Dictionary of Organic Compounds

FIFTH EDITION

SEVENTH SUPPLEMENT

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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 these compounds. The absence of such information should not however be taken as an indication of safety in use or misuse.

Contents

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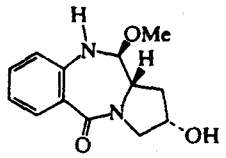
Abbeymycin **A-70001**

1,2,3,10,11,11a-Hexahydro-2-hydroxy-11-methoxy-5H-pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 9CI

[108073-64-9]



$C_{13}H_{16}N_2O_3$ M 248.281

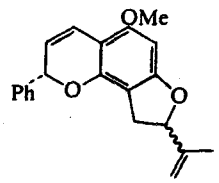
Anthramycin-type antibiotic. Prod. by *Streptomyces* AB 999F-52. Exhibits weak antibacterial activity. Platelets ($CHCl_3$/MeOH). Mp 142-144° dec. $[\alpha]_D^{25}$ +303° (c, 0.741 in H_2O).

Hochlowski, J.E. *et al*, *J. Antibiot.*, 1987, **40**, 145 (*isol, struct, props*)

Abbottin **A-70002**

8,9-Dihydro-5-methoxy-8-(1-methylethenyl)-2-phenyl-2H-furo[2,3-h]-1-benzopyran, 9CI

[106327-62-2]

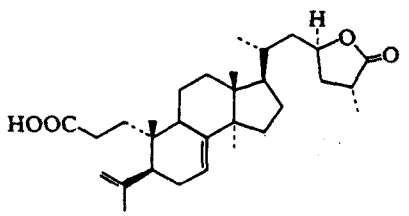


$C_{21}H_{20}O_3$ M 320.387

Isol. from *Tephrosia abbottiae*. Red viscous oil.

Gomez-Garibay, F. *et al*, *Chem. Ind. (London)*, 1986, 827 (*isol*)

Abiesolidic acid **A-70003**



$C_{30}H_{46}O_4$ M 470.691

Constit. of *Abies sibirica*.

Me ester: [108195-55-7]. Cryst. (Et_2O/pet. ether). Mp 154-155°. $[\alpha]_D^{21}$ +10.3° (c, 3.86 in $CHCl_3$).

Raldugin, V.A. *et al*, *Khim. Prir. Soedin.*, 1986, **22**, 688; *Chem. Nat. Compd.*, p. 645 (*isol, cryst struct*)

8,11,13-Abietatriene-7,18-diol **A-70004**

$C_{20}H_{30}O_3$ M 318.455

7α-form

Constit. of pollen grains of *Cedrus deodara*. Needles (Me_2CO). Mp 89°. $[\alpha]_D^{20}$ −3.3° (c, 0.46 in EtOH).

Ohmoto, T. *et al*, *Chem. Pharm. Bull.*, 1987, **35**, 229.

8,11,13-Abietatriene-12,18-diol **A-70005**

18-Hydroxyferruginol

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

Constit. of *Torreya nucifera*. Cryst. (Me_2CO). Mp 180-181°. $[\alpha]_D^{25}$ +70.3° (c, 0.37 in EtOH).

18-Aldehyde: 12-Hydroxy-8,11,13-abietatrien-18-al. ***18-Oxoferruginol***.

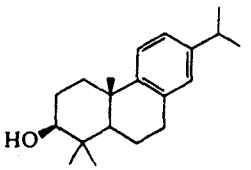
$C_{20}H_{28}O_2$ M 300.440

Constit. of *Torreya nucifera*. Cryst. (hexane). Mp 139-141°. $[\alpha]_D$ +69.6° (c, 1.05 in $CHCl_3$).

Fukushima, I. *et al*, *Agric. Biol. Chem.*, 1968, **32**, 1103 (*isol, struct*)

Harrison, L.J. *et al*, *Phytochemistry*, 1987, **26**, 1211 (*deriv*)

8,11,13-Abietatrien-3-ol **A-70006**



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

3β-form [78078-41-8]

Constit. of *Nepeta tuberosa*. Cryst. (hexane). Mp 109-111° (nat.), Mp 136.5-138° (synthetic). $[\alpha]_D$ +37.26° (c, 0.95 in $CHCl_3$), $[\alpha]_D$ +50.4° ($CHCl_3$).

Ac: Mp 112-114°. $[\alpha]_D$ +58.9° ($CHCl_3$).

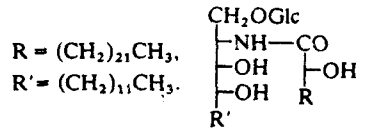
Matsumoto, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 581 (*synth, pmr*)

Urones, J.G. *et al*, *Phytochemistry*, 1988, **27**, 523 (*isol*)

Acanthocerebroside *A* **A-70007**

1-Glucopyranosyl-2-(2-hydroxytetracosanoylamino)-1,3,4-hexadecanetriol

[110744-71-3]



$C_{46}H_{91}NO_{10}$ M 818.226

Cerebroside from the starfish *Acanthaster planci*. Needles + $3H_2O$ (MeOH). Mp 209-210°. $[\alpha]_D$ +2.4° (c, 0.81 in propanol).

Kawano, Y. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 19 (*isol, pmr, cmr, struct*)

Acanthocerebroside *B* **A-70008**

1-Glucopyranosyl-2-(2-hydroxyhexadecanoylamino)-1,3,4-docesanetriol

[110744-72-4]

As Acanthocerebroside *A*, A-70007 with

$$R = -(CH_2)_{13}CH_3,\ R' = (CH_2)_{11}CH_3$$

$C_{44}H_{87}NO_{10}$ M 790.172

Cerebroside from the starfish *Acanthaster planci*. Needles + $1H_2O$ (MeOH). Mp 218-219°. $[\alpha]_D$ +7.8° (c, 0.24 in propanol).

Kawano, Y. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 19 (*isol, pmr, cmr, struct*)

Acanthocerebroside *C* **A-70009**

1-Glucopyranosyl-2-(2-hydroxyhexadecanoylamino)-13-docosene-1,3,4-triol

[110744-73-5]

As Acanthocerebroside *A*, A-70007 with

R = $(CH_2)_{13}CH_3$, R′ = $-(CH_2)_8CH{=}CH(CH_2)_7CH_3$ (*Z*-)

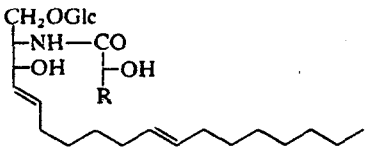
$C_{44}H_{85}NO_{10}$ M 788.156

Cerebroside from the starfish *Acanthaster planci*. Needles (MeOH). Mp 203-204°. $[\alpha]_D$ +18.3° (c, 1.24 in propanol).

Kawano, Y. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 19 (*isol, pmr, cmr, struct*)

Acanthocerebroside *D* **A-70010**

[110744-74-6]



R = $-(CH_2)_{19}CH_3$

$C_{46}H_{87}NO_9$ M 798.195

Cerebroside from the starfish *Acanthaster planci*. Needles + $2H_2O$ (MeOH). Mp 198-199°. $[\alpha]_D$ +1.1° (c, 0.3 in propanol).

Kawano, Y. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 19 (*isol, pmr, cmr, struct*)

Acanthocerebroside *E* **A-70011**

[110744-75-7]

As Acanthocerebroside *D*, A-70010 with

R = $-(CH_2)_{20}CH_3$

$C_{47}H_{89}NO_9$ M 812.221

Cerebroside from the starfish *Acanthaster planci*. Needles + $3H_2O$ (MeOH). Mp 194-195°. $[\alpha]_D$ +1.0° (c, 0.3 in propanol).

Kawano, Y. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 19 (*isol, pmr, cmr, struct*)

Acanthocerebroside *F* **A-70012**

[110744-76-8]

As Acanthocerebroside *D*, A-70010 with

R = $(CH_2)_{21}CH_3$

$C_{48}H_{91}NO_9$ M 826.248

Cerebroside from the starfish *Acanthaster planci*. Needles + $2H_2O$ (MeOH). Mp 193-194°. $[\alpha]_D$ +1.2° (c, 0.5 in propanol).

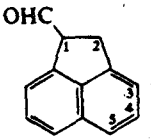
Kawano, Y. *et al*, *Justus Liebigs Ann. Chem.*, 1988, 19 (*isol, pmr, cmr, struct*)

1-Acenaphthenecarboxaldehyde **A-70013**

Updated Entry replacing A-00061

1-Formylacenaphthene

[37977-48-3]



$C_{13}H_{10}O$ M 182.221

(±)-*form*

Yellowish needles (Et_2O/pet. ether). Mp 99.5-100.5°. $Bp_{0.1}$ 154°.

Oxime:

$C_{13}H_{11}NO$ M 197.236

Yellow needles (C_6H_6). Mp 152°.

Feiser, L. *et al*, *J. Am. Chem. Soc.*, 1940, **62**, 49 (*synth*)
Ger. Pat., 2 064 279, (*1972*); *CA*, **77**, 114126r (*synth*)
Raffaelli, A. *et al*, *Synthesis*, 1988, 893 (*synth, deriv, ir, pmr*)

1-Acenaphthenecarboxylic acid, 8CI **A-70014**

Updated Entry replacing A-00062

1,2-Dihydro-5-acenaphthylenecarboxylic acid, 9CI. 1-Acenaphthoic acid

[6833-51-8]

$C_{13}H_{10}O_2$ M 198.221

(±)-*form*

Needles (EtOH aq. or Et_2O/pet. ether). Mp 163-164°.

Nitrile: 1-Cyanoacenaphthene.

$C_{13}H_9N$ M 179.221

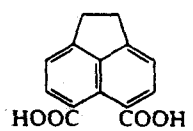
Cryst. (pet. ether). Mp 68°.

Julia, M. *et al*, *Bull. Soc. Chim. Fr.*, 1952, 1065 (*synth*)
Canceid, J. *et al*, *Bull. Soc. Chim. Fr.*, 1973, 2727 (*synth*)
Fay, C.K. *et al*, *J. Org. Chem.*, 1973, **38**, 3122 (*pmr*)
Raffaelli, A. *et al*, *Synthesis*, 1988, 893 (*nitrile*)

5,6-Acenaphthenedicarboxylic acid, 8CI **A-70015**

1,2-Dihydro-5,6-acenaphthylenedicarboxylic acid, 9CI

[5698-99-7]



$C_{14}H_{10}O_4$ M 242.231

Mp 294°.

Dinitrile: [86528-79-2]. *5,6-Dicyanoacenaphthene.*

$C_{14}H_8N_2$ M 204.231

Cryst. (CH_2Cl_2). Mp 310-311° (charred before melting).

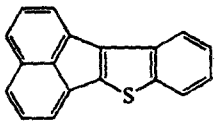
Bis(dimethylamide): [31458-06-7].

$C_{18}H_{20}N_2O_2$ M 296.368

Solid (EtOH aq.). Mp 112-114°.

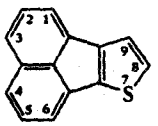
Freund, M. *et al*, *Justus Liebigs Ann. Chem.*, 1913, **399**, 182 (*deriv, synth*)
Carpino, L.A. *et al*, *J. Org. Chem.*, 1964, **29**, 2824 (*synth*)
Trost, B.M. *et al*, *J. Am. Chem. Soc.*, 1971, **93**, 737 (*synth, ir, pmr, ms*)
Rieke, L.I. *et al*, *J. Org. Chem.*, 1983, **48**, 2949 (*deriv, synth, ir, ms*)

Acenaphtho[1,2-*b*]benzo[*d*]thiophene A-70016



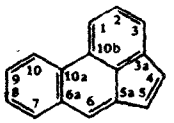
$C_{18}H_{10}S$ M 258.337
Solid. Mp 125°.
Kar, G.K. *et al*, *Org. Prep. Proced. Int.*, 1988, **20**, 213.

Acenaphtho[1,2-*b*]thiophene A-70017
[1969-60-4]



$C_{14}H_8S$ M 208.277
Yellow needles (pet. ether). Mp 73-74° (67°).
Hauptmann, S. *et al*, *J. Prakt. Chem.*, 1969, **311**, 614 (*synth, uv*)
Kar, G.K. *et al*, *Org. Prep. Proced. Int.*, 1988, **20**, 213 (*synth*)

Acephenanthrylene, 9CI A-70018
[201-06-9]



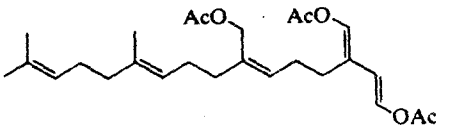
$C_{16}H_{10}$ M 202.255
Yellowish cryst. (MeOH). Mp 143-144°.
Laarhoven, W.H. *et al*, *Recl. Trav. Chim. Pays-Bas*, 1976, **95**, 165 (*synth, uv, pmr*)
Chung, Y.-S. *et al*, *J. Org. Chem.*, 1987, **52**, 1284 (*synth, pmr*)

Acetamide, 9CI A-70019
Updated Entry replacing A-00092
[60-35-5]

H_3CCONH_2

C_2H_5NO M 59.068
Solubiliser, plasticiser, stabiliser, used industrially as solv. in molten form. Dissolves virtually all classes of organic and inorganic compds. Deliquescent, hexagonal cryst. Odourless when pure but usually has characteristic "mouse" odour. V. sol. H_2O, EtOH, sol. $CHCl_3$, prac. insol. Et_2O. Mp 82-83°. Bp 222°, Bp_5 92°. Triboluminescent.
▷Mild irritant, exp. carcinogen. AB4025000.
B,$^1/_2$*HBr:* [20731-46-8]. Reagent for brominating acid-sensitive compds. Needles. Mp 138-139°.
Picrate: Mp 117°.
N-*Chloro: see N-Chloroacetamide, C-00656*
N-*Bromo: see N-Bromoacetamide, B-01883*
N-*Iodo: see N-Iodoacetamide, I-00357*
N-*Ac: see Diacetamide, D-00497*
N-*Me:* [79-16-3].
C_3H_7NO M 73.094
Bp_8 65°.
▷AC5960000.
N-*Di-Me:* [127-19-5].
C_4H_9NO M 87.121
Bp 179-181°, Bp_{10} 68-69°.
▷AB7700000.
Org. Synth., Coll. Vol., **1**, 3 (*synth*)
Robson, J.H. *et al*, *J. Am. Chem. Soc.*, 1955, **77**, 498 (*deriv*)
Marakami, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1962, **35**, 11 (*synth*)
Ueki, M. *et al*, *Bull. Chem. Soc. Jpn.*, 1971, **44**, 1108 (*deriv*)
Ottersen, T., *Acta Chem. Scand., Ser. A*, 1975, **29**, 944 (*cryst struct*)
Kerridge, D.H., *Chem. Soc. Rev.*, 1988, **17**, 181 (*rev*)
Fieser, M. *et al*, *Reagents for Organic Synthesis*, Wiley, 1967-84, **1**, 3.
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 332.

1-Acetoxy-7-acetoxymethyl-3-acetoxymethylene-11,15-dimethyl-1,6,10,14-hexadecatetraene A-70020



$C_{26}H_{38}O_6$ M 446.583
Compd. not named in the paper, not indexed by *CA*. Metab. of *Penicillus dumetosus*. Antibacterial and antifungal. Oil. $[\alpha]_D^{25}$ +17° (c, 1.3 in $CHCl_3$).
Paul, V.J. *et al*, *Tetrahedron*, 1984, **40**, 2913.

2-Acetyl-3-aminobenzofuran A-70021
1-(3-Amino-2-benzofuranyl)ethanone, 9CI. 3-Amino-2-benzofuryl methyl ketone
[49615-96-5]

$C_{10}H_9NO_2$ M 175.187
Cryst. (EtOH). Mp 153-154°.
Gewald, K. *et al*, *J. Prakt. Chem.*, 1973, **315**, 779 (*synth*)
Bachechi, F. *et al*, *Acta Crystallogr., Sect. C*, 1988, **44**, 1449 (*cryst struct*)

2-Acetyl-3-aminopyridine A-70022
1-(3-Amino-2-pyridinyl)ethanone, 9CI. 3-Amino-2-pyridinyl methyl ketone, 8CI
[13210-25-8]

$C_7H_8N_2O$ M 136.153
Yellow plates (pet. ether). Mp 66-67° (63-64°).
2,4-Dinitrophenylhydrazone; B,HCl: [13385-49-4]. Needles (AcOH). Mp 276-277°.
Picrate: [51460-34-5]. Yellow prisms (EtOH aq.). Mp 200-201°.

Atkinson, C.M. *et al*, *J. Chem. Soc.* (*C*), 1966, 2053 (*synth*)
Edward, J.T. *et al*, *J. Heterocycl. Chem.*, 1973, **10**, 1047 (*synth*)

2-Acetyl-5-aminopyridine **A-70023**
1-(5-Amino-2-pyridinyl)ethanone, *9CI*. *5-Amino-2-pyridinyl methyl ketone*, *8CI*
[51460-32-3]
$C_7H_8N_2O$ M 136.153
Mp 108-109°.
B,HCl: [34689-84-4]. Mp 208-210° dec.
Picrate: [51460-36-7]. Yellow needles (EtOH aq.). Mp 191-192°.
N-*Ac:* [31557-77-4].
$C_9H_{10}N_2O_2$ M 178.190
Cryst. (C_6H_6). Mp 114-116°.
Edward, J.T. *et al*, *J. Heterocycl. Chem.*, 1973, **10**, 1047 (*synth*)
Cooper, G.H. *et al*, *J. Chem. Soc.* (*C*), 1971, 772, 3257 (*synth*)

3-Acetyl-2-aminopyridine **A-70024**
1-(2-Amino-3-pyridinyl)ethanone, *9CI*. *2-Amino-3-pyridinyl methyl ketone*
[65326-33-2]
$C_7H_8N_2O$ M 136.153
Mp 136°.
Güngör, T. *et al*, *J. Organomet. Chem.*, 1981, **215**, 139 (*synth, pmr*)

3-Acetyl-4-aminopyridine **A-70025**
1-(4-Amino-3-pyridinyl)ethanone, *9CI*. *4-Amino-3-pyridinyl methyl ketone*
[53277-43-3]
$C_7H_8N_2O$ M 136.153
Cryst. (C_6H_6). Mp 165-166°.
Clark, B.A.J. *et al*, *Tetrahedron*, 1974, **30**, 475 (*synth*)

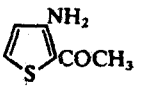
4-Acetyl-2-aminopyridine **A-70026**
1-(2-Amino-4-pyridinyl)ethanone, *9CI*. *2-Amino-4-pyridinyl methyl ketone*
[42182-25-2]
$C_7H_8N_2O$ M 136.153
Cryst. (toluene). Mp 133-133.5°.
Oxime: [80882-45-7]. Cryst. (EtOAc). Mp 215-217°.
N^2,N^2-*Di-Me:* [80882-53-7].
$C_9H_{12}N_2O$ M 164.207
Cryst. Mp 37-42°.
N^2,N^2-*Di-Me, oxime:* [80882-54-8]. Pale-yellow cryst. (toluene). Mp 145-148°.
LaMattina, J.L., *J. Heterocycl. Chem.*, 1983, **20**, 533 (*synth*)

4-Acetyl-3-aminopyridine **A-70027**
1-(3-Amino-4-pyridinyl)ethanone, *9CI*. *3-Amino-4-pyridinyl methyl ketone*
[13210-52-1]
$C_7H_8N_2O$ M 136.153
Yellow plates (pet. ether). Mp 91-92° (87°).
2,4-Dinitrophenylhydrazone; B,HCl: [13210-54-3]. Pale-yellow needles (AcOH). Mp 287-288° dec.
Picrate: [51460-35-6]. Yellow leaflets (EtOH aq.). Mp 189-191°.

Atkinson, C.M. *et al*, *J. Chem. Soc.* (*C*), 1966, 2053 (*synth*)
Edward, J.T. *et al*, *J. Heterocycl. Chem.*, 1973, **10**, 1047 (*synth*)

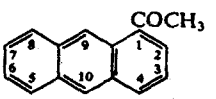
5-Acetyl-2-aminopyridine **A-70028**
1-(6-Amino-3-pyridinyl)ethanone, *9CI*. *6-Amino-3-pyridinyl methyl ketone*, *8CI*
[19828-20-7]
$C_7H_8N_2O$ M 136.153
Cryst. (Me_2CO/hexane or Et_2O). Mp 122° (89-90°).
B,HCl: [19828-21-8]. Cryst. (MeOH/Et_2O). Mp 194°.
N-*Oxide:* [49647-13-4].
$C_7H_8N_2O_2$ M 152.152
Cryst. (Me_2CO aq.) (as hydrochloride). Mp 190-191° (hydrochloride).
Swiss Pat., 452 525, (*1968*); *CA*, **69**, 96488 (*synth*)
Korytnyk, W. *et al*, *J. Med. Chem.*, 1973, **16**, 959 (*synth*)

2-Acetyl-3-aminothiophene **A-70029**
1-(3-Amino-2-thienyl)ethanone, *9CI*
[31968-33-9]



C_6H_7NOS M 141.187
Needles (pet. ether). Mp 82-83° (89-90°).
Huddleston, P.R. *et al*, *Synth. Commun.*, 1979, **9**, 732 (*synth*)

1-Acetylanthracene **A-70030**
1-(1-Anthracenyl)ethanone, *9CI*. *1-Anthryl methyl ketone*, *8CI*
[7396-21-6]



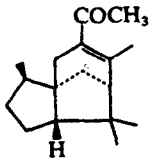
$C_{16}H_{12}O$ M 220.270
Cryst. (EtOH). Mp 110.5-111°.
2,4-Dinitrophenylhydrazone: Cryst. (Py/EtOH). Mp 260°.
Gore, P.H. *et al*, *J. Org. Chem.*, 1957, **22**, 135.
Bassilios, H.F. *et al*, *Recl. Trav. Chim. Pays-Bas*, 1963, **82**, 298 (*synth*)
Gore, P.H. *et al*, *J. Chem. Soc.* (*C*), 1966, 1729 (*synth, deriv, uv, ir*)

2-Acetylanthracene **A-70031**
1-(2-Anthracenyl)ethanone, *9CI*. *2-Anthryl methyl ketone*, *8CI*
[10210-32-9]
$C_{16}H_{12}O$ M 220.270
Cryst. (C_6H_6). Mp 195.5-196°.
2,4-Dinitrophenylhydrazine: Cryst. (Py). Mp 297°.
Gore, P.H. *et al*, *J. Org. Chem.*, 1957, **22**, 135.
Gore, P.H. *et al*, *J. Chem. Soc.* (*C*), 1966, 1729 (*synth, deriv, uv, ir*)

Acetylcedrene A-70032

Vertofix. Lixetone

[32388-55-9]



$C_{17}H_{26}O$ M 246.392

Perfumery ingredient. Bp_4 120-122°, $Bp_{0.01}$ 84-86°. $[\alpha]_D^{25}$ −38.5° (neat). n_D^{20} 1.5152.

Kitchens, G.C. *et al, J. Org. Chem.*, 1972, **37**, 6 (*synth, ir, ms, pmr*)

McAndrew, B.A. *et al, J. Chem. Soc., Perkin Trans. 1*, 1983, 1373 (*synth*)

2-Acetyl-5-chloropyridine A-70033

1-(5-Chloro-2-pyridinyl)ethanone, 9CI

[94952-46-2]

C_7H_6ClNO M 155.584

Eur. Pat., 122 056, (*1983*); *CA*, **102**, 132042 (*synth*)

3-Acetyl-2-chloropyridine A-70034

1-(2-Chloro-3-pyridinyl)ethanone, 9CI

[55676-21-6]

C_7H_6ClNO M 155.584

Sainsbury, M. *et al, J. Chem. Soc., Perkin Trans. 1*, 1975, 289.
U.S.P., 4 060 601, (*1977*); *CA*, **88**, 136458 (*synth*)

4-Acetyl-2-chloropyridine A-70035

1-(2-Chloro-4-pyridinyl)ethanone, 9CI. 2-Chloro-4-pyridinyl methyl ketone, 8CI

[23794-15-2]

C_7H_6ClNO M 155.584

Cryst. (pet. ether). Mp 36-39°.

Ger. Pat., 1 811 833, (*1969*); *CA*, **71**, 91325 (*synth*)
LaMattina, J.L., *J. Heterocycl. Chem.*, 1983, **20**, 533 (*synth*)

4-Acetyl-3-chloropyridine A-70036

1-(3-Chloro-4-pyridinyl)ethanone, 9CI. 3-Chloro-4-pyridinyl methyl ketone

[78790-82-6]

C_7H_6ClNO M 155.584

Liq. Bp_2 81°, $Bp_{0.1}$ 55°.

LaMattina, J.L. *et al, J. Org. Chem.*, 1981, **46**, 4179 (*synth*)
Marsais, F. *et al, J. Organomet. Chem.*, 1981, **216**, 139 (*synth*)

5-Acetyl-2-chloropyridine A-70037

1-(6-Chloro-3-pyridinyl)ethanone, 9CI

[55676-22-7]

C_7H_6ClNO M 155.584

Mp 104°.

Phenylhydrazone: Pale-yellow cryst. Mp 164°.

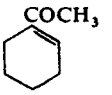
Binz, A. *et al, Justus Liebigs Ann. Chem.*, 1931, **487**, 127 (*synth*)
Sainsbury, M. *et al, J. Chem. Soc., Perkin Trans. 1*, 1975, 289.

1-Acetylcyclohexene A-70038

Updated Entry replacing A-00249

1-(1-Cyclohexen-1-yl)ethanone, 9CI. 3,4,5,6-Tetrahydroacetophenone

[932-66-1]



$C_8H_{12}O$ M 124.182

Bp_{22} 85-88°. n_D^{20} 1.488.

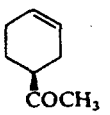
Oxime: [23042-98-0].
$C_8H_{13}NO$ M 139.197
Cryst. (C_6H_6/ligroin). Mp 99°.

2,4-Dinitrophenylhydrazone: Mp 204-205° (196-197°).

Org. Synth., Coll. Vol., **3**, 22 (*synth*)
Ferres, H., *J. Chem. Soc., Perkin Trans. 2*, 1973, 936 (*synth*)
Hasbrouck, R. *et al, J. Org. Chem.*, 1973, **38**, 2103 (*synth*)
Zhang, P. *et al, Synth. Commun.*, 1986, **16**, 957 (*synth, ir, uv*)

4-Acetylcyclohexene A-70039

3-Cyclohexenyl methyl ketone. 1',2',3',6'-Tetrahydroacetophenone



(S)-form

$C_8H_{12}O$ M 124.182

(S)-form

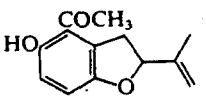
$[\alpha]_D^{23}$ −116.3° (c, 1.25 in $CHCl_3$) (~99% opt. pure).

Ceder, O. *et al, Acta Chem. Scand., Ser. B*, 1976, **30**, 908 (*synth, ir, pmr, ms*)
Brown, H.C. *et al, J. Am. Chem. Soc.*, 1987, **109**, 5420 (*synth, ir, pmr*)

4-Acetyl-2,3-dihydro-5-hydroxy-2-isopropenylbenzofuran A-70040

1-[2,3-Dihydro-5-hydroxy-2-(1-methylethenyl)-4-benzofuranyl]ethanone, 9CI. 4-Acetyl-2-isopropenyl-2,3-dihydro-5-benzofuranol

[110694-79-6]



$C_{13}H_{14}O_3$ M 218.252

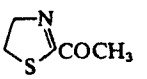
Isol. from *Lasiolaena morii*. Cryst. (hexane). Mp 75-76°.

Bohlmann, F. *et al, Phytochemistry*, 1982, **21**, 161 (*isol*)
Yamaguchi, S. *et al, Bull. Chem. Soc. Jpn.*, 1986, **59**, 3983 (*synth, struct*)

2-Acetyl-4,5-dihydrothiazole A-70041

1-(4,5-Dihydro-2-thiazolyl)ethanone, 9CI. Methyl 2-thiazolin-2-yl ketone, 8CI. 2-Acetyl-2-thiazoline

[29926-41-8]



C_5H_7NOS M 129.176

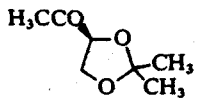
Roasted meat-like flavour ingredient. Mp 25-26°. Bp_{11} 94°. n_D^{20} 1.5294.

Oxime: [37112-89-3].
$C_5H_8N_2OS$ M 144.191
Cryst. (CCl_4). Mp 178-179° dec.

Doornbos, T. *et al*, *Recl. Trav. Chim. Pays-Bas*, 1972, **91**, 711 (*synth, deriv, ir, pmr, uv, ms*)
U.S.P., 3 778 518, (*1973*); *CA*, **80**, 69405e (*props*)

4-Acetyl-2,2-dimethyl-1,3-dioxolane A-70042

1-(2,2-Dimethyl-1,3-dioxolan-4-yl)ethanone, 9CI



$C_7H_{12}O_3$ M 144.170

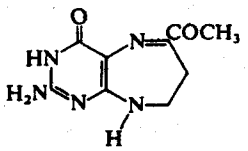
(*S*)-form [99566-52-6]
Chiral intermed. Oil. $[\alpha]_D$ −65° (c, 1.5 in C_6H_6), $[\alpha]_D$ −82° (c, 3.3 in $CHCl_3$). 96% enantiomeric excess. Previous syntheses claimed a lower opt. rotn.

Tanner D. *et al*, Synth. Commun.1986, **16**, 1517 (*synth, pmr, bibl*)

6-Acetylhomopterin A-70043

6-Acetyl-2-amino-1,7,8,9-tetrahydro-4H-pyrimido[4,5-b][1,4]diazepin-4-one, 9CI

[80003-63-0]



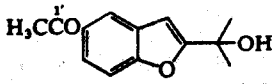
$C_9H_{11}N_5O_2$ M 221.218
Naturally occurring diazepine from *Drosophila melanogaster*. Intermed. involved in the biosynth. of Drosopterin, D-60521 . Greenish-yellow cryst.

Wiederrecht, G.J. *et al*, *J. Biol. Chem.*, 1981, **256**, 10399 (*isol, struct, ms, pmr*)
Jacobson, K.B. *et al*, *Biochemistry*, 1982, **21**, 5700 (*isol, struct, pmr, cmr, uv*)
Boyle, P.H. *et al*, *Tetrahedron Lett.*, 1987, **28**, 5331 (*synth*)

5-Acetyl-2-(1-hydroxy-1-methylethyl)-benzofuran A-70044

1-[2-(1-Hydroxy-1-methylethyl)-5-benzofuranyl]-ethanone, 9CI. 5-Acetyl-2-(2-hydroxyisopropyl)-benzofuran

[64165-99-7]



$C_{13}H_{14}O_3$ M 218.252
Isol. from *Podachaenium eminens, Fleischmanniopsis leucocephala, Smallanthus fruticosus, Stylotrichium rotundifolium* and other plants. Cryst. (Et_2O/pet. ether). Mp 73°.

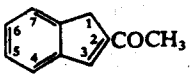
1'-Alcohol: 5-(1-Hydroxyethyl)-2-(1-hydroxy-1-methylethyl)benzofuran.
$C_{13}H_{16}O_3$ M 220.268
Constit. of *Smallanthus fruticosus*. Oil. No opt. rotn. reported.

Bohlmann, F. *et al*, *Phytochemistry*, 1977, **16**, 1304; 1978, **17**, 2101; 1980, **19**, 973; 1981, **20**, 1887 (*isol, ir, ms, struct*)
Schneiders, G.E. *et al*, *Synth. Commun.*, 1980, **10**, 699 (*synth*)

2-Acetyl-1*H*-indene A-70045

1-(1H-Inden-2-yl)ethanone, 9CI. Inden-2-yl methyl ketone

[43073-11-6]



$C_{11}H_{10}O$ M 158.199
Cryst. (Et_2O/hexane). Mp 62° (56-58°). Originally reported (1921) as having Mp 122°; this was a trimer.

Doyle, P. *et al*, *Tetrahedron Lett.*, 1973, 2903 (*synth*)
Marx, J.N. *et al*, *Synth. Commun.*, 1973, **3**, 95 (*synth, pmr*)
Eliasson, B. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1981, 403 (*cmr*)
Satoh, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1987, **60**, 1839 (*synth, ir, pmr, ms*)

3-Acetyl-1*H*-indene A-70046

1-(1H-Inden-3-yl)ethanone, 9CI. Inden-3-yl methyl ketone, 8CI. 1-Acetylindene

[28529-48-8]

$C_{11}H_{10}O$ M 158.199
Mp 65-66° (52-54°).

Uhde, W. *et al*, *Chem. Ber.*, 1970, **103**, 2675 (*synth, struct*)
Craig, J.C. *et al*, *J. Org. Chem.*, 1974, **39**, 1669 (*synth*)

6-Acetyl-1*H*-indene A-70047

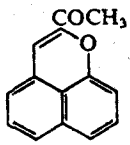
1-(1H-Inden-6-yl)ethanone, 9CI. Inden-6-yl methyl ketone

$C_{11}H_{10}O$ M 158.199
Liq. Bp_3 143-145°.

2,4-Dinitrophenylhydrazone: Cryst. (Py). Mp 265-270°.

Kumazawa, Z. *et al*, *Agric. Biol. Chem.*, 1961, **25**, 798 (*synth*)

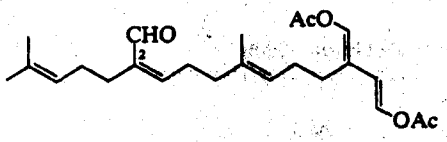
2-Acetylnaphtho[1,8-*bc*]pyran A-70048



$C_{14}H_{10}O_2$ M 210.232
Yellow-orange microcryst. (pet. ether).

Buisson, J.-P. *et al*, *J. Heterocycl. Chem.*, 1988, **25**, 539 (*synth, pmr, uv*)

12-(Acetyloxy)-10-[(acetyloxy)methylene]-6-methyl-2-(4-methyl-3-pentenyl)-2,6,11-dodecatrienal, 9CI A-70049

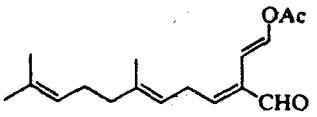


$C_{24}H_{34}O_5$ M 402.530

(*2E*)-form
Metab. of *Penicillus dumetosus*. Oil.

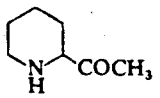
(2Z)-form
Metab. of *P. dumetosus*. Oil.
Paul, V.J. *et al*, *Tetrahedron*, 1984, **40**, 2913.

2-[2-(Acetyloxy)ethenyl]-6,10-dimethyl-2,5,9-undecatrienal, 9CI **A-70050**
[93888-67-6]



$C_{17}H_{24}O_3$ M 276.375
Metab. of algae *Penicillus capitatus* and *Udotea cyathiformis*. Antibacterial and ichthyotoxin. Oil.
Paul, V.J. *et al*, *Tetrahedron*, 1984, **40**, 2913.

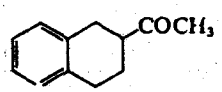
2-Acetylpiperidine **A-70051**
1-(2-Piperidinyl)ethanone, 9CI



$C_7H_{13}NO$ M 127.186
(±)-form [106318-86-9]
Light-yellow oil. Unstable, lib. from HCl salt immed. prior to use.
B,HCl: [106318-66-5]. Powder. Mp 225-228° dec.
Oxime (E-): [106318-67-6].
$C_7H_{14}N_2O$ M 142.200
Solid. Mp 103-105°.
Phenylhydrazone: $Bp_{0.54}$ 143-145°.
tert-*Butylhydrazone:* Oil. $Bp_{0.5}$ 100-105°.
Ethylene ketal: [106318-87-0].
$C_9H_{17}NO_2$ M 171.239
Liq. $Bp_{0.28}$ 55-60°.
Norman, M.H. *et al*, *J. Org. Chem.*, 1987, **52**, 226 (*synth, ir, pmr, cmr*)

3-Acetylpyrrole **A-70052**
Updated Entry replacing A-00414
1-(1H-Pyrrol-3-yl)ethanone, 9CI. Methyl 3-pyrryl ketone. 3-Acetopyrrole
[1072-82-8]
C_6H_7NO M 109.127
Cryst. ($CHCl_3$/pet. ether). Mp 115-116°.
Khan, M.K.A. *et al*, *Tetrahedron*, 1966, **22**, 2095 (*synth*)
Loader, C.E. *et al*, *Tetrahedron*, 1969, **25**, 3879 (*synth, pmr*)
v. Leusen, A.M. *et al*, *Tetrahedron Lett.*, 1972, 5337 (*synth*)
Anderson, H.J. *et al*, *Synth. Commun.*, 1987, **17**, 401 (*synth*)

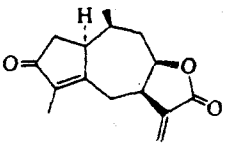
2-Acetyl-1,2,3,4-tetrahydronaphthalene **A-70053**
1-(1,2,3,4-Tetrahydro-2-naphthalenyl)ethanone, 9CI. 2-Acetyltetralin
[35060-50-5]



$C_{12}H_{14}O$ M 174.242

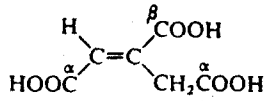
(±)-form
Oil.
2,4-Dinitrophenylhydrazone: Mp 164°.
Ravichandran, K. *et al*, *Heterocycles*, 1987, **26**, 645 (*synth. pmr*)

Achalensolide **A-70054**
Updated Entry replacing A-30038
3-Oxo-4,11(13)-guaiadien-12,8β-olide
[87302-42-9]



$C_{15}H_{18}O_3$ M 246.305
Constit. of *Stevia achalensis*. Cryst. (MeOH/Et_2O). Mp 176-177°. $[\alpha]_D$ +226.8° (c, 0.34 in $CHCl_3$).
3-Deoxo: 4,11(13)-Guaiadien-12,8β-olide. 3-Desoxoachalensolide.
$C_{15}H_{20}O_2$ M 232.322
Constit. of *S. polyphylla*. Oil. $[\alpha]_D^{24}$ +162° (c, 1.55 in $CHCl_3$).
3-Deoxo, 11β,13-Dihydro: 4-Guaien-12,8β-olide. 11β,13-Dihydrodesoxoachalensolide.
$C_{15}H_{22}O_2$ M 234.338
Constit. of *S. polyphylla*.
Oberti, J.C. *et al*, *J. Org. Chem.*, 1983, **48**, 4038 (*isol, struct*)
Zdero, C. *et al*, *Phytochemistry*, 1988, **23**, 2835 (*derivs*)

Aconitic acid **A-70055**
Updated Entry replacing A-00441
1-Propene-1,2,3-tricarboxylic acid, 9CI. Achilleaic acid. Citridinic acid. Equisetic acid. Pyrocitric acid
[499-12-7]



(E)-form

$C_6H_6O_6$ M 174.110
▷UD2380000.
(E)-form [4023-65-8]
Isol. from *Asarum europaeum*, from cane-sugar molasses and other plant sources. Used to prod. unsatd. polyesters. Leaflets (H_2O). Sol. H_2O, EtOH. Mp 194-195° dec. pK_{a1} 2.8 (25°), pK_{a2} 4.46 (25°). Decarboxylates at Mp to Itaconic acid. Mp variable with rate of htg.
α-Mono-Me ester: [65146-88-5].
$C_7H_8O_6$ M 188.137
Prisms (Me_2CO/C_6H_6). Mp 136-137°. Called 3-ester in CA.
β-Mono-Me ester: [65146-89-6].
$C_7H_8O_6$ M 188.137
Prisms (Me_2CO/C_6H_6). Mp 144-145°. Called 2-ester in CA.
γ-Mono-Me ester: [62424-07-1].
$C_7H_8O_6$ M 188.137
Prisms (Me_2CO/C_6H_6). Mp 154-155°. Called 1-ester in CA.
Tri-Me ester: [4271-99-2].
$C_9H_{12}O_6$ M 216.190
Sol. EtOH, Et_2O. Bp 270°, Bp_{14} 161°.

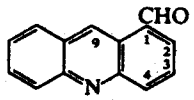
Triamide:
$C_6H_9N_3O_3$ M 171.155
Needles. Sol. hot H_2O, insol. EtOH, Et_2O. Turns brown at 250°. Sinters without melting at 260°.
Anhydride:
$C_6H_4O_5$ M 156.095
Mp 134-135°.

(Z)-form [585-84-2]
Mp 125°. Gives (*E*)-form on heating.
α-Mono-Me ester: [65146-85-2]. Prisms (Me_2CO/C_6H_6). Mp 101-102°.
β-Mono-Me ester: [65146-86-3]. Mp 102-104°.
γ-Mono-Me ester: [65146-87-4]. Prisms (Me_2CO/C_6H_6). Mp 126-127°.
Anhydride: [31511-11-2]. Mp 74°.

Malachowski, R. *et al*, *Ber.*, 1928, **61**, 2521 (*synth, props*)
Krogh, A., *Acta Chem. Scand.*, 1969, **23**, 2932 (*isol*)
Org. Synth., Coll. Vol., **2**, 12 (*synth*)

1-Acridinecarboxaldehyde A-70056

1-Formylacridine
[113139-13-2]



$C_{14}H_9NO$ M 207.231
Pale-green plates (hexane). Mp 118-119°.

Takahashi, K. *et al*, *J. Heterocycl. Chem.*, 1987, **24**, 977 (*synth, pmr*)

2-Acridinecarboxaldehyde A-70057

2-Formylacridine
[113139-14-3]
$C_{14}H_9NO$ M 207.231
Straw-coloured plates (hexane). Mp 196-198°.

Takahashi, K. *et al*, *J. Heterocycl. Chem.*, 1987, **24**, 977 (*synth, pmr*)

3-Acridinecarboxaldehyde A-70058

3-Formylacridine
[113139-15-4]
$C_{14}H_9NO$ M 207.231
Pale-yellow needles (hexanes). Mp 133-134°.

Takahashi, K. *et al*, *J. Heterocycl. Chem.*, 1987, **24**, 977 (*synth, pmr*)

4-Acridinecarboxaldehyde A-70059

4-Formylacridine
[113139-16-5]
$C_{14}H_9NO$ M 207.231
Yellow prisms (hexane). Mp 140-142°.

Takahashi, K. *et al*, *J. Heterocycl. Chem.*, 1987, **24**, 977 (*synth, pmr*)

9-Acridinecarboxaldehyde A-70060

[885-23-4]
$C_{14}H_9NO$ M 207.231
Yellow needles (C_6H_6/pet. ether). Mp 147°.
10-Oxide: [10228-97-4].
$C_{14}H_9NO_2$ M 223.231
Mp 261° (200° dec.).

Chardonnens, L. *et al*, *Helv. Chim. Acta*, 1949, **32**, 656 (*synth, bibl*)
Tsuge, O. *et al*, *Bull. Chem. Soc. Jpn.*, 1965, **38**, 2037 (*synth*)
Kawashima, K. *et al*, *Chem. Pharm. Bull.*, 1978, **26**, 951 (*oxide*)
Faure, R. *et al*, *Chem. Scr.*, 1980, **15**, 62 (*cmr*)

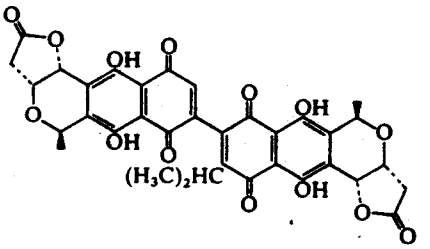
9-Acridinecarboxylic acid, 9CI A-70061

Updated Entry replacing A-00461
[5336-90-3]
$C_{14}H_9NO_2$ M 223.231
Yellow cryst. Spar. sol. H_2O. Mp >300°.
Me ester: [5132-81-0].
$C_{15}H_{11}NO_2$ M 237.257
Mp 127-128°.
▷AR7675000.
Ph ester:
$C_{20}H_{13}NO_2$ M 299.328
Fine needles (hexane/THF). Mp 189-190°.
Chloride: [5132-80-9].
$C_{14}H_8ClNO$ M 241.676
Mp 221-222° (as hydrochloride).
Amide: [35417-96-0].
$C_{14}H_{10}N_2O$ M 222.246
Yellow needles (EtOH). Mp 263-264°.
Nitrile: [42978-64-3]. *9-Cyanoacridine.*
$C_{14}H_8N_2$ M 204.231
Mp 181°.

Lehmstedt, K. *et al*, *Ber.*, 1928, **61**, 2044 (*deriv, synth*)
Albert, A., *The Acridines*, 1951, Arnold, London, 282 (*synth*)
Rauhut, M.M. *et al*, *J. Org. Chem.*, 1965, **30**, 3587 (*deriv, synth*)
White, E.H. *et al*, *J. Am. Chem. Soc.*, 1987, **109**, 5189 (*deriv, synth, ir, pmr*)

β-Actinorhodin A-70062

[109978-15-6]



$C_{35}H_{28}O_{14}$ M 672.598
Anthraquinone. Prod. by *Streptomyces violaceoruber*.

Krone, B. *et al*, *Justus Liebigs Ann. Chem.*, 1987, 751 (*pmr, struct*)

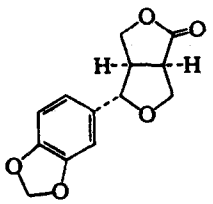
Consult the Dictionary of Antibiotics and Related Substances for a fuller treatment of antibiotics and related compounds.

Acuminatolide A-70063

Updated Entry replacing A-60063

4-(1,3-Benzodioxol-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan-1-one, 9CI

[108645-28-9]



$C_{13}H_{12}O_5$ M 248.235

Constit. of *Helichrysum acuminatum*. Cryst. Mp 118°.

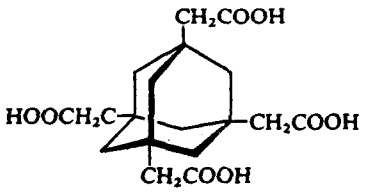
4-Epimer: [28168-96-9]. ***Pluviatide***. From *Zanthoxylum alatum* and *Z. pluviatile*. Needles (MeOH). Mp 162°. $[\alpha]_D$ −35.5° ($CHCl_3$). Epimeric at the aryl group.

Corrie, J.E.T. *et al*, *Aust. J. Chem.*, 1970, **23**, 133 (*isol*)
Dashpande, V.H. *et al*, *Indian J. Chem., Sect. B*, 1977, **15**, 95 (*isol*)
Jakupovic, J. *et al*, *Phytochemistry*, 1987, **26**, 803 (*isol, struct*)

1,3,5,7-Adamantanetetraacetic acid A-70064

Tricyclo[3.3.1.1^{3,7}]decane-1,3,5,7-tetraacetic acid, 9CI
1,3,5,7-Tetrakis(carboxymethyl)adamantane

[84782-76-3]



$C_{18}H_{24}O_8$ M 368.383

Cryst. (AcOH). Mp >300°.

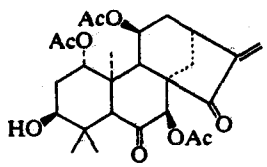
Tetranitrile: [84782-75-2]. *Tricyclo[3.3.1.1^{3,7}]decane-1,3,5,7-tetraacetonitrile. 1,3,5,7-Tetrakis(cyanomethyl)adamantane.*
$C_{18}H_{20}N_4$ M 292.383
Cryst. (AcOH). Mp 266-268°.

Tetrakis(dimethylamide):
$C_{26}H_{44}O_4N_4$ M 476.658
Oil. $Bp_{0.1}$ 345-350° (oven).

Naemura, K. *et al*, *Tetrahedron*, 1986, **42**, 1763 (*synth, ir*)

Adenanthin A-70065

[109974-30-3]



$C_{26}H_{34}O_9$ M 490.549

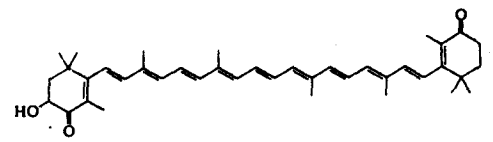
ent-Kaurene terpenoid antibiotic. Isol. from *Rabdosia adenantha*. Possesses bacteriostatic, antiinflammatory and antitumour props. Mp 255° dec. $[\alpha]_D^{13}$ −76° (c, 0.25 in $CHCl_3$).

Xu, Y.-L. *et al*, *Tetrahedron Lett.*, 1987, **28**, 499 (*isol, struct*)

Adonirubin A-70066

3-Hydroxy-β,β-carotene-4,4'-dione. Phoenicoxanthin

[4418-72-8]



$C_{40}H_{52}O_3$ M 580.849

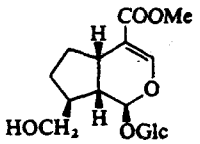
Red pigment from feathers of flamingos (e.g. *Phoenicopterus ruber*) and from flowers of *Adonis annua*. Red gum. λ_{max} 478 nm (C_6H_6).

Cooper, R.D.G. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1975, 2195.

Adoxoside A-70067

Updated Entry replacing A-50069

[42830-26-2]



$C_{17}H_{26}O_{10}$ M 390.386

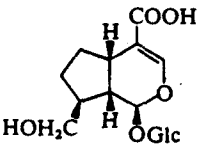
Constit. of *Adoxa moschatellina*. Amorph.

Penta-Ac: Cryst. Mp 140.5-141.5°. $[\alpha]_D^{22}$ −63° (c, 1 in $CHCl_3$).

6β-Hydroxy: [110559-86-9]. ***6β-Hydroxyadoxoside***.
$C_{17}H_{26}O_{11}$ M 406.386
Constit. of *Castilleja integra*. Foam. $[\alpha]_D^{27}$ −83.4° (c, 0.43 in MeOH).

Jensen, S.R. *et al*, *Biochem. Syst. Ecol.*, 1979, **7**, 103 (*isol*)
Damtoft, S. *et al*, *Phytochemistry*, 1981, **20**, 2717 (*cmr*)
Gardner, D.R. *et al*, *J. Nat. Prod.*, 1987, **50**, 485 (*isol*)

Adoxosidic acid A-70068



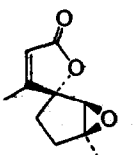
$C_{16}H_{24}O_{10}$ M 376.360

Constit. of *Castilleja integra* and *Fouquieria columnaris*.

Jensen, S.R. *et al*, *Biochem. Syst. Ecol.*, 1979, **7**, 103 (*isol*)
Jensen, S.R. *et al*, *Phytochemistry*, 1982, **21**, 1623 (*isol*)
Gardner, D.R. *et al*, *J. Nat. Prod.*, 1987, **50**, 485 (*isol*)

Adriadysiolide A-70069

[113540-73-1]



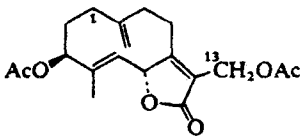
$C_{10}H_{12}O_3$ M 180.203

Constit. of a *Dysidea* sp. of the Adriatic Sea. Powder. Mp 76-77°. $[\alpha]_{435}^{20}$ +2.1° (c, 0.625 in MeOH).

Mancini, I. *et al*, *Helv. Chim. Acta*, 1987, **70**, 2011.

Afraglaucolide A-70070

[115346-35-5]



$C_{19}H_{24}O_6$ M 348.395

1α-Hydroxy: [115367-47-0]. ***1α-Hydroxyafraglaucolide***.
$C_{19}H_{24}O_7$ M 364.394
Constit. of *Artemisia afra*.

1β-Hydroxy: [115346-39-9]. ***1β-Hydroxyafraglaucolide***.
$C_{19}H_{24}O_7$ M 364.394
Constit. of *A. afra*.

1α-Hydroxy, 13-de-Ac: [115334-66-2]. *13-Desacetyl-1α-hydroxyafraglaucolide*.
$C_{17}H_{22}O_6$ M 322.357
Constit. of *A. judaica*.

1β-Hydroxy, 13-de-Ac: 13-Desacetyl-1β-hydroxyafraglaucolide.
$C_{17}H_{22}O_6$ M 322.357
Constit. of *A. judaica*. Oil.

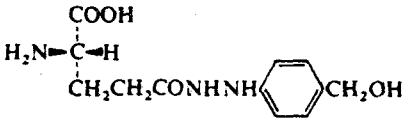
Khafagy, S.M. *et al*, *Phytochemistry*, 1988, **27**, 1125 (*isol*)
Jakupovic, J. *et al*, *Phytochemistry*, 1988, **27**, 1129 (*isol*)

Agaritine A-70071

Updated Entry replacing A-00625

β-N-(γ-Glutamyl)-4-hydroxymethylphenylhydrazine. Glutamic acid 5-2-(α-hydroxy-p-tolyl)hydrazide, *8CI*

[2757-90-6]



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

▷MA1284000.

(S)-form

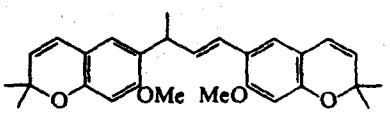
L-form

Constit. of some members of the family *Agaricaceae*, notably *Agaricus bisporus*. Cryst. (EtOH/butanol). Mp 205-209°. $[\alpha]_D^{25}$ +7° (c, 0.8 in H_2O). pK_{a1} 3.4, pK_{a2} 8.86 (H_2O).

Daniels, E.G. *et al*, *J. Org. Chem.*, 1962, **23**, 3229 (*isol, synth*)
Levenberg, B., *J. Biol. Chem.*, 1964, **239**, 2267 (*isol, struct*)
Datta, S. *et al*, *Helv. Chim. Acta*, 1987, **70**, 1261 (*synth, ir, pmr, bibl*)

Agerasanin A-70072

[116397-92-3]

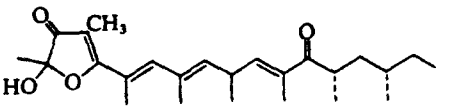


$C_{28}H_{32}O_4$ M 432.558

Constit. of *Ageratina arsenii*.

Fang, N. *et al*, *Phytochemistry*, 1988, **27**, 1902.

Aglajne 2 A-70073



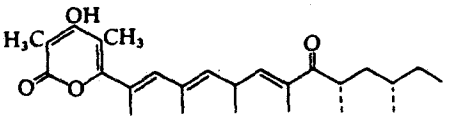
$C_{25}H_{38}O_4$ M 402.573

Constit. of the mollusc *Aglaja depicta* and its prey *Bulla striata*.

Ac: Oil. $[\alpha]_D^{20}$ +46° (c, 1.3 in $CHCl_3$).

Cimino, G. *et al*, *J. Org. Chem.*, 1987, **52**, 5326.

Aglajne 3 A-70074



$C_{26}H_{38}O_4$ M 414.584

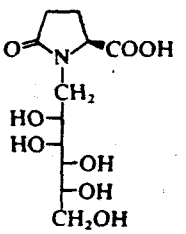
Constit. of the molusc *Aglaja depicta* and its prey *Bulla striata*. Oil. $[\alpha]_D^{20}$ +105° (c, 0.8 in $CHCl_3$).

Cimino, G. *et al*, *J. Org. Chem.*, 1987, **52**, 5326.

Agropinic acid A-70075

1-(2-Carboxy-5-oxo-1-pyrrolidinyl)-1-deoxy-D-mannitol, *9CI*

[74474-75-2]

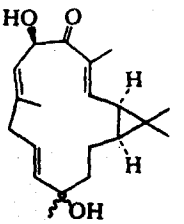


$C_{11}H_{19}NO_8$ M 293.273

Opine found in plant tumours.

Tate, M.E. *et al*, *Carbohydr. Res.*, 1982, **104**, 105 (*synth*)
Chilton, W.S. *et al*, *Biochemistry*, 1984, **23**, 3290 (*cd*)
Chilton, W.S. *et al*, *J. Bateriol.*, 1984, **158**, 650 (*deriv, struct, metab*)
Chilton, W.S. *et al*, *Phytochemistry*, 1985, **24**, 2945.

Agroskerin A-70076



$C_{20}H_{30}O_3$ M 318.455

Constit. of *Agrostistachys hookeri*. Resin. $[\alpha]_D$ −54° (c, 0.1 in $CHCl_3$).

Choi, Y.-H. *et al*, *J. Nat. Prod.*, 1988, **51**, 110.