

Dictionary of Organic Compounds

FIFTH EDITION

SECOND SUPPLEMENT

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CHAPMAN AND HALL

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Fifty years of "Heilbron"

The first volume of the first edition of the *Dictionary of Organic Compounds* was published 50 years ago, in October 1934. The idea for such a dictionary came from H. M. Bunbury of ICI, but it was in conjunction with Ian Heilbron, Professor of Organic Chemistry at the University of Manchester, that it came to life, and it was realized through Heilbron's ability to marshal academic resources, principally from the Universities of Manchester and Liverpool, to undertake the massive job of authorship. When published the work was an immediate success, and new editions were called for in 1943, 1953, 1965 and most recently, 1982. Sir Ian Heilbron maintained close links with the publication until close to his death in 1959.

Perhaps remarkably, the scope and general appearance of "Heilbron" have stayed virtually constant throughout its half-century history. Despite the inclusion of many new substances and the recent employment of computer aided methods of compilation and manufacture, nothing has swayed the publishers or editors from ensuring that "Heilbron" remained a carefully selected, expertly compiled and clearly presented dictionary for practising organic chemists. Thus the Preface from the first edition in 1934 could nearly have sufficed as the Preface for the fifth edition in 1982. Then, Sir Ian wrote:

"The growth of Organic Chemistry during the past half-century has proceeded with such remarkable rapidity, and the output of research is to-day so immense, that the search in the reference literature for data concerning any specific compound is frequently both a lengthy and difficult undertaking. The present Dictionary, which is the only one of its kind in the English language, aims at providing a concise, up-to-date, but at the same time adequate work of reference in which the subject matter is presented in a readily accessible form for all general purposes. It has been designed to meet the general requirements both of academic research workers and of those engaged in the various branches of the organic chemical industry. A careful method of selection has been adopted in order to avoid the inclusion of matter either relatively unimportant or of a highly specialized nature."

Of course, the *detail* of the new, fifth edition of "Heilbron" and its Supplements has changed radically following the recent developments in analytical and synthetic organic chemistry, in response to industrial and environmental interests, and in recognition of an information age increasingly influenced by the use of computers. "Heilbron" will continue to evolve. There will undoubtedly be a sixth edition, although its form, content and size will most likely be determined by its complementary relationship to a computer-based information service. What is certain is that the name "Heilbron" will continue to be associated with the provision to chemists of reliable yet selective compound information.

Richard Stileman
March 1984

Note to Readers

Always use the latest Supplement

Supplements are published in the middle of each year and contain new and updated Entries derived from the primary literature of the preceding year. The second and subsequent Supplements have cumulative indexes derived from the Entries in *all* the Supplements. Searching the entire Supplement series is facilitated by consulting first the indexes in the latest Supplement.

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New compounds for DOC 5

The Editor is always pleased to receive comments on the selection policy of DOC 5, and in particular welcomes specific suggestions for compounds or groups of compounds to be considered for inclusion in the annual Supplements.

Write to

The Editor, DOC 5
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Caution

Treat all organic compounds as if they have dangerous properties.

The information contained in this volume has been compiled from sources believed to be reliable. However, no warranty, guarantee, or representation is made by the Publisher as to the correctness or sufficiency of any information herein; and the Publisher assumes no responsibility in connection therewith.

The specific information in this publication on the hazardous and toxic properties of certain compounds is included to alert the reader to possible dangers associated with the use of those compounds. The absence of such information should not however be taken as an indication of safety in use or misuse.

Second Supplement

Introduction

For detailed information about how to use DOC 5, see the Introduction in Volume 1 of the Main Work.

1. Using DOC 5 Supplements

As in the Main Work volumes, every Entry is numbered to assist ready location. The DOC Number consists of a letter of the alphabet followed by a five-digit number. In this second supplement the first digit is invariably 2. Cross-references within the text to Entries having numbers beginning with zero refer to Main Work Entries and with 1 refer to the first supplement.

Where a supplement Entry contains additional or corrected information referring to an Entry in the Main Work or first supplement, the whole Entry is reprinted, with the accompanying statement "Updated Entry replacing . . .". In such cases, the new Entry contains all of the information which appeared in the former Entry, except for any which has been deliberately deleted. In such cases there is therefore no necessity for the user to consult the Main Work or previous supplements.

2. Literature Coverage

In compiling this Supplement the primary literature has been surveyed to mid-1983. A considerable number of compounds from the older literature have also been included for the first time.

3. Spelling of chemical names

American spelling of chemical names has been adopted in its entirety for this and subsequent DOC supplements. The most important consequence of this change is that all sulfur compounds are now spelled with f in place of ph. (Previously f was used where *Chemical Abstracts* was quoted, otherwise ph.)

English spelling has been retained for words other than chemical names.

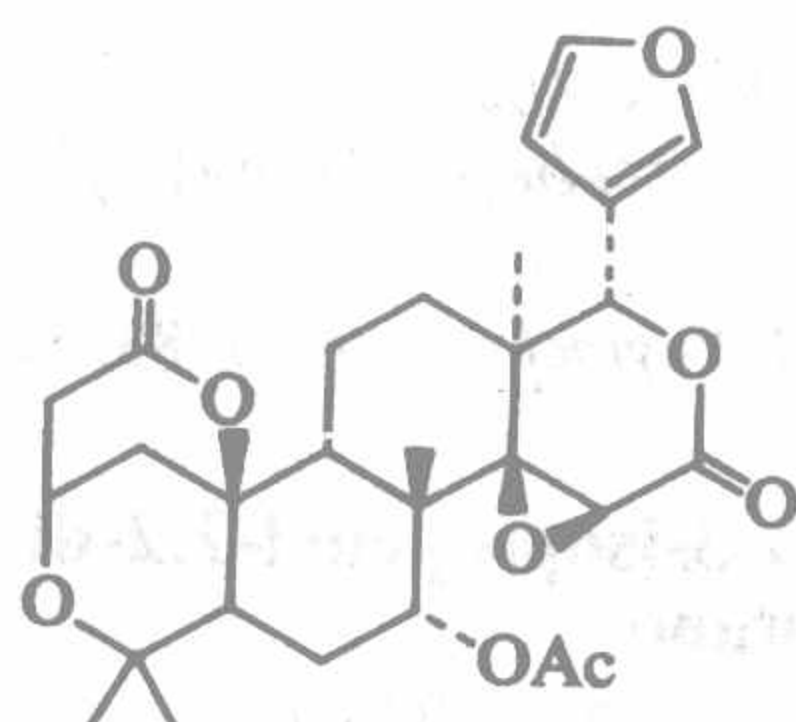
Contents

Second Supplement Entries	<i>page 1</i>
Name Index	477
Molecular Formula Index	597
Chemical Abstracts Service Registry Number Index	729

A

1(10→19)Abeo-7-acetoxyisoobacun-3,10-olide
[85643-98-7]

A-20001



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

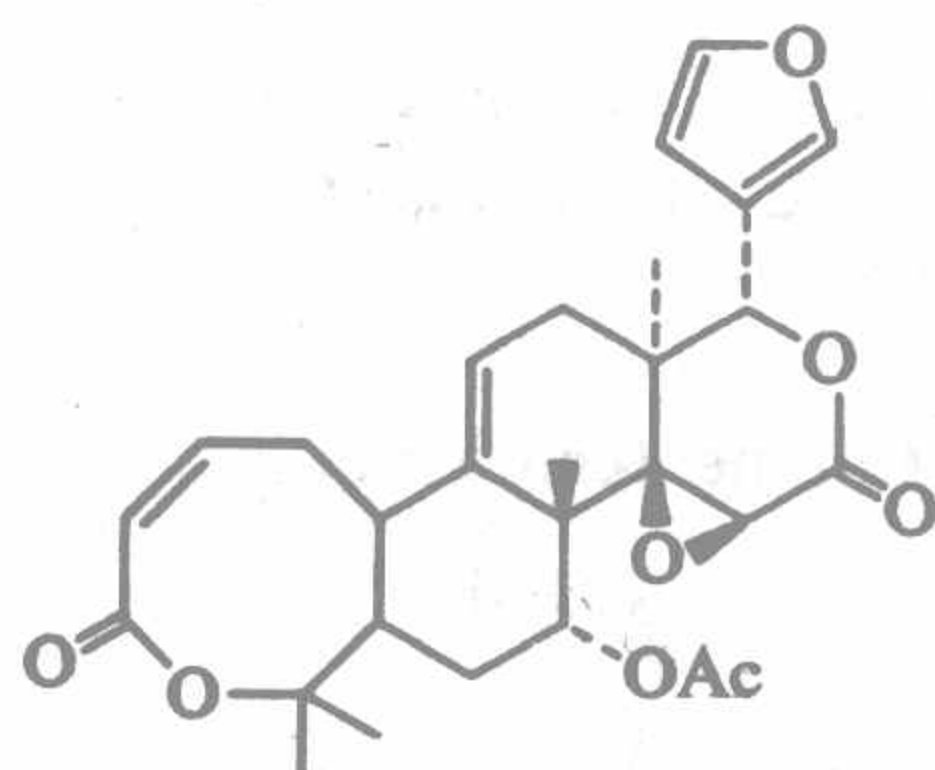
(7 α ,10 β)-form

Constit. of a *Citrus-Poncirus* hybrid. Cryst. (MeOH).
Mp 271-4°.

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

1(10→19)Abeo-7-acetoxy-9(11)-obacunene
[85643-97-6]

A-20002



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

7 α -form

Constit. of a *Citrus-Poncirus* hybrid.

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

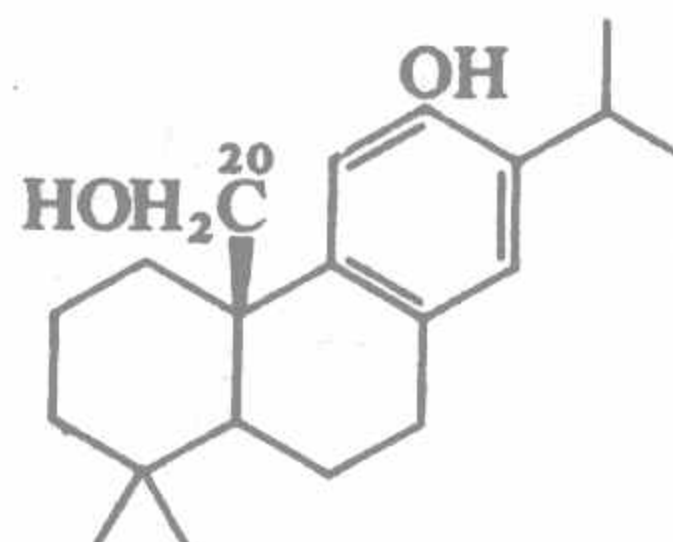
8,11,13-Abietatriene-12,20-diol

A-20003

Updated Entry replacing P-10215

Pisiferol

[24035-36-7]



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

Constit. of *Chamaecyparis pisifera*. Cryst. (C_6H_6 /Et₂O).

20-Aldehyde: [24035-37-8]. **12-Hydroxy-8,11,13-abietatrien-20-al.** *Pisiferol*. Constit. of *C. pisifera*. Cryst.
Mp 63.6-65°. $[\alpha]_D^{25} +164^\circ$ (c, 0.6 in MeOH).

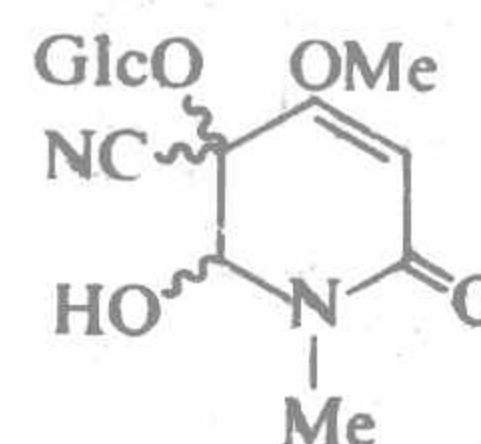
Yatagi, M. *et al*, *Phytochemistry*, 1979, **18**, 176; 1980, **19**, 1149 (isol)

Matsumoto, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 1599; 1983, **56**, 2018 (synth)

Acalyphin

[81861-72-5]

A-20004



$C_{14}H_{20}N_2O_9$ M 360.320

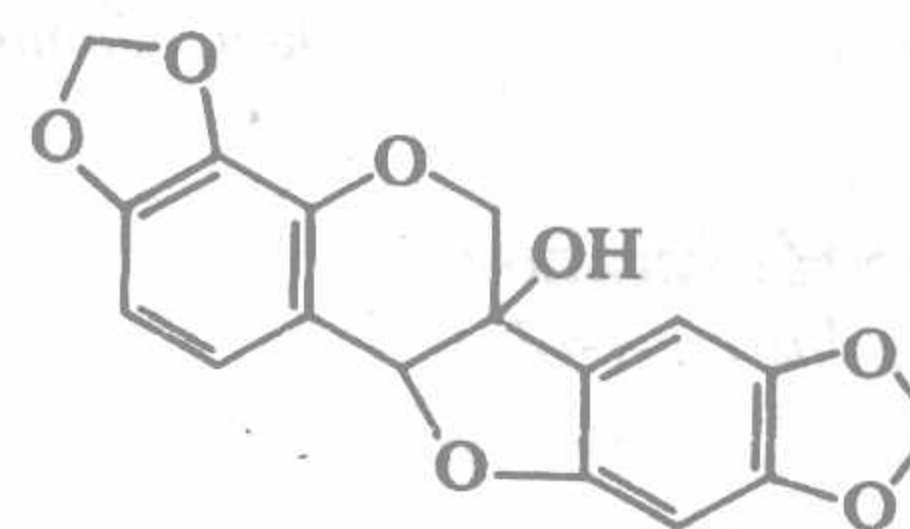
Cyanogenic glucoside from *Acalypha indica*. Hygroscopic powder. Mp 185-6°.

Nahrstedt, A. *et al*, *Phytochemistry*, 1982, **21**, 101.

Acanthocarpan

A-20005

6 α -Hydroxy,3,4:8,9-dimethylenedioxypterocarpan



$C_{17}H_{12}O_7$ M 328.278

Constit. of *Tephrosia bidwilli* and *Caragana acanthophylla*. $[\alpha]_D -259^\circ$ (c, 0.23 in MeOH).

Ingham, J.L. *et al*, *Phytochemistry*, 1982, **21**, 2969.

Acarnidines

A-20006

$HN=C(NH_2)NH(CH_2)_5NR(CH_2)_3NHCOCH=C(CH_3)_2$

R = $H_3C(CH_2)_{10}CO-$

$H_3C(CH_2)_3CH=CH(CH_2)_3CO-(Z)$ or

$H_3CCH_2(CH=CHCH_2)_2CH_2CH=CH(CH_2)_2CO-(all-Z)$

Isol. from *Acarus erithacus* (red-orange sponge). Anti-viral and antimicrobial compounds.

Carter, G.T. *et al*, *J. Am. Chem. Soc.*, 1978, **100**, 4302 (isol)

Blunt, J.W. *et al*, *Tetrahedron Lett.*, 1982, **23**, 2793 (synth)

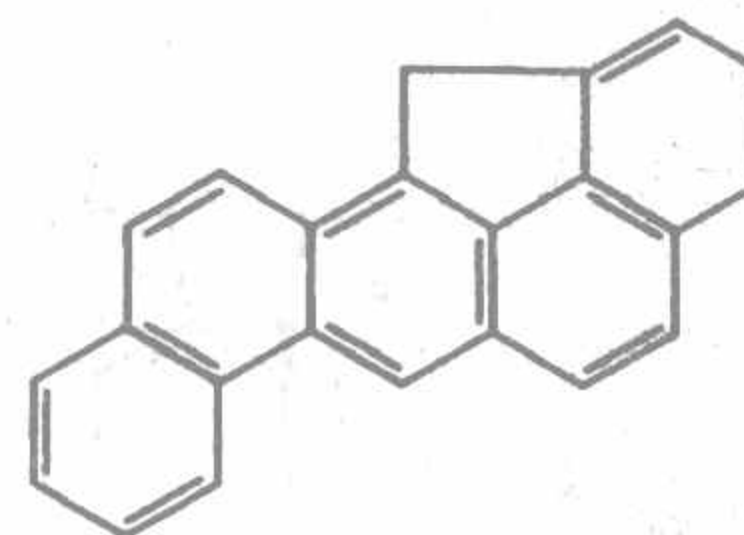
13H-Acenaphtheno[1,8-ab]phenanthrene

A-20007

Updated Entry replacing A-00075

1,9-Methylene-1,2,5,6-dibenzanthracene. 1,14-Methylenedibenz[a,h]anthracene

[201-42-3]



$C_{23}H_{14}$ M 290.364

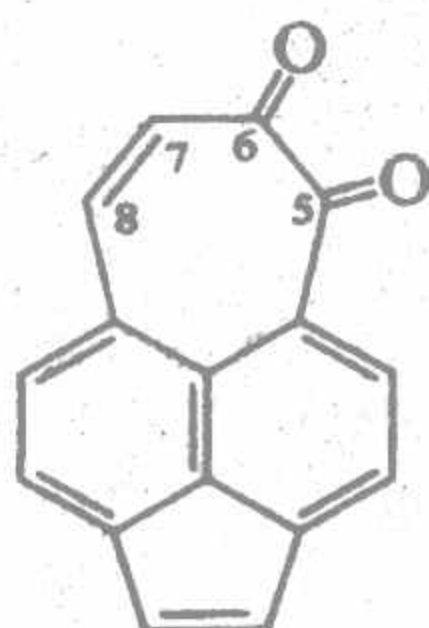
Greenish-yellow prisms (C_6H_6 /pet. ether). Mp 266-7°.

▷HN0175000.

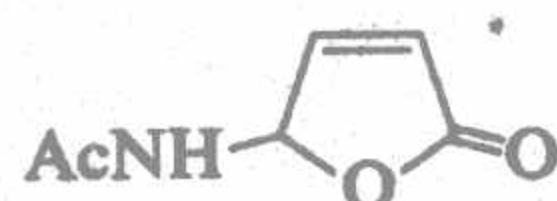
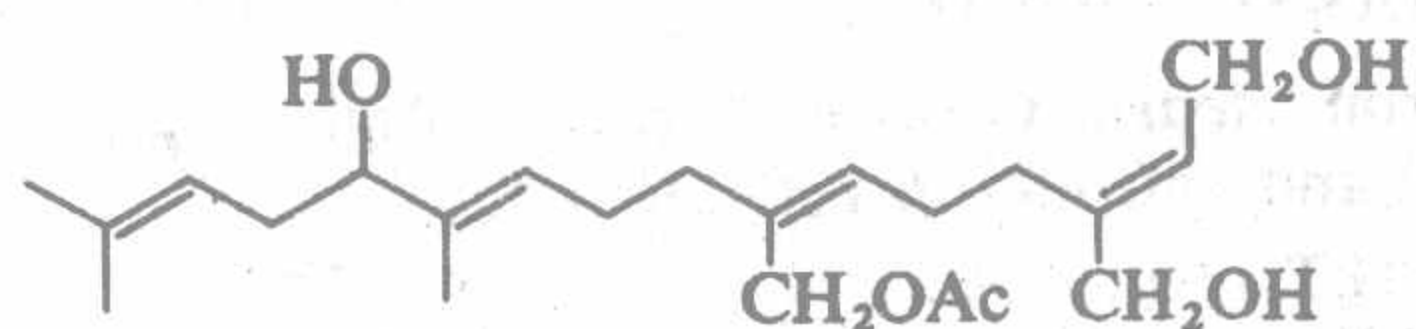
Dipicrate: Orange needles (C_6H_6). Mp 201°.

Fieser, L.F. *et al*, *J. Am. Chem. Soc.*, 1935, **57**, 1681 (synth)

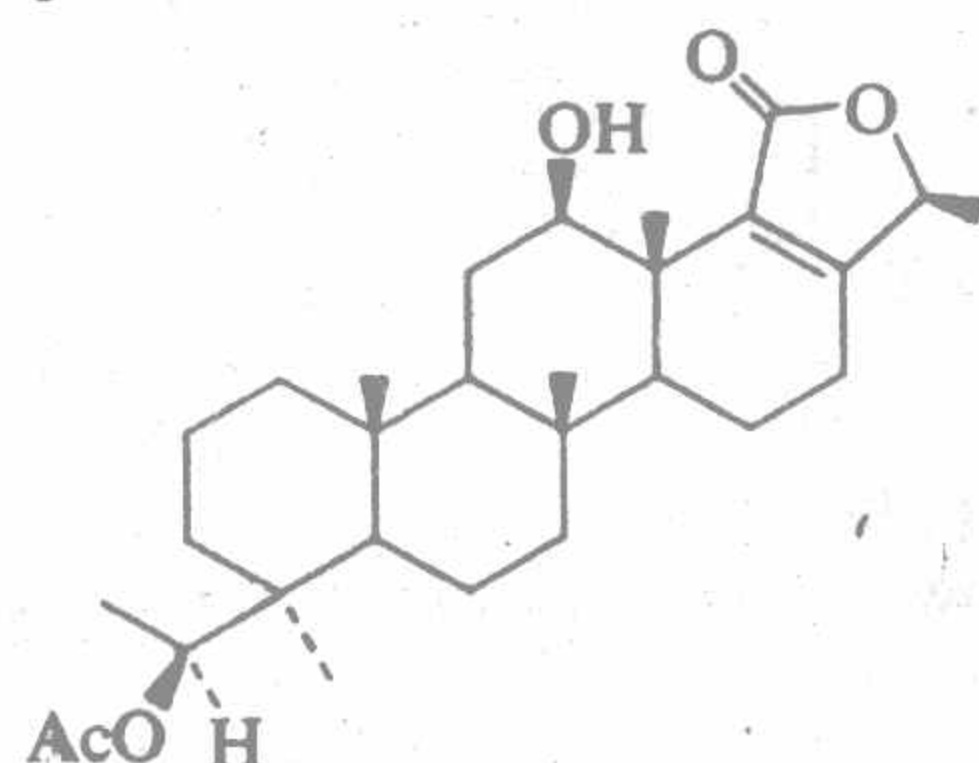
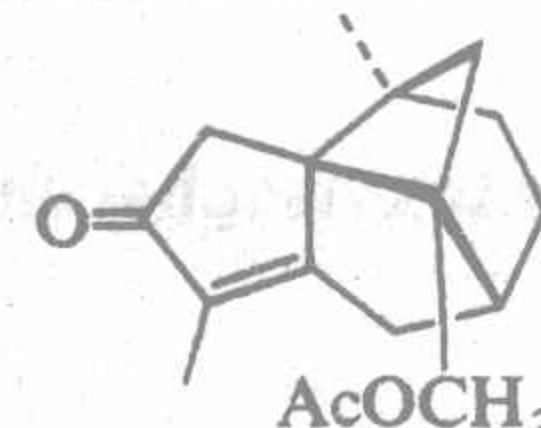
Buchta, E. *et al*, *Chem. Ber.*, 1963, **96**, 2093 (synth)

Ray, J.K. *et al*, *J. Org. Chem.*, 1983, 48, 1352 (*synth*)Croft, K.D. *et al*, *J. Chem. Soc., Perkin Trans. I*, 1983, 155.**5,6-Acepleiadylenedione****A-20008** $C_{16}H_8O_2$ M 232.238Purple-red needles (C_6H_6 /hexane). Mp 145° dec. Unstable.Tsunetsugu, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1983, 28.**5,8-Acepleiadylenedione****A-20009** $C_{16}H_8O_2$ M 232.238Purple-red needles (C_6H_6 /hexane). Mp 186° dec.Tsunetsugu, J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1983, 28.**5-Acetamido-2(5H)-furanone****A-20010**

4-Acetamido-2-buten-4-olide

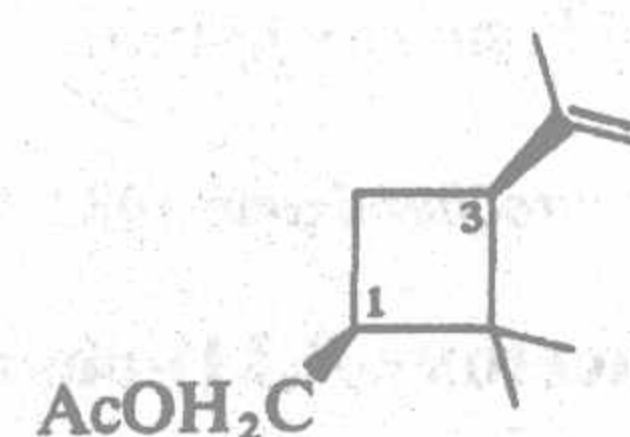
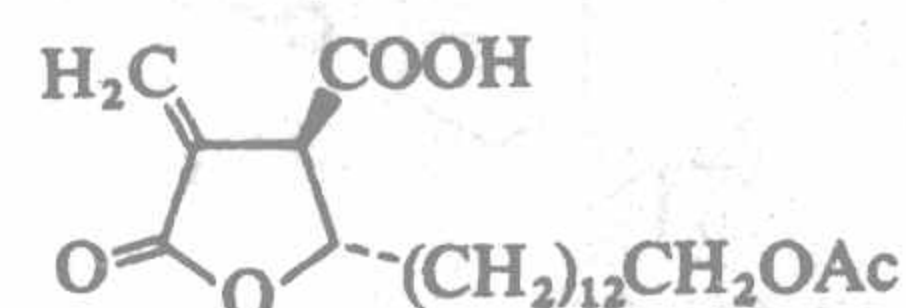
 $C_6H_7NO_3$ M 141.126Mycotoxin produced by the mould *Fusarium nivale* on *Festuca arundinacea*. Affects cattle. Cryst. (Me_2CO). Mp 115-116.5°. $[\alpha]_D \pm 0^\circ$ (c, 2.0 in H_2O).Yates, S.G. *et al*, *Phytochemistry*, 1968, 7, 139 (*isol*, *struct*)Ružić-Toroš, Ž. *et al*, *Acta Crystallogr., Sect. B*, 1982, 38, 1664 (*cryst struct*)**19-Acetoxy-12,20-dihydroxygeranylnerol****A-20011** $C_{22}H_{36}O_5$ M 380.523Constit. of *Lasiolaena morii*. Gum.Bohlmann, F. *et al*, *Phytochemistry*, 1982, 21, 161.**20-Acetoxy-12-hydroxy-20,24-dimethyl-25-nor-17-scalaren-18,24-olide****A-20012**

[85735-14-4]

 $C_{29}H_{44}O_5$ M 472.664**(12β,20S,24S)-form**Constit. of a *Carteriospongia* sp. Cryst. (Et_2O /pet. ether). Mp 252-4°. $[\alpha]_D +20^\circ$ (c, 3.3 in $CHCl_3$).**12-Acetoxy-4-jungistueben-3-one****A-20013** $C_{17}H_{22}O_3$ M 274.359Constit. of *Jungia stuebelii*. Gum. $[\alpha]_D^{24} +10^\circ$ (c, 0.15 in $CHCl_3$).Bohlmann, F. *et al*, *Phytochemistry*, 1983, 22, 1201.**1-Acetoxyethyl-3-isopropenyl-2,2-dimethylcyclobutane****A-20014**

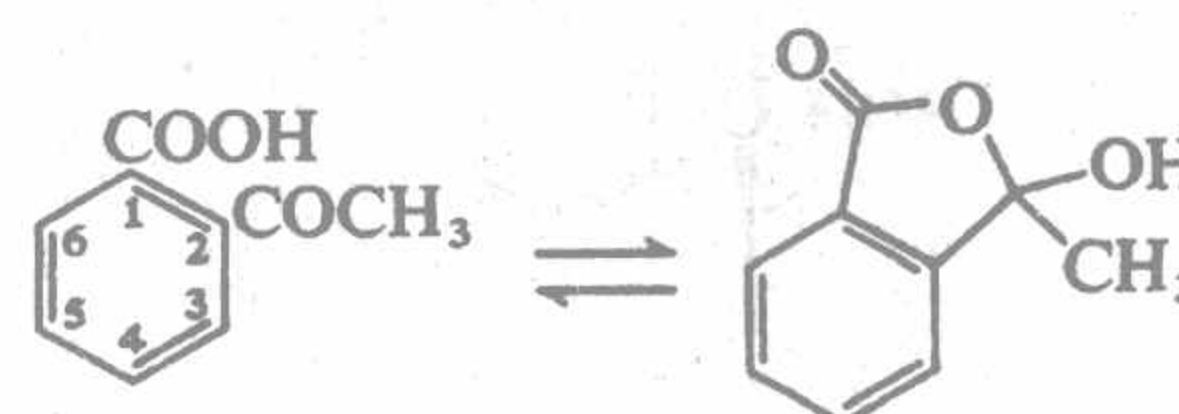
2,2-Dimethyl-3-(1-methylethenyl)cyclobutanemethanol acetate

[28465-10-3]

 $C_{12}H_{20}O_2$ M 196.289**(1R,3S)-form**Sex attractant of the citrus mealybug *Phanococcus citri*.Bierl-Leonhardt, B.A. *et al*, *Tetrahedron Lett.*, 1981, 22, 389 (*isol*, *synth*, *specta*)**13-Acetoxyprotolichesterinic acid****A-20015** $C_{21}H_{34}O_6$ M 382.496See Protolichesteric acid, P-10254. Metab. from *Neuropogon trachycarpus*. Mp 94-6°.Ghogamu, R.T. *et al*, *Phytochemistry*, 1982, 21, 2355.**2-Acetylbenzoic acid, 9CI****A-20016**

3-Hydroxy-3-methylphthalide. Acetophenone-2-carboxylic acid

[577-56-0]

 $C_9H_8O_3$ M 164.160

Cryst. (pet. ether). Mp 117-8°. Exists as phthalide in solid state and non-aq. soln., and as 2-acetylbenzoic acid only in aq. alkaline soln.

Me ester: [1077-79-8]. Liq. Bp₂ 94-5°.Riemschneider, R. *et al*, *Chem. Ber.*, 1959, 92, 1705 (*synth*)Newman, M.S., *J. Chem. Educ.*, 1977, 54, 191 (*synth*)Panetta, C.A. *et al*, *Synthesis*, 1977, 43 (*use*)Tyman, J.H.P. *et al*, *Spectrochim. Acta, Part A*, 1977, 33, 479 (*struct*, *pmr*, *cmr*, *ms*, *ir*)Durrani, A.A. *et al*, *J. Chem. Soc., Perkin Trans. I*, 1979, 2069 (*synth*, *pmr*)

3-Acetylbenzoic acid, 9CI

A-20017

Acetophenone-3-carboxylic acid

[586-42-5]

 $C_9H_8O_3$ M 164.160

Cryst. Mp 172° (166°).

Me ester: [21860-07-1]. Cryst. (Et₂O). Mp 45-6°.*Chloride*: [31076-85-4]. Liq. Bp_{0.4} 120°.*Ph ester*: [31076-87-6]. Cryst. (MeOH). Mp 75°.Rupe, H. *et al*, *Ber.*, 1900, 33, 3408 (*synth*)Durif-Verambon, B. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 4452 (*synth*)Exner, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, 36, 534 (*ir*)Bromilow, J. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1981, 753 (*cmr*)**4-Acetylbenzoic acid, 9CI**

A-20018

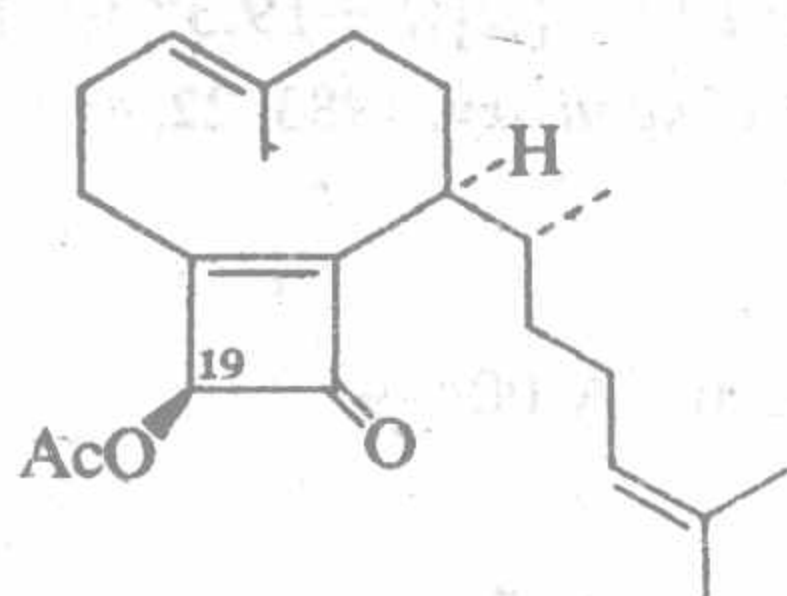
Acetophenone-4-carboxylic acid

[586-89-0]

 $C_9H_8O_3$ M 164.160Cryst. (H₂O). Mp 209-10°.*2,4-Dinitrophenylhydrazone*: Orange needles (AcOH). Mp 280° dec.*Me ester*: [3609-53-8]. Needles (C₆H₆/hexane), plates (CCl₄ or hexane). Mp 95-95.5°.*Ph ester*: [31076-86-5]. Cryst. (EtOH). Mp 122°.Bergmann, E.D. *et al*, *J. Org. Chem.*, 1959, 24, 549 (*synth*)Smisman, E.E. *et al*, *J. Org. Chem.*, 1968, 33, 4231 (*synth*)Durif-Verambon, B. *et al*, *Bull. Soc. Chim. Fr.*, 1970, 4452 (*synth*)Exner, O. *et al*, *Collect. Czech. Chem. Commun.*, 1971, 36, 534 (*ir*)Bromilow, J. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1981, 753 (*cmr*)**Acetylcoriacenone**

A-20019

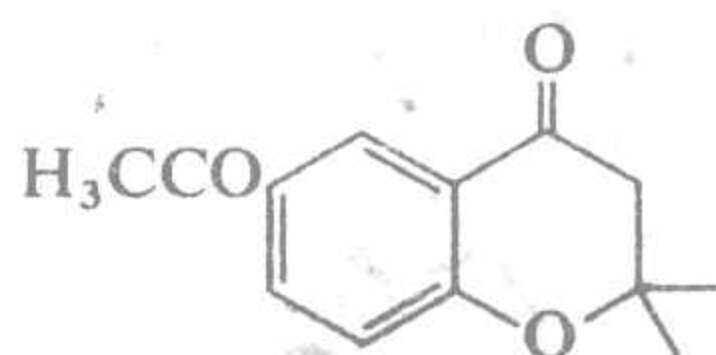
[85612-73-3]

 $C_{22}H_{32}O_3$ M 344.493Constit. of *Pachydictyon coriaceum*. Oil.*19-Epimer*: Isoacetylcoriacenone. Constit. of *P. coriaceum*. Oil.Ishitsuka, M. *et al*, *J. Org. Chem.*, 1983, 48, 1937.**6-Acetyl-2,3-dihydro-2,2-dimethyl-4H-1-benzopyran-4-one, 9CI**

A-20020

6-Acetyl-2,2-dimethyl-4-chromanone

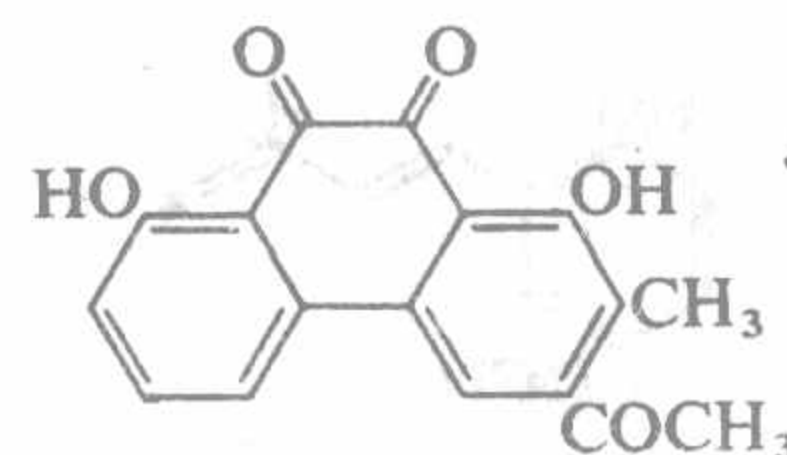
[68799-41-7]

 $C_{13}H_{14}O_3$ M 218.252Constit. of *Ambrosia cumanaensis* and *Gnoxys psilophylla*. Cryst. (Et₂O/pet. ether). Mp 96°.Bohlmann, F. *et al*, *Phytochemistry*, 1977, 16, 575, 1979, 18, 339 (*isol*)Bohlmann, F. *et al*, *Chem. Ber.*, 1981, 114, 147 (*synth*)**3-Acetyl-1,8-dihydroxy-2-methylphenanthraquinone**

A-20021

Haloquinone

[80902-01-8]

 $C_{17}H_{12}O_5$ M 296.279Isol. from *Streptomyces venezuelae* ssp. *xanthophaeus*.

Active against gram-positive bacteria and halobacteria and weakly active against gram-negative bacteria. Acts on DNA synthesis. Powder. Mp 226°. Red in acid soln., blue in alkali.

Di-Me ether: [80902-05-2]. Mp 192°.Ewersmeyer-Wenk, B. *et al*, *J. Antibiot.*, 1981, 34, 1531 (*isol*)Krone, B. *et al*, *J. Antibiot.*, 1981, 34, 1538 (*struct*)**Acetyl methanesulfonate**

A-20022

Acetic acid anhydride with methanesulfonic acid, 9CI

[5539-53-7]

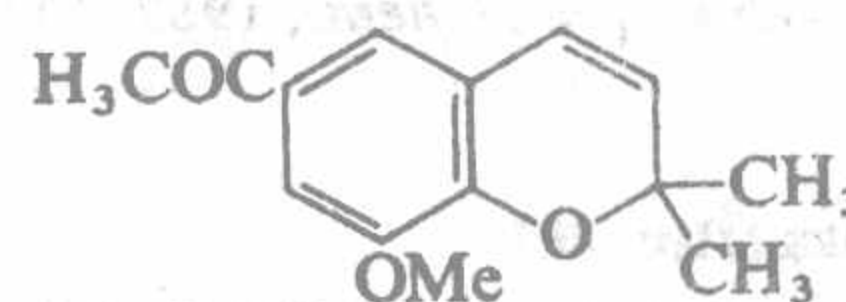
AcOSO₂Me $C_3H_6O_4S$ M 138.138Readily cleaves aliphatic ethers. Bp_{0.05} 100°, Bp_{0.001} 70-2°.Boehme, H. *et al*, *Justus Liebigs Ann. Chem.*, 1965, 688, 78 (*synth*)Karger, M.H. *et al*, *J. Org. Chem.*, 1971, 36, 528, 532, 540 (*synth, use*)Corey, E.J. *et al*, *Tetrahedron Lett.*, 1973, 3153 (*use*)Modi, M.N. *et al*, *Indian J. Chem.*, 1973, 11, 1049 (*synth*)Fieser, M. *et al*, *Reagents for Organic Synthesis*, Wiley, 1967-82, 5, 5 (*use*)**6-Acetyl-8-methoxy-2,2-dimethyl-2H-1-benzopyran**

A-20023

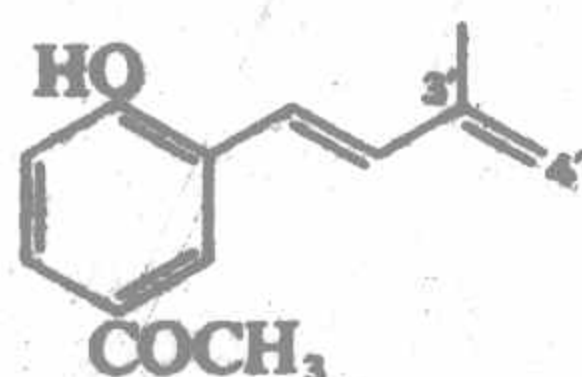
Updated Entry replacing A-00325

*6-Acetyl-8-methoxy-2,2-dimethyl-2H-chromene**Acetovanillochromene*

[34155-83-4]

 $C_{14}H_{16}O_3$ M 232.279Constit. of *Ageratina scorodonioides* and *Eupatorium riparium*. Oil.*5-Hydroxy*: [61670-29-9]. *6-Acetyl-5-hydroxy-8-methoxy-2,2-dimethyl-2H-1-benzopyran*. Isol. from *Flourensia cernua* and *A. spp.* Needles (Et₂O/pet. ether). Mp 88°.*5-Methoxy*: [62458-48-4]. *6-Acetyl-5,8-dimethoxy-2,2-dimethyl-2H-1-benzopyran*. Constit. of *A. scorodonioides*. Cryst. (Et₂O/pet. ether). Mp 63°.Taylor, D.R. *et al*, *Phytochemistry*, 1971, 10, 1665 (*isol*)Bohlmann, F. *et al*, *Chem. Ber.*, 1977, 110, 295, 301 (*isol*)Bohlmann, F. *et al*, *Phytochemistry*, 1978, 17, 566 (*isol*)Bohlmann, F. *et al*, *Justus Liebigs Ann. Chem.*, 1980, 185 (*synth*)Ahlualia, V.K. *et al*, *Indian J. Chem., Sect. B*, 1982, 21, 1039 (*synth*)

4-Acetyl-2-(3-methyl-1,3-butadienyl)phenol A-20024
 1-[4-Hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]ethanone, 9CI. 4-Hydroxy-3-(3-methyl-1,3-butadienyl)-acetophenone
 [26932-04-7]



$C_{13}H_{14}O_2$ M 202.252

Constit. of the roots of *Helianthella uniflora*. Cryst. (Et_2O). Mp 137-8°.

Bohlmann, F. *et al*, *Chem. Ber.*, 1970, **103**, 90; 1972, **105**, 863 (isol, uv, synth)

Acetyl nitrite, 8CI

A-20025

Acetic acid anhydride with nitrous acid, 9CI
 [5813-49-0]

AcONO

$C_2H_3NO_3$ M 89.051

Nitrosating agent. Green solid at -196°, green liq. at -78°, pale-brown unstable liq. at r.t. Dec. by light.

▷ Vapour highly explosive

Kyte, A.B. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 74 (synth, nmr, use)

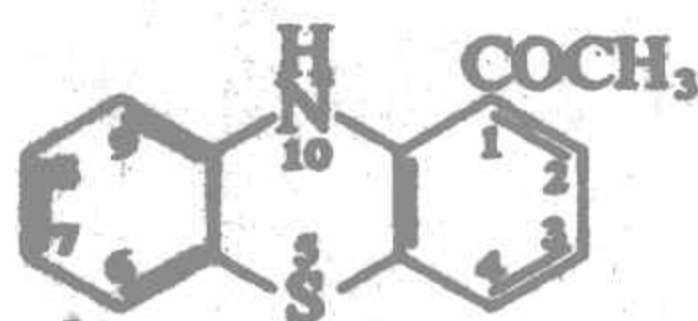
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd Ed., Butterworths, London and Boston, 1979, 364.

Hazards in the Chemical Laboratory, (Bretherick, L., Ed.), 3rd Ed., Royal Society of Chemistry, London, 1981, 164.

1-Acetylphenothiazine, 8CI

A-20026

1-(10H-Phenothiazin-1-yl)ethanone, 9CI
 [83161-97-1]



$C_{14}H_{11}NOS$ M 241.307

Cryst. (C_6H_6). Mp 99-101°.

Ueno, Y., *Justus Liebigs Ann. Chem.*, 1982, 1573 (synth)

2-Acetylphenothiazine, 8CI

A-20027

1-(10H-Phenothiazin-2-yl)ethanone, 9CI
 [6631-94-3]

$C_{14}H_{11}NOS$ M 241.307

Yellow-orange needles ($EtOAc$ /hexane). Mp 192-3°.

N-Ac: 2,10-Diacetylphenothiazine. Needles ($EtOH$). Mp 105-6°.

Baltzly, M. *et al*, *J. Am. Chem. Soc.*, 1946, **68**, 2673.

3-Acetylphenothiazine, 8CI

A-20028

1-(10H-Phenothiazin-3-yl)ethanone, 9CI

$C_{14}H_{11}NOS$ M 241.307

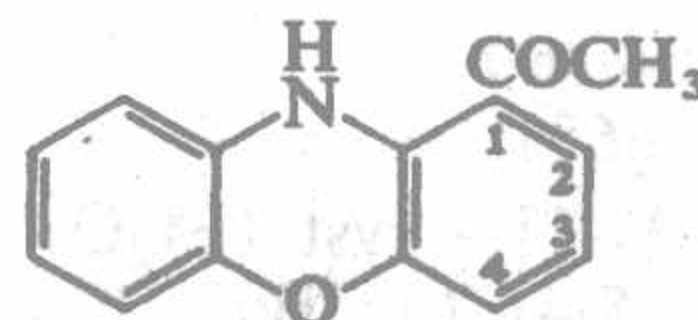
Cryst. (C_6H_6). Mp 177-8°.

Ueno, Y., *Justus Liebigs Ann. Chem.*, 1982, 1573 (synth)

1-Acetylphenoxazine

A-20029

1-(10H-Phenoxazin-1-yl)ethanone, 9CI
 [83620-89-7]



$C_{14}H_{11}NO_2$ M 225.246

Yellow cryst. Mp 156°.

Ueno, Y., *Monatsh. Chem.*, 1982, **113**, 855 (synth)

2-Acetylphenoxazine

A-20030

1-(10H-Phenoxazin-2-yl)ethanone, 9CI

$C_{14}H_{11}NO_2$ M 225.246

Greenish-yellow cryst. Mp 211-3°.

Vanderhaeghe, H., *J. Org. Chem.*, 1960, **25**, 747.

3-Acetylphenoxazine

A-20031

1-(10H-Phenoxazin-3-yl)ethanone, 9CI

[83620-90-0]

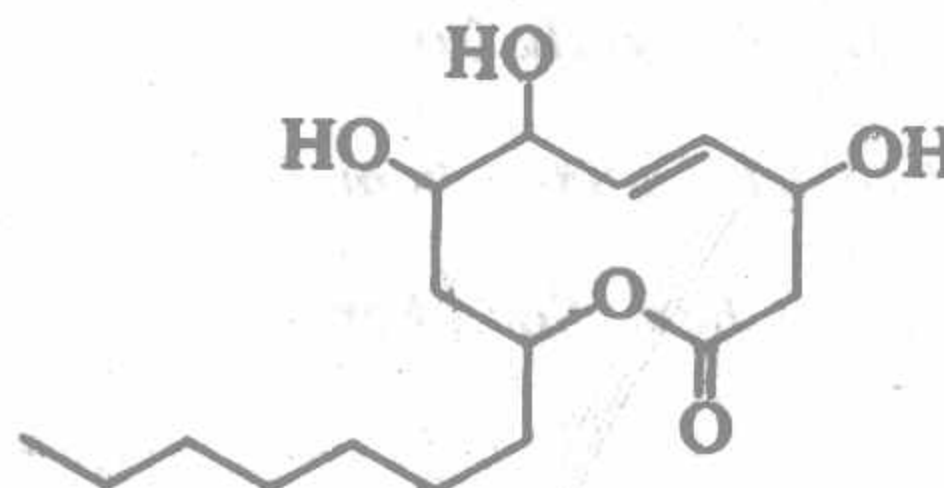
$C_{14}H_{11}NO_2$ M 225.246

Yellow cryst. Mp 186°.

Ueno, Y., *Monatsh. Chem.*, 1982, **113**, 855 (synth)

Achaetolide

A-20032



$C_{16}H_{28}O_5$ M 300.394

Metab. from *Achaetomium cristalliferum*. Cryst.

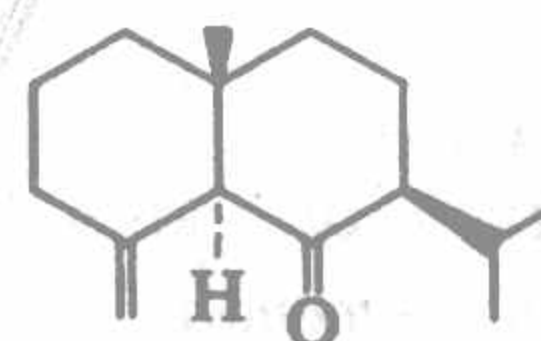
(Me_2CO). Mp 122°. $[\alpha]_D^{21} -19.3^\circ$ (c, 1.46 in $EtOH$).

Bodo, B. *et al*, *Phytochemistry*, 1983, **22**, 447.

Acolamone

A-20033

Updated Entry replacing A-00439
 [39012-14-1]



$C_{15}H_{24}O$ M 220.354

Constit. of *Acorus calamus*. Liq.

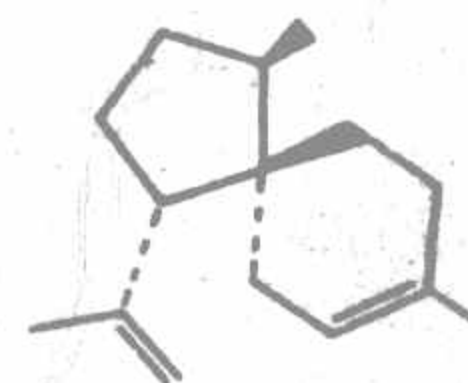
Niwa, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2930 (isol)

Banerjee, A.K. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1982, 2547 (synth)

α -Acoradiene

A-20034

Updated Entry replacing A-00443
 [24048-44-0]



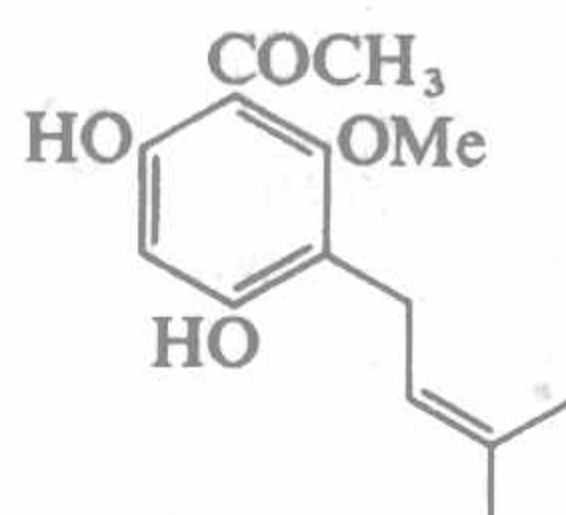
$C_{15}H_{24}$ M 204.355

Constit. of *Juniperus rigida*. Oil. $[\alpha]_D -20^\circ$.

Tomita, B. *et al*, *Tetrahedron Lett.*, 1970, 143 (*isol*)
 Oppolzer, W. *et al*, *Helv. Chim. Acta*, 1983, **66**, 522 (*synth*)
 Solas, D. *et al*, *J. Org. Chem.*, 1983, **48**, 670 (*synth*)

Acronylin**A-20035**

1-[(4,6-Dihydroxy-2-methoxy-3-(3-methyl-2-butenyl)-phenyl)ethanone, 9Cl. 4,6-Dihydroxy-3-isopentenyl-2-methoxyacetophenone
 [27364-64-3].



$C_{14}H_{18}O_4$ M 250.294

Isol. from *Acronychia laurifolia*. Cryst. (C_6H_6 /EtOAc).
 Mp 128-9°.

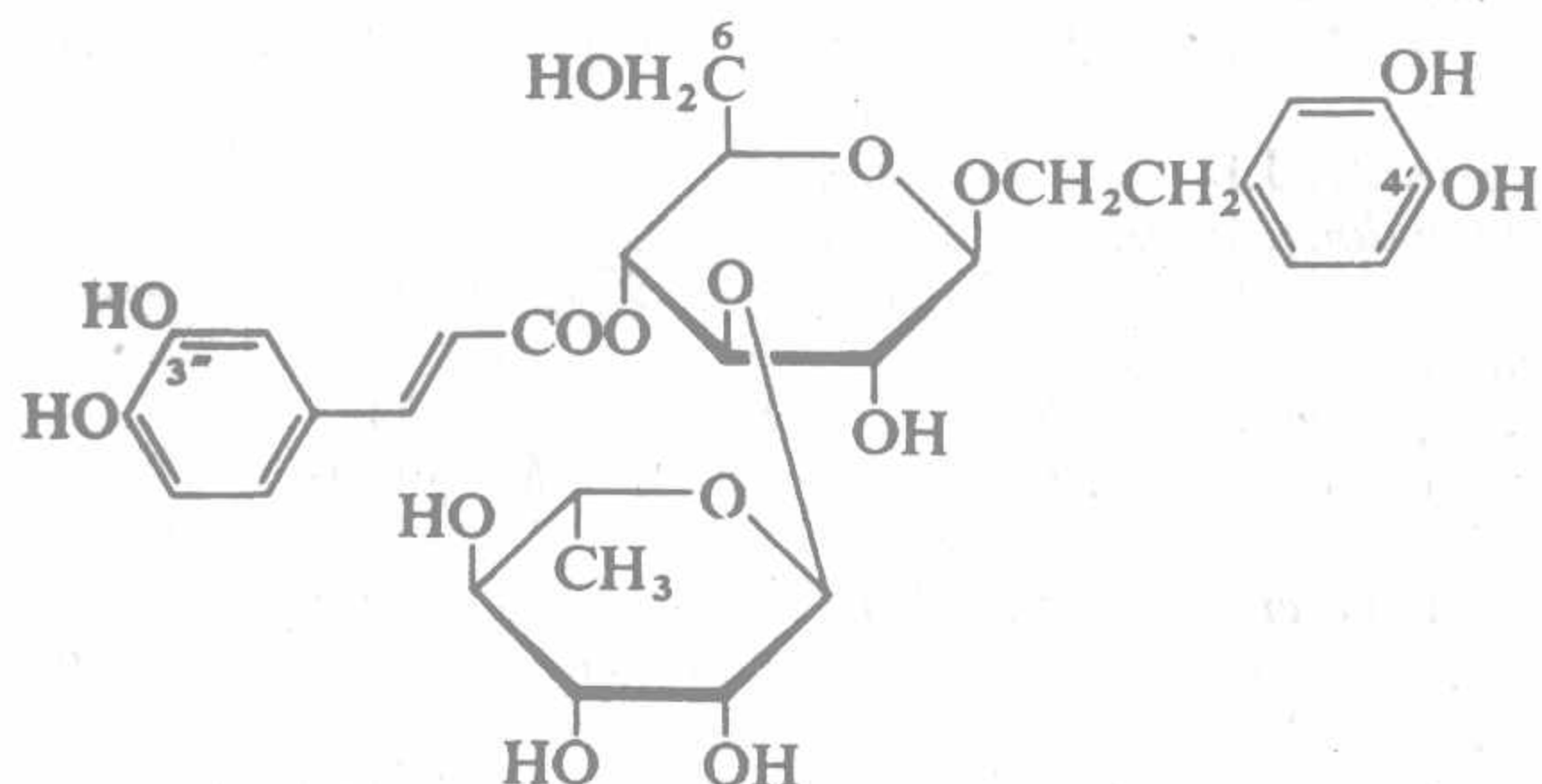
O-Demethyl: [27364-71-2]. 6-Demethylacronylin.

Constit. of the root bark of *A. laurifolia*. Mp 154° dec.

Biswas, G.K. *et al*, *Chem. Ind. (London)*, 1970, 654 (*isol, struct, uv*)

Jain, A.C. *et al*, *Tetrahedron*, 1972, **28**, 5589 (*synth*)

Banerji, J. *et al*, *Indian J. Chem., Sect. B*, 1973, **11**, 693 (*deriv*)

Acteoside**A-20036**

$C_{29}H_{36}O_{15}$ M 624.594

Glycoside from *Leucosceptum japonicum* and other plants.

3''-Me ether: *Leucosceptoside A*. Isol. from *L. japonicum*.

4',3''-Di-Me ether: *Martynoside*. Glycoside from *Martynia louisiana* and *L. japonicum*.

6-O-Apiofuranoside: *Leucosceptoside B*. From *L. japonicum*.

Miyase, T. *et al*, *Chem. Pharm. Bull.*, 1982, **30**, 2732 (*isol, bibl*)

Actinomycin D, 9Cl, 8Cl**A-20037**

Updated Entry replacing A-00486

*Actinomycin C*₁. *Dactinomycin*

[50-76-0]

As *Actinomycin C*₂, A-00483 with

A = X = Sar
 B = Y = L-Pro
 C = Z = D-Val

$C_{62}H_{86}N_{12}O_{16}$ M 1255.432

Isol. from *Actinomyces* spp. Antibiotic active against gram-positive bacteria and tumours. Red rhomboids +3H₂O (EtOH). Mp 241.5-243° dec. $[\alpha]_D^{28}$ -315° (c, 0.25 in MeOH).

Di-Me ester; B,HCl: Mp 251-3°. $[\alpha]_D^{20}$ -130° (CHCl₃).

▷Exp. carcinogen and teratogen

Bullock, E. *et al*, *J. Chem. Soc.*, 1957, 3280 (*struct, uv*)

Brockmann, H. *et al*, *Naturwissenschaften*, 1964, **51**, 382, 384 (*synth*)

Meienhofer, J., *J. Am. Chem. Soc.*, 1970, **92**, 3771 (*synth*)

Lackner, H., *Chem. Ber.*, 1971, **104**, 3653 (*synth, ir, ms, nmr*)

Lackner, H., *Tetrahedron Lett.*, 1971, 2221 (*struct, pmr, conformn*)

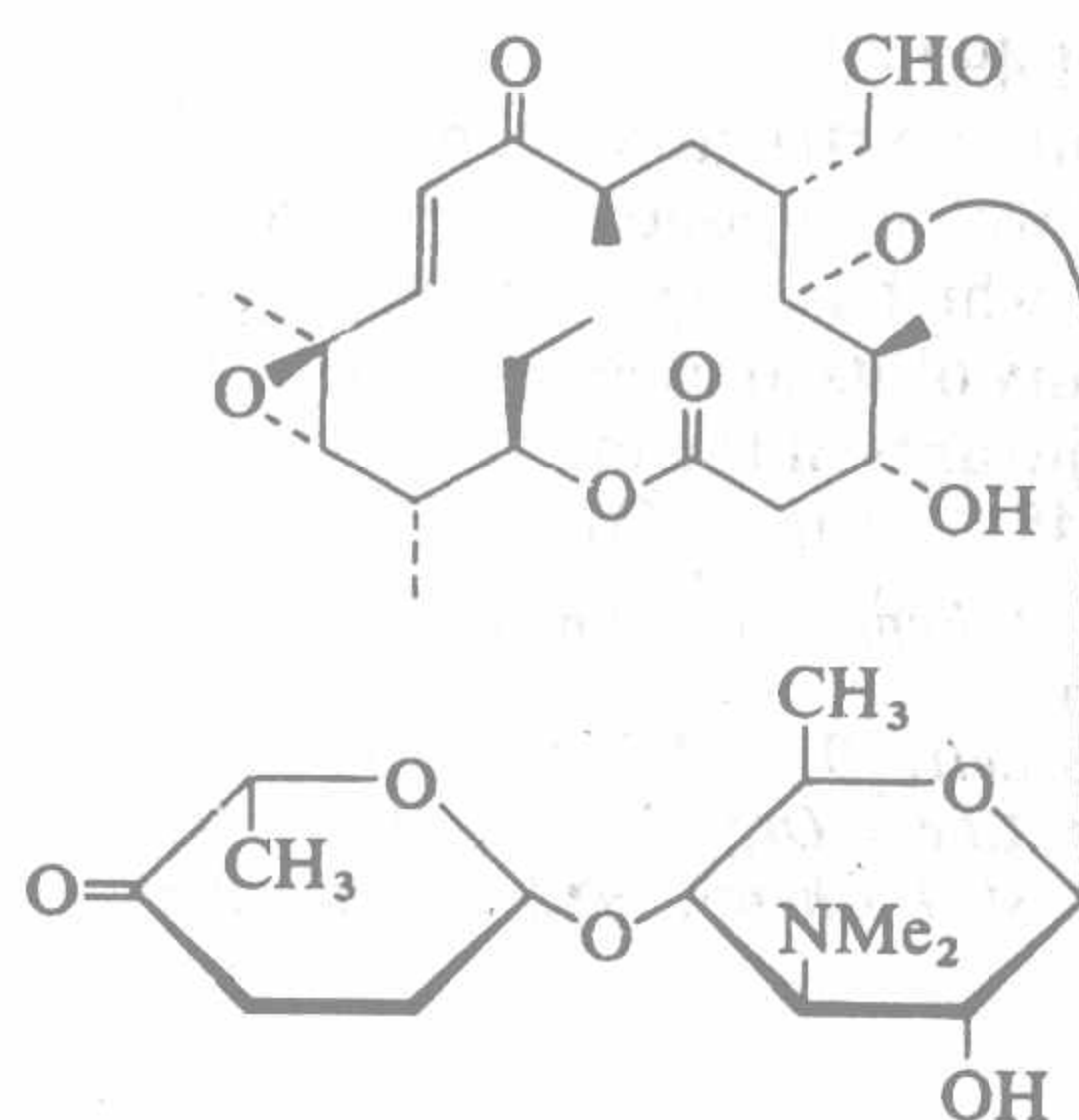
Hollstein, U. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 8036 (*cmr, struct*)

Nakajima, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 3237 (*synth*)

Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 343.

Acumycin**A-20038**

[25999-30-8]



Absolute configuration

$C_{37}H_{59}NO_{12}$ M 709.873

Macrolide antibiotic. Isol. from *Streptomyces griseoflavus*. Prisms (EtOAc). Mp 230-3°.

Bickel, H. *et al*, *Helv. Chim. Acta*, 1962, **45**, 1396 (*isol*)

Clardy, J. *et al*, *Tetrahedron, Suppl.*, 1981, No. 9, 37, 91 (*struct*)

Adamantane**A-20039**

Updated Entry replacing A-00526

Tricyclo[3.3.1.1^{3,7}]decane, 9Cl

[281-23-2]



$C_{10}H_{16}$ M 136.236

Present in petroleum. Cryst. with camphoraceous odour (Me₂CO or by subl.). Mp 268°.

Landa, S. *et al*, *CA*, 1933, **27**, 2792 (*isol*)

Prelog, V. *et al*, *Ber.*, 1941, **74**, 1769 (*synth, props*)

Fort, R.C. *et al*, *Chem. Rev.*, 1964, **64**, 277 (*rev*)

Ault, A. *et al*, *J. Chem. Educ.*, 1969, **46**, 612 (*synth*)

Perkins, R.R. *et al*, *Org. Magn. Reson.*, 1976, **8**, 165 (*cmr*)

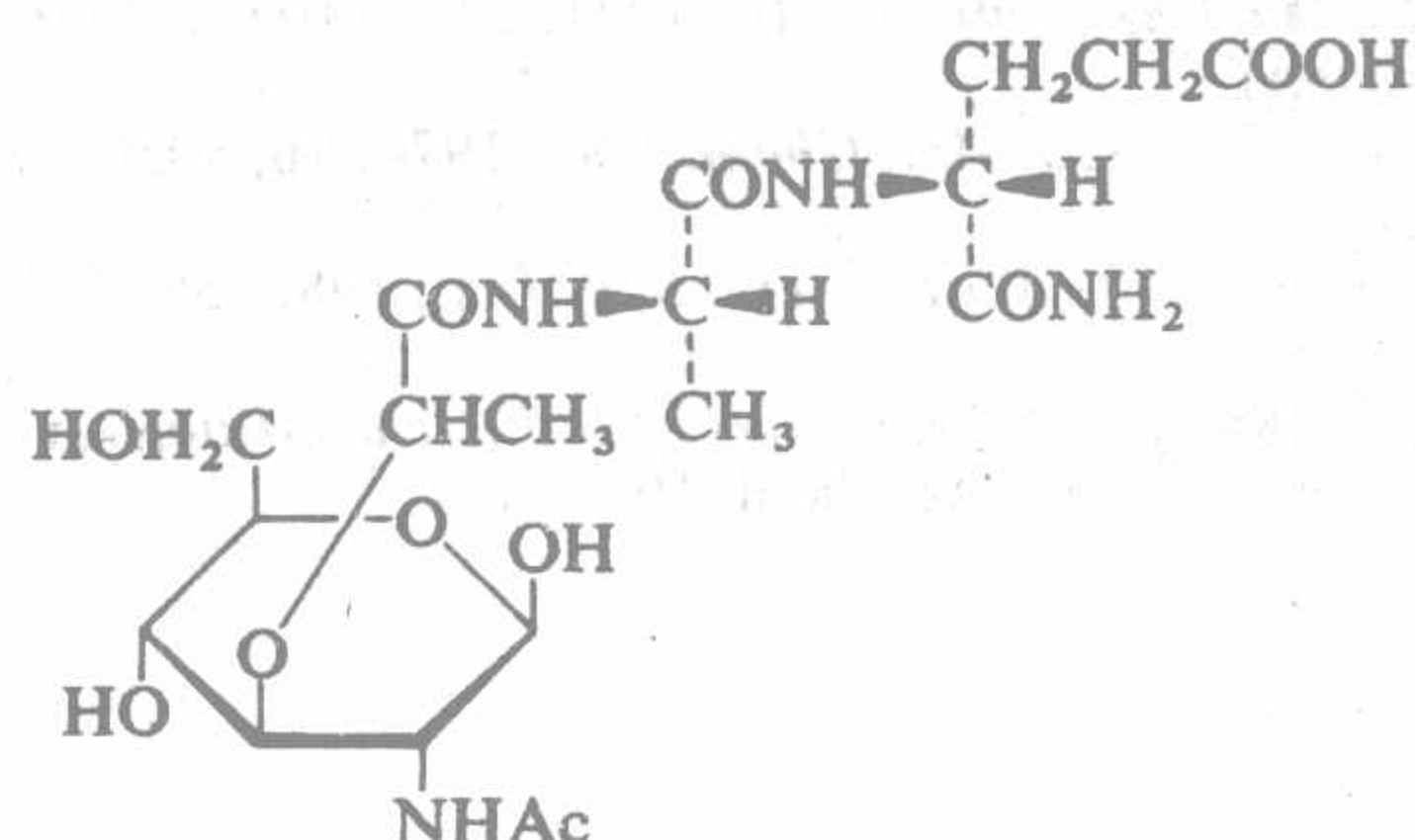
Org. Synth., Coll. Vol., **5**, 16 (*synth*)

Adjuvant peptide**A-20040**

Updated Entry replacing A-10040

N²-[N-(N-Acetylmuramoyl)-L-alanyl-D-α-glutamine, 9Cl. N-Acetylmuramyl-L-alanyl-D-isoglutamine. Muramyl dipeptide. MDP

[53678-77-6]

C₁₉H₃₂N₄O₁₁ M 492.482

Identified as the minimum structural constit. of the mycobacterial cell wall component of Freund's complete adjuvant which is necessary for adjuvant activity. It and many of its analogues have been investigated as adjuvants in the immunisation of animals. $[\alpha]_D^{25} +44^\circ$ (c, 1 in AcOH).

Lefrancier, P. *et al*, *Int. J. Pept. Protein Res.*, 1977, 9, 249; 1978, 11, 289 (*synth*)

Nebelin, E. *et al*, *FEBS Lett*, 1979, 107, 254 (*ms*)

Lefrancier, P., *Fortschr. Chem. Org. Naturst.*, 1981, 40, 1 (*rev*)

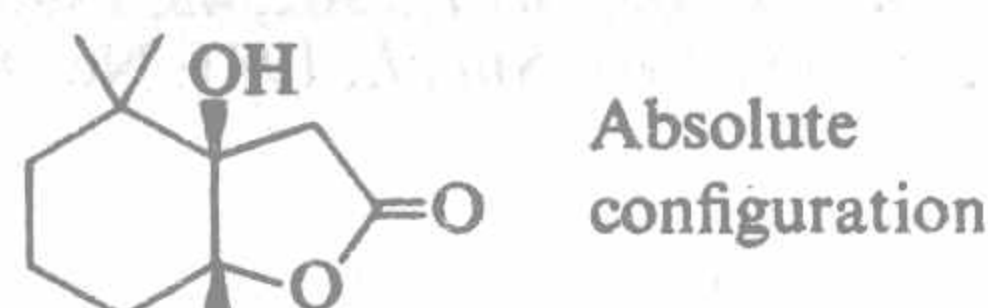
Chapman, B.E. *et al*, *Aust. J. Chem.*, 1982, 35, 489 (*pmr*)

Aeginetolide**A-20041**

Updated Entry replacing A-00597

Hexahydro-3a-hydroxy-4,4,7a-trimethyl-2(3H)-benzofuranone, 9Cl

[53337-93-2]



Absolute configuration

C₁₁H₁₈O₃ M 198.261

Constit. of *Aeginetia indica*. Cryst. Mp 169-70°.

Dighe, S.S. *et al*, *Indian J. Chem.*, 1973, 11, 404; 1974, 12, 413; 1977, 15, 546 (*isol, struct*)

Eschenmoser, W. *et al*, *Helv. Chim. Acta*, 1982, 65, 353 (*struct, synth, abs config*)

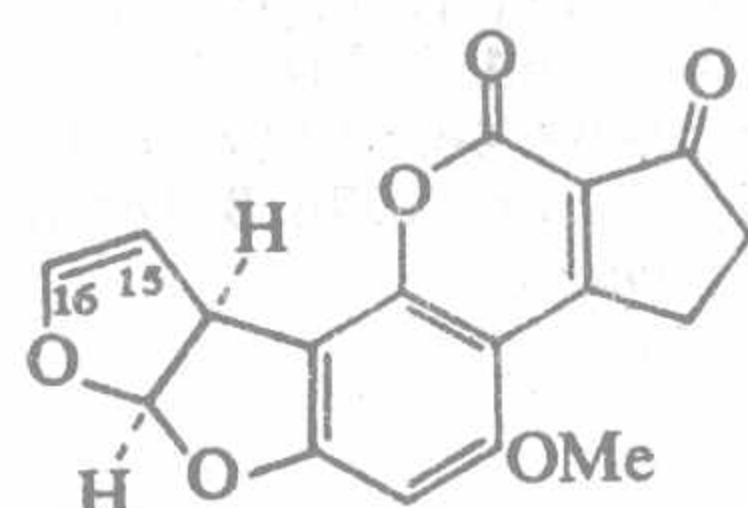
Rubottom, G.M. *et al*, *J. Org. Chem.*, 1983, 48, 422 (*synth*)

Aflatoxin B₁**A-20042**

Updated Entry replacing A-10049

2,3,6a,9a-Tetrahydro-4-methoxycyclopenta[c]furo[3,2':4,5]furo[2,3-h][1]benzopyran-1,11-dione, 9Cl. Aflatoxin; in FB₁. Aflatoxin B

[1162-65-8]

(-)-form
Absolute configurationC₁₇H₁₂O₆ M 312.278

Member of a group of closely related secondary fungal metab. shown to be mycotoxins.

▷GY1925000.

(-)-form

Isol. from *Aspergillus flavus* and *A. parasiticus*. Toxin causing Turkey X disease. Cryst. exhibiting blue fluor. Mp 268-9° dec. $[\alpha]_D^{25} -562^\circ$ (c, 0.115 in CHCl₃).

▷Extremely carcinogenic

15,16-Dihydro: [7220-81-7]. Aflatoxin B₂. Metab. of *A. flavus*. Mycotoxin. Yellow cryst. with blue fluor. (MeOH). Mp >310° dec. $[\alpha]_D^{23} -492^\circ$ (c, 0.1 in CHCl₃).

▷Carcinogenic

15,16-Dihydro, 16-hydroxy: [17878-54-5]. Aflatoxin B_{2a}. Dihydrohydroxyaflatoxin B₁. Metab. of *A. flavus*. Mycotoxin. Cryst. with blue fluor. (CHCl₃). Mp 217° (240° dec.).

▷Carcinogenic

De-O-Methyl: [32217-02-4]. Aflatoxin P₁. Metab. of Aflatoxin B₁. Pale-yellow needles (MeOH/C₆H₆/hexane). Mp >320°. $[\alpha]_D^{20} -574^\circ$ (c, 0.08 in MeOH).

▷Carcinogenic. GY1775000.

(±)-form [10279-73-9]

Mp 255-6°.

15,16-Dihydro: Cryst. with blue fluor. (CHCl₃/MeOH). Mp 303-6° dec.

v. Soest, T.C. *et al*, *Acta Crystallogr., Sect. B*, 1970, 26, 1940, 1947 (*cryst struct*)

Asao, T. *et al*, *J. Am. Chem. Soc.*, 1963, 85, 1705; 1965, 87, 882 (*struct, isol, ir, uv, ms, nmr*)

Dutton, M.F. *et al*, *Biochem. J.*, 1966, 101, 21P (*deriv*)

Brechbühler, S. *et al*, *J. Org. Chem.*, 1967, 32, 2641 (*abs config*)

Roberts, J.C. *et al*, *J. Chem. Soc. (C)*, 1968, 22 (*synth, uv, ir, ms*)

Heathcote, J.B. *et al*, *Tetrahedron*, 1969, 25, 1497; *Chem. Ind. (London)*, 1976, 270 (*biosynth*)

Büchi, G. *et al*, *J. Am. Chem. Soc.*, 1971, 93, 746 (*synth, uv, ms*)

Büchi, G. *et al*, *Life Sci.*, 1973, 13, 1143 (*synth*)

Pachler, K.G.R. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1976, 1182 (*cmr, biosynth*)

Cox, R.H. *et al*, *J. Org. Chem.*, 1977, 42, 112 (*cmr*)

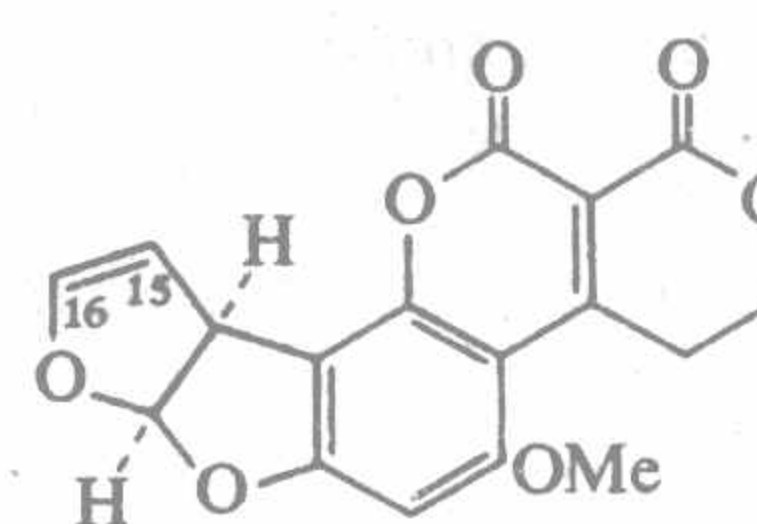
Simpson, T.J. *et al*, *J. Chem. Soc., Chem. Commun.*, 1982, 631; 1983, 338 (*biosynth*)

Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 344.

Aflatoxin G₁**A-20043**

Updated Entry replacing A-00613

[1165-39-5]



Absolute configuration

C₁₇H₁₂O₇ M 328.278

Isol. from *Aspergillus flavus* and *A. parasiticus*. Mycotoxin. Needles (MeOH) exhibiting green fluor. Mp 247-50°. $[\alpha]_D^{23} -556^\circ$ (c, 0.1 in CHCl₃).

▷Carcinogenic. LV1720000.

15,16-Dihydro: [7241-98-7]. Aflatoxin G₂. Minor constit. of *A. flavus*. Mycotoxin. Cryst. with green fluor. (EtOH). Mp 237-40°. $[\alpha]_D^{23} -473^\circ$ (c, 0.084 in CHCl₃).

▷Carcinogenic, extremely poisonous

15,16-Dihydro, 16-hydroxy: [20421-10-7]. Aflatoxin G_{2a}. Metab. of *A. flavus*. Cryst. with green fluor. Mp 190° dec.

▷Carcinogen

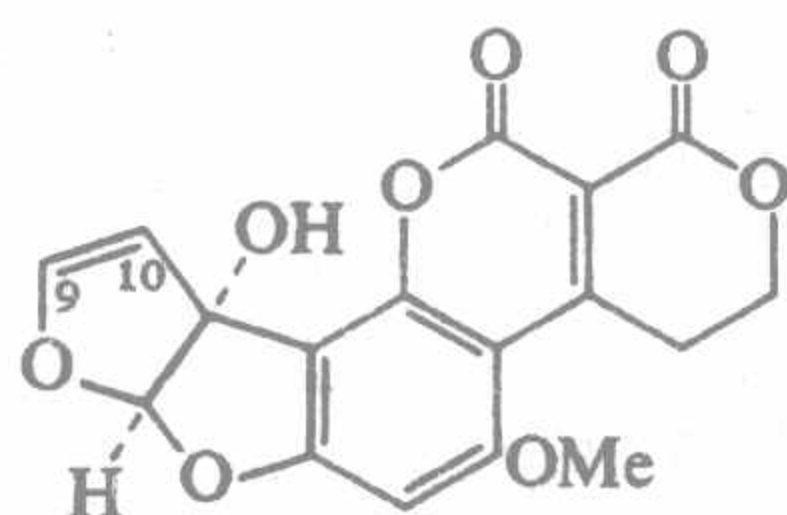
Nesbitt, B.E. *et al*, *Nature (London)*, 1962, **195**, 1062 (*isol*)
 Asao, T. *et al*, *J. Am. Chem. Soc.*, 1963, **85**, 1706; 1965, **87**, 882
 (*isol, uv, ir, ms, nmr, struct*)
 Dutton, M.F. *et al*, *Biochem. J.*, 1966, **101**, 21P (*deriv*)
 Brechbühler, S. *et al*, *J. Org. Chem.*, 1967, **32**, 2641 (*abs config*)
 Büchi, G. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 746 (*uv, ms, synth*)
 Heathcote, J.B. *et al*, *Chem. Ind. (London)*, 1976, 270 (*biosynth*)
 Cox, R.H. *et al*, *J. Org. Chem.*, 1977, **42**, 112 (*cmr*)
 Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 344.

Aflatoxin GM₁

A-20044

Updated Entry replacing A-00616

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



Absolute configuration

C₁₇H₁₂O₈ M 344.277

Metab. of *Aspergillus flavus*. Mycotoxin. Cryst. (CHCl₃). Mp 276°.

▷Carcinogenic

Ac: Mp 280°.

9,10-Dihydro: Aflatoxin GM₂. Minor metab. of *A. flavus*. Mp 270-2°.

Heathcote, J.B. *et al*, *Tetrahedron*, 1969, **25**, 1497 (*isol, uv, struct*)

Heathcote, J.B. *et al*, *Biochem. Soc. Trans.*, 1974, **2**, 301 (*deriv*)

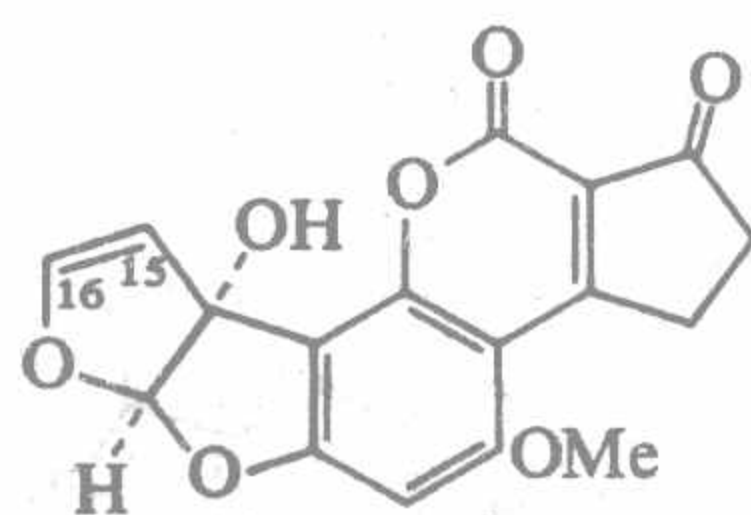
Heathcote, J.B. *et al*, *Chem. Ind. (London)*, 1976, 270 (*synth*)

Aflatoxin M₁

A-20045

Updated Entry replacing A-10050

[6795-23-9]

C₁₇H₁₂O₇ M 328.278

Minor metab. of *Aspergillus flavus*, also found in the milk of cows and sheep fed toxic meal. Mycotoxin. Cryst. (MeOH) exhibiting blue-violet fluor. Mp 299° dec. [α]_D²⁰ -280° (c, 0.1 in DMF).

▷Carcinogenic

Ac: Oil.

15,16-Dihydro: [6885-57-0]. Aflatoxin M₂. Trace metab. of *A. flavus*. Mycotoxin. Cryst. with violet fluor. (MeOH/CHCl₃). Mp 293° dec.

▷Carcinogenic

Holzappel, C.W. *et al*, *Tetrahedron Lett.*, 1966, 2799 (*isol, struct*)

Büchi, G. *et al*, *J. Am. Chem. Soc.*, 1969, **91**, 5408; 1971, **93**, 746 (*uv, ms, nmr, synth*)

Heathcote, J.B. *et al*, *Chem. Ind. (London)*, 1976, 270 (*biosynth*)

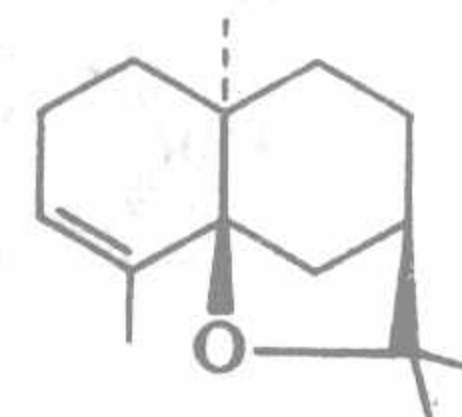
Büchi, G. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 3497 (*synth*)
 Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 345.

α-Agarofuran

A-20046

Updated Entry replacing A-00627

[5956-12-7]

C₁₅H₂₄O M 220.354

Constit. of Agar wood oil (from fungus infected *Aquillaria agallocha*. Oil. Bp₆ 134°. [α]_D +37.1° (c, 6.1 in CHCl₃).

3α,4α-Epoxy: Constit. of *Alpinia japonica*. Oil. [α]_D²⁵ -20.8° (c, 0.4 in EtOH).

Maheshwari, M.L. *et al*, *Tetrahedron*, 1963, **19**, 1077 (*isol*)

Barrett, H.C. *et al*, *J. Am. Chem. Soc.*, 1967, **89**, 5665 (*struct*)

Marshall, J.A. *et al*, *J. Org. Chem.*, 1968, **33**, 435 (*synth*)

Huffmann, J.W. *et al*, *J. Org. Chem.*, 1976, **41**, 3705 (*synth*)

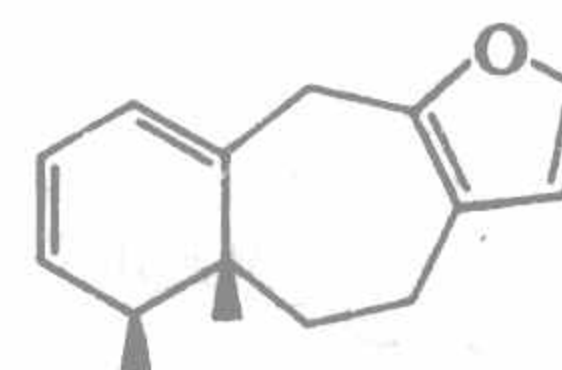
Itohawa, H. *et al*, *Chem. Pharm. Bull.*, 1980, **28**, 681 (*isol*)

Huffman, J.W. *et al*, *J. Org. Chem.*, 1982, **47**, 3254 (*synth*)

Agassizin

A-20047

[79827-32-0]

C₁₅H₁₈O M 214.307

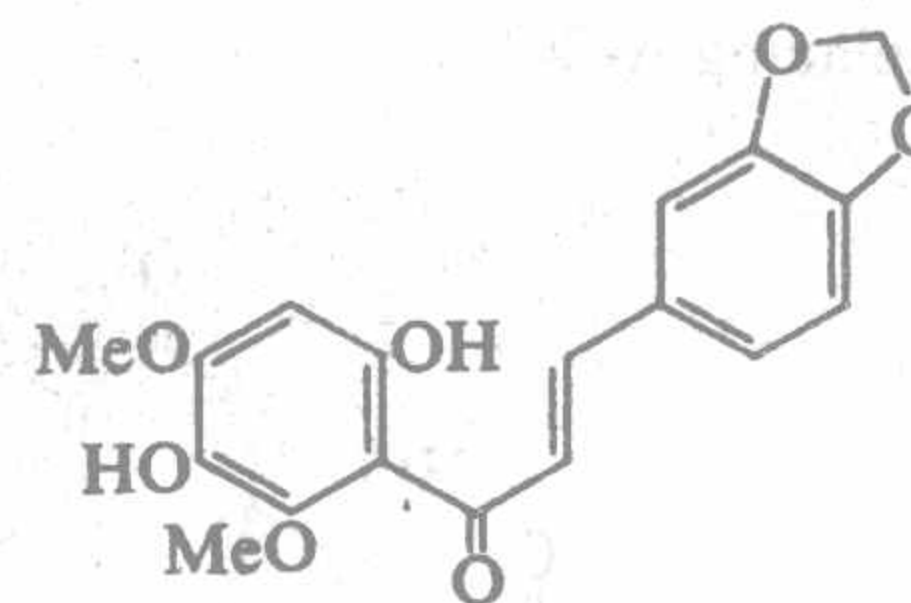
Constit. of the nudibranch *Hypselodoris* spp. Oil. [α]_D -94° (c, 1.2 in MeOH).

Hochlowski, J.E. *et al*, *J. Org. Chem.*, 1982, **47**, 88.

Agestricin A

A-20048

3-(1,3-Benzodioxol-5-yl)-1-(3,6-dihydroxy-2,4-dimethoxyphenyl)-2-propen-1-one, 9Cl. 3',6'-Dihydroxy-2',4'-dimethoxy-3,4-methylenedioxychalcone
 [85563-73-1]

C₁₈H₁₆O₇ M 344.320

Constit. of *Ageratum strictum*. Dark-red cryst. (Me₂CO/Et₂O). Mp 190-2°.

Quijano, L. *et al*, *Phytochemistry*, 1982, **21**, 2575.

The symbol ▷ in Entries highlights hazard or toxicity information