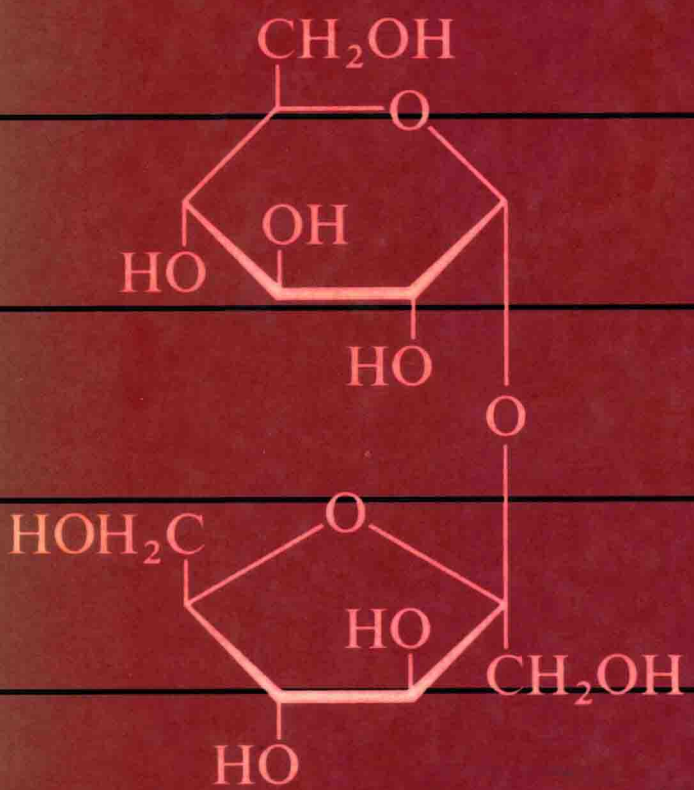
Carbohydrates

Edited by P.M. Collins



CHAPMAN AND HALL CHEMISTRY SOURCEBOOKS

Carbohydrates

Edited by

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Preface

This is the largest volume yet to be published in the series *Chapman and Hall Chemistry Sourcebooks*. The aim of this series is to provide carefully tailored information to individual workers in particular areas of chemistry and biochemistry.

The information in this volume is partially derived from the Fifth Edition of the *Dictionary of Organic Compounds*, published in 1982, and its annual supplements. Each individual entry has, however, been reviewed and updated, and a large number of totally new entries have been added. In addition, many hundreds of additional synonyms and derivative molecular formulae have been added to the existing entries, thus considerably enhancing the utility of the Name and Molecular Formula Indexes.

A new and important additional index to be found in this volume is the Type of Compound Index in which most carbohydrates in the dictionary are classified under one or more of 102 headings according to structural type. This is the first DOC publication to contain this index, which it is anticipated will be of considerable value to carbohydrate chemists.

The coverage of entries in this sourcebook is as follows. The monosaccharides are extensively documented together with a full range of their derivatives, including deoxy, aminodeoxy and halogenodeoxy sugars, diuloses, glyconic acids, etc. The selection of derivatives has been made with the carbohydrate chemist interested in synthesis principally in mind. There is an extensive range of disaccharides and their derivatives but only the most important oligo- and polysaccharides are covered. The glycosides chosen for inclusion were selected from the many known examples because they are abundant in nature and/or have unusual structures. Numerous further simple glycosides, especially plant glucosides, are recorded in the parent *Dictionary of Organic Compounds* but it is felt that they would be out of place here as holding little interest for the 'mainstream' carbohydrate chemist. There is extensive coverage of the important nucleosides and glycoside antibiotics.

With a work of this kind, some omissions are inevitable, but it is hoped that most users will find nearly every compound of interest to them. As the intention is to produce periodical revised editions as demand permits, users are strongly encouraged to communicate their comments on compound selection to the Editor or Publishers.

P. M. Collins

Introduction

1. Using the Sourcebook

The *Sourcebook* is arranged alphabetically by entry name. Every entry is numbered to assist ready location. Many compounds are included as derivatives of main entry compounds: the extensive indexing of the *Sourcebook* means that these can be readily located through the Name, Molecular Formula Index or Type of Compound Index.

Indexes

There are four printed indexes: a Name Index which lists every compound name or synonym in alphabetical order; a Molecular Formula Index which lists all molecular formulae, including those of derivatives, in Hill convention order; a CAS Registry Number Index listing all CAS numbers included in the *Sourcebook* in serial order, and a Type of Compound Index in which compounds are listed by structural type. All indexes refer to the entry number. In the Name Index an entry number which follows immediately upon an index term means that the term itself is used as the entry name but an entry number which is preceded by the word '*see*' means that the term is a synonym to an entry name. In all indexes an entry number which is preceded by the word '*in*' refers the reader to a specified stereoisomer or derivative which is to be found embeded within the entry.

2. Chemical Names and Synonyms

The *Sourcebook* contains a wide range of synonyms which may be (a) those found in the primary literature, (b) *Chemical Abstracts* names or (c) names added editorially to achieve as much consistency as possible with other closely related substances.

Names corresponding to those used by CAS during the 8th and 9th index periods (1967–71 and 1972–76 respectively) are labelled with the suffixes 8CI, 9CI respectively. Names first introduced by CAS since 1976 are referred to as 9CI since there have been no substantial changes of CA nomenclature since that date affecting organic compounds.

If a compound cannot be located immediately in the main body of the entries, it is important to use the indexes.

3. Bibliographic References

The selection of references is made with the aim of facilitating entry into the literature for the user who wishes to locate more detailed information about a particular compound. Reference contents are frequently indicated using suffixes. In general recent references are preferred to older ones, and the number of references quoted does not necessarily indicate the relative importance of a compound.

Journal abbreviations generally follow the practice of the Chemical Abstracts Service Source Index (CASSI). In patent references, no distinction is made between patent applications and granted patents.

4. Further Information

For further information about the presentation of data in this and other sourcebooks, see the introduction to the *Dictionary of Organic Compounds*, Fifth Edition and supplements.

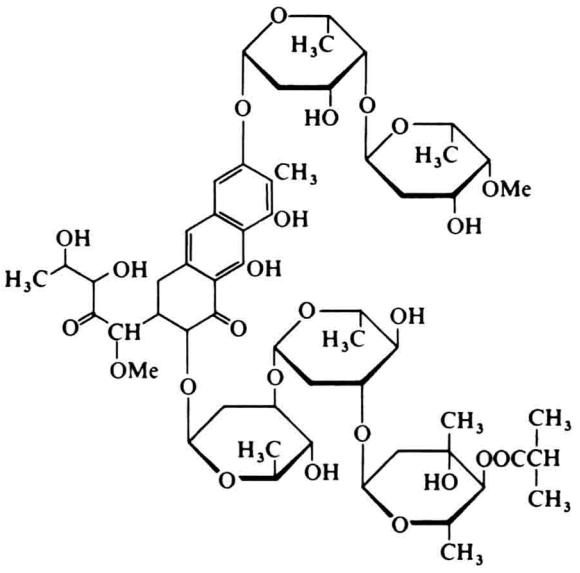
Contents

A

Aburamycin *C* **A-00001**

Deacetylchromomycin A_2

[37847-80-6]



$C_{57}H_{84}O_{25}$ M 1169.276

Chromomycin-type antibiotic. Produced by *Streptomyces* spp. Cancerostatic antibiotic. Yellow amorph. powder. $[\alpha]_D$ −17° (EtOH).

Per-Ac: Mp 219-221°. $[\alpha]_D$ −18° ($CHCl_3$).

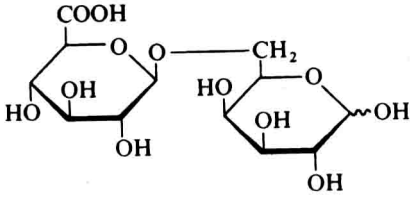
Berlin, Y.A. *et al*, *Nature (London)*, 1968, **218**, 193 (*isol, struct*)

Acaciabiuronic acid **A-00002**

[7264-19-9]

-form

6-O-β-D-Glucopyranuronosyl-D-galactose, 9CI, 8CI



$C_{12}H_{20}O_{12}$ M 356.283

Isol. from hydrol. products of gum acacia. Mp 118-119° (hydrate). $[\alpha]_D$ +11.6° → −8.6° (H_2O).

α-form [52554-59-3]

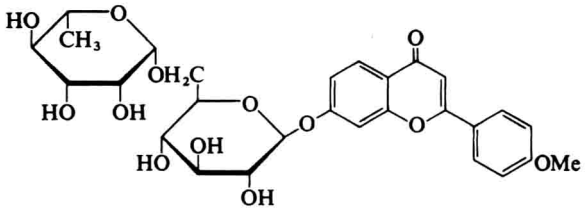
1,2:3,4-Di-O-isopropylidene, 2',3',4'-tri-Ac, Me ester: Mp 114-115°. $[\alpha]_D$ −65° (c, 4.5 in $CHCl_3$).

Goebel, W.F. *et al*, *J. Biol. Chem.*, 1938, **124**, 207 (*isol*)
De, K.K. *et al*, *Carbohydr. Res.*, 1967, **4**, 177.
Peciar, C. *et al*, *Chem. Zvesti*, 1974, **28**, 83 (*config, pmr*)

Acaciin **A-00003**

7-[[6-O-(6-Deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-5-hydroxy-2-(4-methoxyphenyl)-4H-1-benzopyran-4-one, 9CI. Linarin, 8CI

[480-36-4]



$C_{28}H_{32}O_{13}$ M 576.553

Constit. of leaves of *Robinia pseudoacacia*. Needles (Py aq.). Mp 263°. $[\alpha]_D$ −85.3° (Py), −99.5° (AcOH).

Hepta-Ac: Mp 135°.

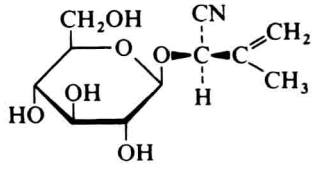
Me ether: Mp 279-280°.

Wagner, H. *et al*, *Tetrahedron Lett.*, 1968, 1635 (*synth*)
Plouvier, V., *C. R. Hebd. Seances Acad. Sci.*, 1969, **269**, 646 (*isol*)
Schmid, R.D., *Tetrahedron*, 1972, **28**, 3259 (*ms*)

Acacipetalin, 9CI **A-00004**

2-(β-D-Glucopyranosyloxy)-3-methyl-(R)-3-buteneni-trile, 9CI

[644-68-8]



Absolute configuration

$C_{11}H_{17}NO_6$ M 259.258

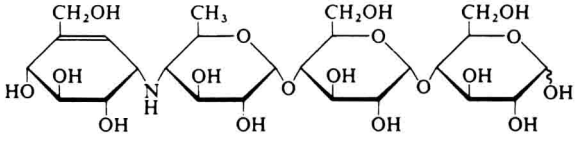
Constit. of *Acacia sieberiana*, *A. hebeclada* and *A. constricta*.

Butterfield, C.S. *et al*, *Phytochemistry*, 1975, **14**, 993 (*struct, biosynth, pmr, ms*)
Seigler, D.S. *et al*, *Phytochemistry*, 1975, **14**, 1419.
Seigler, D.S. *et al*, *Phytochemistry*, 1976, **15**, 219 (*isol*)

Acarbose, BAN **A-00005**

O-4,6-Dideoxy-4-[[4,5,6-trihydroxy-3-(hydroxy-methyl)-2-cyclohexen-1-yl]amino]-α-D-glucopyranosyl-(1→4)-O-α-D-glucopyranosyl-(1→4)-D-glucose, 9CI

[56180-94-0]



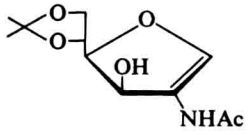
$C_{25}H_{43}NO_{18}$ M 645.611

A potent inhibitor of glucosidases and saccharases. Used for treatment of diabetes, hyperlipidaemia and obesity.

Ger. Pat., 23 467 782, (*1975*); *CA*, **83**, 56721s

Block, K. *et al*, *Carbohydr. Res.*, 1984, **132**, 142 (*nmr*)

2-Acetamido-1,4-anhydro-2-deoxy-5,6-*O*-isopropylidene-*arabino*-hex-1-enitol A-00006



$C_{11}H_{17}NO_5$ M 243.259

D-form [66335-63-5]

Plates (MeOH/Et_2O). Mp 152°. $[\alpha]_D^{25}$ −1° (c, 0.5 in MeOH).

*3-O-(2-Acetamido-2,3-dideoxy-5,6-O-isopropylidene-α-D-*erythro*-hex-2-enofuranosyl)*: [73745-59-2]. *2-Acetamido-3-O-(2-acetamido-2,3-dideoxy-5,6-O-isopropylidene-α-D-*erythro*-hex-2-enofuranosyl)-1,4-anhydro-2-deoxy-5,6-O-isopropylidene-D-*arabino*-hex-1-enitol.* Amorph. solid. $[\alpha]_D^{25}$ −81.7° (c, 1.0 in $CHCl_3$).

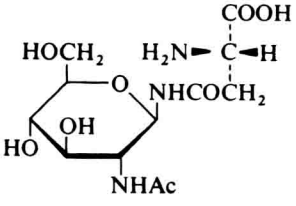
*3-O-(2-Acetamido-2,3-dideoxy-5,6-O-isopropylidene-β-D-*erythro*-hex-2-enofuranosyl)*: [73836-73-4]. *2-Acetamido-3-O-(2-acetamido-2,3-dideoxy-5,6-O-isopropylidene-β-D-*erythro*-hex-2-enofuranosyl)-1,4-anhydro-2-deoxy-5,6-O-isopropylidene-D-*arabino*-hex-1-enitol.* Plates (Et_2O/EtOH). Mp 198-199°. $[\alpha]_D^{25}$ +7.6° (c, 1.0 in $CHCl_3$).

Hasegawa, A. *et al*, *Carbohydr. Res.*, 1979, **74**, 341; 1978, **63**, 91; 1980, **79**, 255 (*synth, ms, pmr*)

N-(2-Acetamido-2-deoxy-β-D-glucopyranosyl)-L-asparagine, 9CI A-00007

2-Acetamido-1β-(L-β-aspartamido)-1,2-dideoxy-D-glucose

[2776-93-4]



$C_{12}H_{21}N_3O_8$ M 335.313

Found in hydrolysates of glycopeptides/glycoproteins. Needles (EtOH). Mp 255-258° dec. $[\alpha]_D^{22}$ +23.6° (c, 1 in H_2O).

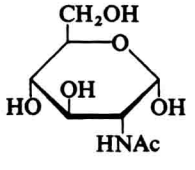
Hydrate: Plates (EtOH aq.). Mp 215-222° dec. $[\alpha]_D^{24}$ +23.2° (c, 1.5 in H_2O).

Marks, G.S. *et al*, *Biochem. J.*, 1963, **87**, 274 (*isol, struct*)
Tsukamoto, H. *et al*, *Biochem. Biophys. Res. Commun.*, 1964, **15**, 151 (*synth*)

2-Acetamido-2-deoxyglucose A-00008

2-(Acetylamino)-2-deoxyglucose, 9CI. N-*Acetylglucosamine*

[7512-17-6]



α-D-Pyranose-*form*

$C_8H_{15}NO_6$ M 221.210

D-form

The polysaccharide Chitin is composed of β-(1→4)-linked *N*-acetyl-D-glucosamine units. Mp 205°. $[\alpha]_D$ +64° → +41° (H_2O).

Di-Et dithioacetal: Mp 121-122°. $[\alpha]_D$ −24° (H_2O).

Di-Et dithioacetal, 5,6-O-isopropylidene: Mp 39-40°. $[\alpha]_D^{20}$ +9° (c, 1 in H_2O).

Di-Et dithioacetal, 5,6-O-isopropylidene, 3,4-di-Me: [18422-19-0]. Mp 120-121°. $[\alpha]_D^{20}$ +13.6° (c, 1 in H_2O).

Di-Et dithioacetal, 3,4,5,6-tetra-Ac: Mp 126-127°. $[\alpha]_D$ −32° ($CHCl_3$).

3-Benzoyl: Mp 198° dec. $[\alpha]_D^{20}$ +35° (c, 0.85 in 50% dioxan aq.).

D-Pyranose-form

4,6-O-Isopropylidene: 2-Acetamido-2-deoxy-4,6-O-isopropylidene-D-glucopyranose. Mp 189-190°. $[\alpha]_D^{20}$ +57.5° (c, 1.0 in MeOH).

3,4,6-Tribenzyl: [37169-61-2]. Mp 218-219°. $[\alpha]_D^{20}$ +71.3° (c, 1.08 in $CHCl_3$).

3-Me ether: see 2-Acetamido-2-deoxy-3-O-methylglucose, A-00009

4-Me ether: see 2-Acetamido-2-deoxy-4-O-methylglucose, A-00010

6-Me ether: see 2-Acetamido-2-deoxy-6-O-methylglucose, A-00011

3,4-Di-Me ether: see 2-Acetamido-2-deoxy-3-O-methylglucose, A-00009

3,6-Di-Me ether: see 2-Acetamido-2-deoxy-3-O-methylglucose, A-00009

4,6-Di-Me ether: see 2-Acetamido-2-deoxy-4-O-methylglucose, A-00010

3,4,6-Tri-Me ether: see 2-Acetamido-2-deoxy-3-O-methylglucose, A-00009

Methyl glycoside: see Methyl 2-acetamido-2-deoxyglucopyranoside, M-00059

Benzyl glycoside: see Benzyl 2-amino-2-deoxyglucopyranoside, B-00015

α-D-Pyranose-form

Mp 202-204°. $[\alpha]_D$ +82° → +40.2° (H_2O).

1-Ac: see 1-O-Acetyl-2-amino-2-deoxyglucose, A-00017

1,3,4,6-Tetra-Ac: Mp 139°. $[\alpha]_D$ +92° ($CHCl_3$).

1-Benzoyl: Mp 192-193°. $[\alpha]_D^{20}$ +190° (c, 0.83 in MeOH).

1-Benzoyl,3,4,6-tri-Ac: Mp 161-162°. $[\alpha]_D^{20}$ +114° (c, 1.2 in $CHCl_3$).

1-Benzoyl, 3,4,6-tribenzyl: Mp 118-119°. $[\alpha]_D^{20}$ +171° (c, 0.54 in $CHCl_3$).

β-D-Pyranose-form

Mp 182-184°. $[\alpha]_D$ −21.5° → +40.4° (H_2O).

1,3,4,6-Tetra-Ac: Mp 187-189°. $[\alpha]_D$ +1.2° ($CHCl_3$).

1-Benzoyl: Mp 154-160°. $[\alpha]_D^{20}$ −38° (c, 0.82 in $CHCl_3$).

1-Benzoyl, 3,4,6-tribenzyl: Mp 147-148°. $[\alpha]_D^{20}$ −11.1° (c, 0.54 in $CHCl_3$).

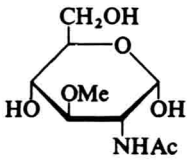
α-D-Furanose-form

1-Benzoyl, 3,5,6-tri-Ac: $[\alpha]_D^{20}$ +110° (c, 0.3 in $CHCl_3$).

Foster, A.B. *et al*, *Adv. Carbohydr. Chem.*, 1952, **7**, 247 (*rev*)
Jeanloz, R.W., *J. Am. Chem. Soc.*, 1952, **74**, 4597.
Kuhn, R. *et al*, *Chem. Ber.*, 1953, **86**, 722.
Jeanloz, R.W., *Adv. Carbohydr. Chem.*, 1958, **13**, 189.
Johnson, L.N. *et al*, *Nature (London)*, 1964, **202**, 588
Harrison, R. *et al*, *J. Org. Chem.*, 1965, **30**, 2317.
Inch, T.D. *et al*, *J. Org. Chem.*, 1966, **31**, 1823.
Heynes, K. *et al*, *Chem. Ber.*, 1967, **100**, 2655.

Cerezo, A.S., *Chem. Ind. (London)*, 1971, 96 (*pmr*)
Bundle, D.R. *et al*, *Can. J. Chem.*, 1973, **51**, 3812 (*cmr*)
Hasegawa, A. *et al*, *Carbohydr. Res.*, 1973, **29**, 209.

2-Acetamido-2-deoxy-3-*O*-methylglucose A-00009



α-D-Pyranose-*form*

$C_9H_{17}NO_6$ M 235.236

D-form

Mp 195-196° (183-185°). $[\alpha]_D$ +33° (H_2O).

4-Me: [53684-98-3]. *2-Acetamido-2-deoxy-3,4-di-O-methyl-D-glucose.* Mp 173-175°. $[\alpha]_D^{26}$ +64° → +48° (1 d) (c, 0.81 in $CHCl_3$).

6-Me: 2-Acetamido-2-deoxy-3,6-di-O-methyl-D-glucose. Mp 232-233°. $[\alpha]_D$ +90° → +37° (H_2O).

4,6-Di-Me: 2-Acetamido-2-deoxy-3,4,6-tri-O-methyl-D-glucose. Mp 234°. $[\alpha]_D$ +75° → +44.8° (H_2O).

Jeanloz, R.W., *Adv. Carbohydr. Chem.*, 1958, **13**, 189.
Horton, D., *The Amino Sugars*, (*Jeanloz, R.W., Ed.*), 1969, Academic Press, **1A**, 1

2-Acetamido-2-deoxy-4-*O*-methylglucose A-00010

$C_9H_{17}NO_6$ M 235.236

D-form

Mp 211-215° dec. $[\alpha]_D$ +79° → +69° (H_2O).

6-Me: 2-Acetamido-2-deoxy-4,6-di-O-methyl-D-glucose. Mp 227-228°. $[\alpha]_D$ +88° → +68° (H_2O).

Jeanloz, R.W., *Adv. Carbohydr. Chem.*, 1958, **13**, 189.
Horton, D., *The Amino Sugars*, (*Jeanloz, R.W., Ed.*), 1969, Academic Press, **1A**, 1

2-Acetamido-2-deoxy-6-*O*-methylglucose A-00011

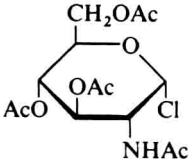
$C_9H_{17}NO_6$ M 235.236

D-form

Mp 224-225°. $[\alpha]_D$ +74° → +48° (H_2O).

Jeanloz, R.W., *Adv. Carbohydr. Chem.*, 1958, **13**, 189.
Horton, D., *The Amino Sugars*, (*Jeanloz, R.W., Ed.*), 1969, Academic Press, *1A*, 1

2-Acetamido-2-deoxy-3,4,6-tri-*O*-acetylglucopyranosyl chloride, 8CI A-00012



$C_{14}H_{20}ClNO_8$ M 365.767

α-D-form [3068-34-6]

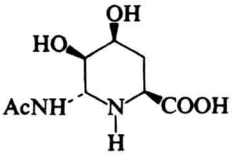
Mp 127-128° (133-134° dec.). $[\alpha]_D^{24}$ +110° (c, 1.1 in $CHCl_3$).

Micheel, F. *et al*, *Chem. Ber.*, 1957, **90**, 521 (*struct, ir*)
Conchie, J. *et al*, *Methods Carbohydr. Chem.*, 1963, **2**, 332 (*synth*)
Org. Synth., 1966, **46**, 1 (*synth*)
Horton, D. *et al*, *J. Org. Chem.*, 1967, **32**, 1073 (*pmr*)
Horton, D., *Methods Carbohydr. Chem.*, 1972, **6**, 282 (*synth*)
Pravdic, N. *et al*, *Carbohydr. Res.*, 1975, **45**, 302.
Nashed, M.A. *et al*, *Carbohydr. Res.*, 1980, **82**, 237 (*synth*)

6-Acetamido-4,5-dihydroxy-2-piperidinecarboxylic acid A-00013

N-(*5-Amino-4-carboxy-4,5-dideoxy-β-ribopyranosyl*)-*acetamide*, *9CI. Siastatin* B

[54795-58-3]



Relative configuration

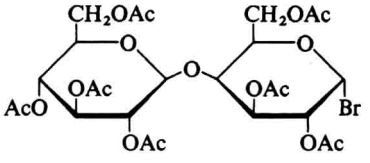
$C_8H_{14}N_2O_5$ M 218.209

Isol. from *Streptomyces verticillus* var. *quintum*. Needles. Mp 137° dec. $[\alpha]_D^{25}$ +57.2° (c, 1 in H_2O).

Umezawa, H. *et al*, *J. Antibiot.*, 1974, **27**, 963 (*isol, ir, props*)
Aoyagi, T. *et al*, *Experientia*, 1975, **31**, 896 (*struct*)

Acetobromocellobiose A-00014

Hepta-O-acetyl-α-D-cellobiosyl bromide



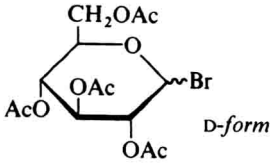
$C_{26}H_{35}BrO_{17}$ M 699.456

Mp 183°. $[\alpha]_D^{20}$ +95.8° ($CHCl_3$).

Brauns, D.H., *J. Am. Chem. Soc.*, 1923, **45**, 2388.
Haynes, L.J. *et al*, *Adv. Carbohydr. Chem.*, 1955, **10**, 207.

Acetobromoglucose A-00015

2,3,4,6-Tetra-O-acetylglucosyl bromide



D-*form*

$C_{14}H_{19}BrO_9$ M 411.203

α-D-Pyranose-form [572-09-8]

Mp 88-89°. $[\alpha]_D^{20}$ +194° (c, 3.9 in $CHCl_3$).

β-D-Pyranose-form [6919-96-6]

Mp 92°. $[\alpha]_D^{20}$ −16° → +77° ($CHCl_3$).

α-L-Pyranose-form

Mp 88°. $[\alpha]_D^{17.5}$ −192.7° (Et_2O).

α-D,L-Pyranose-form

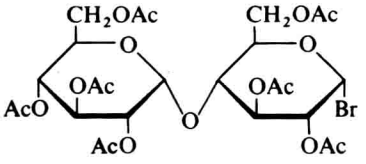
Mp 85°.

Barczai-Martos, M. *et al*, *Nature (London)*, 1950, **165**, 369 (*synth*)
Haynes, L.J. *et al*, *Adv. Carbohydr. Chem.*, 1955, **10**, 207 (*rev*)
Weygand, F. *et al*, *Chem. Ber.*, 1958, **91**, 2534.
Lemieux, R.U., *Methods Carbohydr. Chem.*, 1972, **6**, 292.
Bock, K. *et al*, *Acta Chem. Scand., Ser. B*, 1974, **28**, 1041 (*synth, pmr*)

Acetobromomaltose A-00016

4-O-(2,3,4,6-Tetra-O-acetyl-α-D-glucopyranosyl)-tri-O-acetyl-α-D-glucopyranosyl bromide, 9CI. Hepta-O-acetyl-4-O-α-D-glucopyranosyl-α-D-glucopyranosyl bromide, 8CI

[14257-35-3]



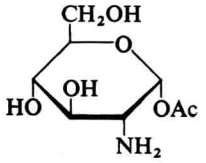
$C_{26}H_{35}BrO_{17}$ M 699.456

Mp 112-113°. $[\alpha]_D^{20}$ +180.1° ($CHCl_3$).

Brauns, D.H., *J. Am. Chem. Soc.*, 1929, **51**, 1820 (*synth*)
Haynes, L.J. *et al*, *Adv. Carbohydr. Chem.*, 1955, **10**, 207 (*rev*)
Szabo, F. *et al*, *Acta Chim. (Budapest)*, 1970, **64**, 67; *CA*, **73**, 4149k (*synth*)
Mori, M., *Chem. Pharm. Bull.*, 1974, **22**, 1331.

1-*O*-Acetyl-2-amino-2-deoxyglucose A-00017

1-O-Acetylglucosamine



α-D-Pyranose-*form*

$C_8H_{15}NO_6$ M 221.210

α-D-Pyranose-form

N-*Ac: 2-Acetamido-1-O-acetyl-2-deoxy-α-D-glucopyranose*. Mp 169-170°. $[\alpha]_D^{20}$ +149° (c, 0.29 in MeOH).

*2*N,*3-Di-Ac: 2-Acetamido-2-deoxy-1,3-di-O-acetyl-α-D-glucopyranose*. Mp 172-173°. $[\alpha]_D^{20}$ +8° (c, 1.0 in MeOH).

3,4,6-Tri-Ac: 2-Amino-2-deoxy-1,3,4,6-tetra-O-acetyl-α-D-glucopyranose. Mp 143°. $[\alpha]_D$ +25.9° ($CHCl_3$).

3,4,6-Tri-Ac, N-*benzoyl: 2-Benzamido-2-deoxy-1,3,4,6-tetra-O-acetyl-α-D-glucopyranose*. Mp 240°. $[\alpha]_D$ +41.9° ($CHCl_3$).

*2*N,*3-Di-Ac, 4,6-O-isopropylidene: 2-Acetamido-2-deoxy-1,3-di-O-acetyl-4,6-O-isopropylidene-α-D-glucopyranose*. Mp 137-138°. $[\alpha]_D^{20}$ +73° (c, 1.0 in $CHCl_3$).

N-*Ac, 3,4,6-tribenzyl: 2-Acetamido-1-O-acetyl-2-deoxy-3,4,6-tri-O-benzyl-α-D-glucopyranose*. Mp 146-147°. $[\alpha]_D^{20}$ +108° (c, 0.74 in $CHCl_3$).

β-D-Pyranose-form

3,4,6-Tri-Ac: 2-Amino-2-deoxy-1,3,4,6-tetra-O-acetyl-β-D-glucopyranose. Mp 230° (as hydrochloride). $[\alpha]_D$ +29.7° (H_2O).

*2*N,*3,4,6-Tetra-Ac: see 2-Acetamido-2-deoxyglucose, A-00008*

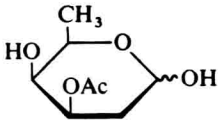
3,4,6-Tri-Ac, N-*benzyloxycarbonyl:* Mp 150-151°. $[\alpha]_D$ +21.5° (Py).

N-*Ac, 3,4,6-tribenzyl: 2-Acetamido-1-O-acetyl-2-deoxy-3,4,6-tri-O-benzyl-β-D-glucopyranose*. Mp 168-169°. $[\alpha]_D^{20}$ +31° (c, 0.9 in $CHCl_3$).

Foster, A.B. *et al*, *Adv. Carbohydr. Chem.*, 1952, **7**, 247.
Harrison, R. *et al*, *J. Org. Chem.*, 1965, **30**, 2317.
Inch, T.D. *et al*, *J. Org. Chem.*, 1966, **31**, 1813.
Hasegawa, A. *et al*, *Carbohydr. Res.*, 1973, **29**, 209.

3-*O*-Acetyl-2,6-dideoxy-*lyxo*-hexopyranose, 9CI A-00018

Chromose D. *3-O-Acetyloliose*



$C_8H_{14}O_5$ M 190.196

D-form [2595-12-2]

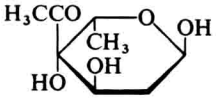
Constit. of the antibiotic Chromomycin. Needles. Mp 118°. $[\alpha]_D^{23}$ +87° (c, 1.5 in H_2O).

α-D-Pyranose-form

Me glycoside: Methyl 3-O-acetyl-2,6-dideoxy-α-D-lyxo-hexopyranoside. Syrup. $[\alpha]_D^{16}$ +142° (c, 2.4 in $CHCl_3$).

Miyamoto, M. *et al*, *Tetrahedron Lett.*, 1964, 2371 (*isol*)
Brimacombe, J.S. *et al*, *Carbohydr. Res.*, 1965, **1**, 128 (*synth*)
Brimacombe, J.S. *et al*, *Chem. Ind. (London)*, 1965, 468
Miyamoto, M. *et al*, *Tetrahedron*, 1966, **22**, 2785.

4-*C*-Acetyl-2,6-dideoxy-*xylo*-hexose A-00019



β-L-pyranose-*form*

$C_8H_{14}O_5$ M 190.196

L-form

Occurs in Quinocycline *B* and Isoquinocycline *B*.

α-L-Pyranose-form

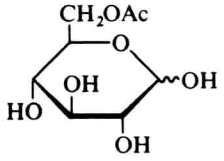
Me glycoside: Methyl 4-C-acetyl-2,6-dideoxy-α-L-xylo-hexopyranoside. Needles (MeOH). Mp 109-112°. $[\alpha]_D^{20}$ −60° (c, 0.1 in $CHCl_3$).

β-L-Pyranose-form

Me glycoside: Methyl 4-C-acetyl-2,6-dideoxy-β-L-xylo-hexopyranoside. Plates. Mp 103-107°. $[\alpha]_D^{20}$ +46° (c, 0.2 in $CHCl_3$).

Matern, U. *et al*, *Eur. J. Biochem.*, 1972, **29**, 1 (*synth, pmr*)

6-*O*-Acetylglucose, 9CI A-00020



$C_8H_{14}O_7$ M 222.194

D-form [7286-45-5]

Produced by *Bacillus megaterium*. Prisms (H_2O). Mp 133°. $[\alpha]_D^{20}$ +48° (c, 4.0 in H_2O).

Phenylhydrazone: Mp 134-136°. $[\alpha]_D^{20}$ −13° (c, 1.3 in H_2O).

α-D-Pyranose-form

Me glycoside: [4201-66-5]. *Methyl 6-O-acetyl-α-D-glucopyranoside*. Oil. $[\alpha]_D^{21}$ +151.1° (c, 1.12 in Me_2CO).

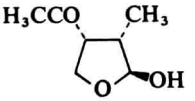
β-D-Pyranose-form

Me glycoside: [20771-12-4]. *Methyl 6-O-acetyl-β-D-glucopyranoside*. Mp 132-134°.

Duff, R.B. *et al*, *Nature (London)*, 1957, **179**, 103 (*isol*)
Lindberg, K.B. *et al*, *Acta Crystallogr., Sect. B*, 1976, **32**, 642 (*cryst struct*)
Wiren, E. *et al*, *Carbohydr. Res.*, 1976, **49**, 201.

4-Acetyl-2-hydroxy-3-methyltetrahydrofuran A-00021

1-(Tetrahydro-5-hydroxy-4-methyl-3-furanyl)-ethanone, 9CI



Absolute configuration

$C_7H_{12}O_3$ M 144.170

(2S,3S,4R)-form [27098-03-9]

Botryodiplodin

Antibiotic metab. of *Botryodiplodia theobromae* and of *Penicillium carneoluteus* and *P. roquefortii*. Shows antifungal and antileukaemic activity. Cryst. (Et_2O). Mp 50-52°. Anomerises in soln. to a mixt. of 2-epimers.

▷OB6005000.

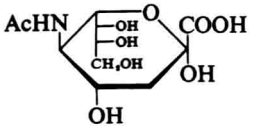
Ac: Cryst. (Et_2O). Mp 45-47°. $[\alpha]_D$ −104° (c, 0.09 in $CHCl_3$).

McCurry, P.M. *et al, J. Am. Chem. Soc.*, 1973, **95**, 5824; *Tetrahedron Lett.*, 1973, 4103 (*synth, stereochem*)
Wilson, S.R. *et al, J. Org. Chem.*, 1975, **40**, 3309 (*synth*)
Sakai, K. *et al, CA*, 1979, **90**, 186692p (*synth, abs config*)
Moreau, S. *et al, J. Org. Chem.*, 1982, **47**, 2358 (*isol, cryst struct*)
Kurth, M.J. *et al, J. Org. Chem.*, 1985, **50**, 1840 (*synth*)

N-Acetylneuraminic acid A-00022

5-(Acetylamino)-3,5-dideoxy-D-glycero-D-galacto-2-nonulosonic acid, 9CI. O-Sialic acid. NANA. Lactaminic acid. Gynaminic acid. Serolactaminic acid

[131-48-6]



α-D-Pyranose-*form*

$C_{11}H_{19}NO_9$ M 309.272

Isol. from milk, clostrum, submaxillary mucin and meconium by acid or enzymic hydrol. of the constit. sialoproteins and oligosaccharides. Edible bird's nest is also a source. Present in urine of patients with sialuria. Mp 185-187° dec. $[\alpha]_D^{22}$ −32° (H_2O).

4-Ac: Mp 199-200°. $[\alpha]_D$ −62° (H_2O).

7-Ac: B-*Sialic acid*. Mp 138-140°. $[\alpha]_D$ +6°.

4,7,8,9-Tetra-Ac, Me ester: Mp 174-175°. $[\alpha]_D^{20}$ −4.8° → −5.2° (c, 0.5 in $CHCl_3$).

2,4,7,8,9-Penta-Ac, Me ester: Methyl 5-N-acetyl-2,4,7,8,9-penta-O-acetylneuraminate. Mp 156-157°. $[\alpha]_D^{20}$ −3.3° (c, 1.0 in $CHCl_3$).

4,7,8,9-Tetrabenzoyl, Me ester: $[\alpha]_D^{20}$ −0.4° (c, 1.0 in $CHCl_3$).

α-D-Pyranose-form

Benzyl glycoside: Mp 194-195°. $[\alpha]_D^{25}$ −7.5° (MeOH).

Benzyl glycoside, Me ester: Mp 85-89°. $[\alpha]_D^{25}$ −3.5° (MeOH).

Me glycoside: Mp 185-188° dec. $[\alpha]_D^{25}$ −16.3° (MeOH).

Me glycoside, Me ester: Mp 166-168° dec. $[\alpha]_D^{25}$ −5.2° (MeOH).

Allyl glycoside: Mp 167-169° dec. $[\alpha]_D$ −14° (MeOH).

Allyl glycoside, Me ester: Mp 154-156°. $[\alpha]_D$ −13° (MeOH).

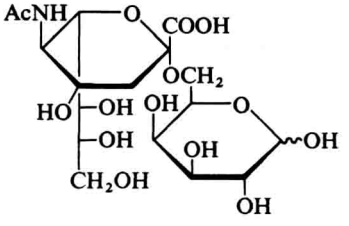
β-D-Pyranose-form

Me glycoside, Me ester: Mp 115-130°. $[\alpha]_D^{20}$ −46° (c, 0.67 in MeOH).

Gottschalk, A., *The Chemistry and Biology of Sialic Acids and Related Substances*, 1960, Cambridge Univ. Press, London (*rev*)
Blix, G. *et al, Methods Carbohydr. Chem.*, 1962, **1**, 246 (*isol*)
Kuhn, R. *et al, Chem. Ber.*, 1966, **99**, 611 (*synth*)
O'Connell, A.M., *Acta Crystallogr., Sect. B*, 1973, **29**, 2320 (*cryst struct*)
Codington, J.F. *et al, Methods Carbohydr. Chem.*, 1976, **7**, 226 (*rev*)
Jaques, L.W. *et al, J. Biol. Chem.*, 1977, **252**, 4533 (*cmr*)
Martin, J.E. *et al, Carbohydr. Res.*, 1977, **56**, 432 (*isol*)
Benzing-Nguyen, L. *et al, J. Org. Chem.*, 1978, **43**, 554 (*synth*)
Eschenfelder, V. *et al, Carbohydr. Res.*, 1980, **78**, 190 (*synth*)
Friebolin, H. *et al, Angew. Chem., Int. Ed. Engl.*, 1980, **19**, 208.
Van der Vleugel, D.J.M. *et al, Carbohydr. Res.*, 1982, **102**, 121 (*Me ester, Me glycoside*)

6-O-(N-Acetyl-α-D-neuraminyl)-D-galactose A-00023

6-O-(5-Acetamido-3,5-dideoxy-α-D-glycero-D-galacto-2-nonulopyranosylonic acid)-D-galactose



$C_{17}H_{29}NO_{14}$ M 471.414

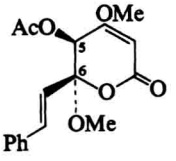
K salt: $[\alpha]_D^{25}$ +16.7° (c, 0.3 in H_2O).

Me ester: $[\alpha]_D^{20}$ +5.4° (c, 0.8 in MeOH).

Me ester, benzyl-β-glycoside: Mp 183-184°. $[\alpha]_D^{20}$ −1.3° (c, 0.95 in MeOH).

Khorlim, A.Ya. *et al, Carbohydr. Res.*, 1971, **19**, 272.
Van Der Vleugel, D.J.M. *et al, Carbohydr. Res.*, 1982, **104**, 221.

5-Acetyloxy-5,6-dihydro-4,6-dimethoxy-6-(2-phenylethenyl)-2H-yl-pyran-2-one, 9CI A-00024



(5S,6S)-*form*
Absolute configuration

$C_{17}H_{18}O_6$ M 318.326

(5S,6S)-form [60037-33-4]

Constit. of the roots of *Piper sanctum*. Needles (EtOH). Mp 178-180°. $[\alpha]_D^{20}$ +380° (c, 0.1 in $CHCl_3$).

(5RS,6RS)-form [60102-66-1]

Cryst. (MeOH). Mp 153-155°.

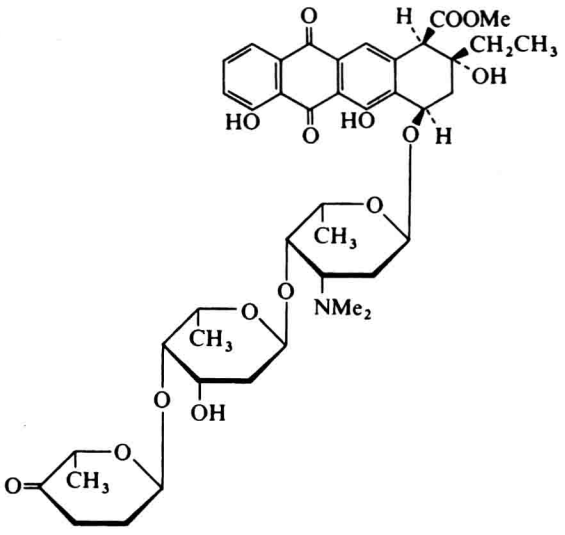
(5RS,6SR)-form

Cryst. (MeOH). Mp 104-105°.

Hänsel, R. *et al, Chem. Ber.*, 1976, **109**, 1617 (*isol, struct*)

Aclacinomycin *A* A-00025

[57576-44-0]



$C_{42}H_{53}NO_{15}$ M 811.878

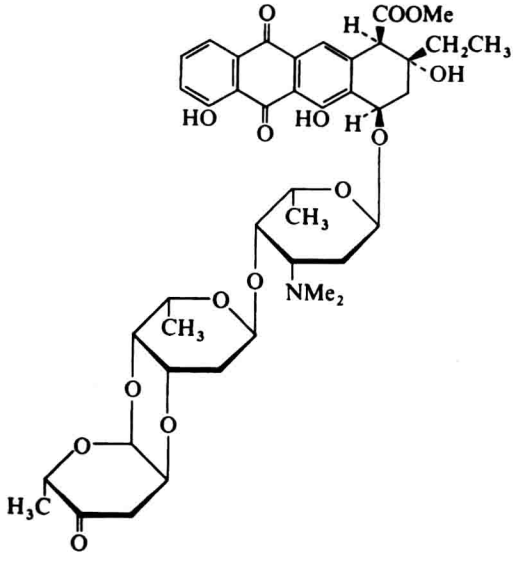
Anthracycline. Isol. from *Streptomyces galilaeus*. Antitumour antibiotic. Yellow powder. Mp 129-135° dec. $[\alpha]_D^{24}$ +29° (c, 1 in $CHCl_3$).

▷QI9279300.

Oki, Y. *et al*, *J. Antibiot.*, 1975, **28**, 830 (*isol, ir, uv, nmr, struct*)

Aclacinomycin *B* A-00026

[57596-79-9]



$C_{42}H_{51}NO_{15}$ M 809.863

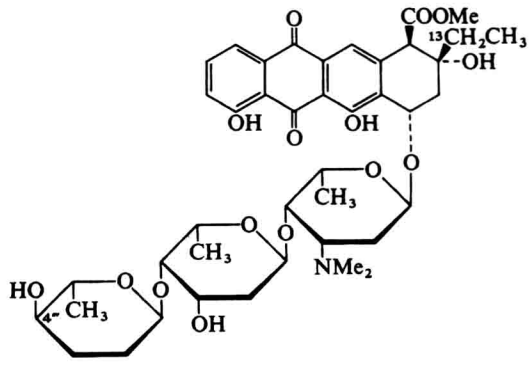
Anthracycline. Isol. from *Streptomyces galilaeus*. Antitumour antibiotic. Yellow powder. Mp 135-145° dec. $[\alpha]_D^{24}$ +3° (c, 1 in $CHCl_3$).

Oki, T. *et al*, *J. Antibiot.*, 1975, **28**, 830 (*isol, ir, uv, nmr, struct*)

Aclacinomycin *M* A-00027

MA 144M$_1$. Antibiotic MA 144M$_1$

[64431-68-1]



$C_{42}H_{55}NO_{15}$ M 813.894

Anthracycline antibiotic. Isol. from *Streptomyces galilaeus*. Antitumour antibiotic. Mp 149-150°. $[\alpha]_D^{22}$ +36.7° (c, 1 in $CHCl_3$).

13-Methyl: ***13-Methylaclacinomycin*** **M**. From *S. galilaeus*. Mp 165°. $[\alpha]_D^{20}$ +53° (c, 1.01 in $CHCl_3$).

4‴-Epimer: [64474-88-0]. ***Aclacinomycin*** **N**. *MA 144N$_1$. Antibiotic MA 144N$_1$*. Isol. from *S. galilaeus*. Antitumour antibiotic. Mp 146-147°. $[\alpha]_D^{22}$ +38.6° (c, 1 in $CHCl_3$).

▷QI9288700.

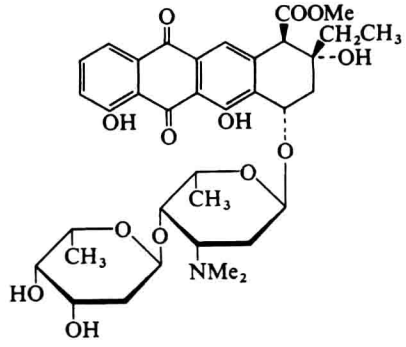
4‴-Epimer, 13-Methyl: ***13-Methylaclacinomycin*** **N**. From *S. galilaeus*. Mp 164.5°. $[\alpha]_D^{20}$ +45.7° (c, 1 in $CHCl_3$).

Oki, T. *et al*, *J. Antibiot.*, 1977, **30**, 683 (*isol*)
Oki, T. *et al*, *J. Antibiot.*, 1979, **32**, 791, 801 (*isol, uv, ir, pmr*)
Soga, K. *et al*, *J. Antibiot.*, 1981, **34**, 770 (*deriv*)
Yoshimoto, A. *et al*, *J. Antibiot.*, 1981, **34**, 951 (*isol, epimer*)

Aclacinomycin *S* A-00028

MA 144S$_1$. Antibiotic MA 144S$_1$

[64431-69-2]



$C_{36}H_{45}NO_{13}$ M 699.750

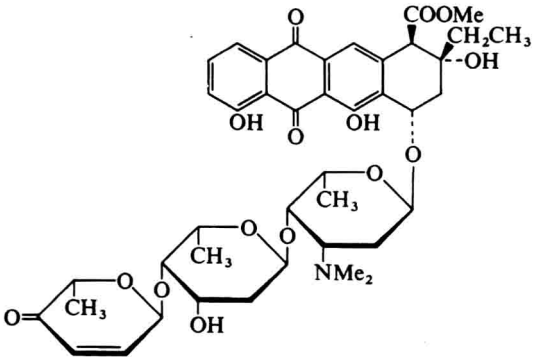
Anthracycline. Isol. from *Streptomyces galilaeus*. Antitumour antibiotic. Mp 145-146°. $[\alpha]_D^{22}$ +90.8° (c, 1 in $CHCl_3$).

Oki, T. *et al*, *J. Antibiot.*, 1977, **30**, 683 (*isol*)
Oki, T. *et al*, *J. Antibiot.*, 1979, **32**, 791, 801 (*isol, uv, ir, pmr, cmr*)
Soga, K. *et al*, *J. Antibiot.*, 1981, **34**, 770 (*deriv*)
Yoshimoto, A. *et al*, *J. Antibiot.*, 1981, **34**, 951 (*isol*)

Aclacinomycin Y A-00029

MA 144Y. Antibiotic MA 144Y

[66789-14-8]



$C_{42}H_{51}NO_{15}$ M 809.863

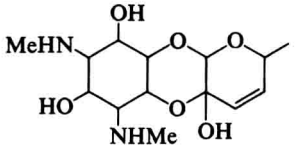
Anthracycline. Isol. from *Streptomyces galilaeus*. Antitumour antibiotic. Mp 153-155°. $[\alpha]_D^{22}$ +66° (c, 1 in $CHCl_3$).

▷QI9279700.

Yoshimoto, A. *et al*, *J. Antibiot.*, 1979, **32**, 472 (*isol*)
Oki, T. *et al*, *J. Antibiot.*, 1979, **32**, 791, 801 (*isol, uv, ir, pmr, cmr*)
Hoshino, T. *et al*, *J. Antibiot.*, 1983, **36**, 1458 (*synth*)

Acmimycin A-00030

[90755-71-8]



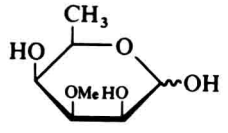
$C_{14}H_{24}N_2O_6$ M 316.353

Aminoglycoside-type antibiotic. Prod. by *Streptomyces* sp. Active against gram-positive and -negative bacteria. Possibly demethoxy deriv. of Spenolimycin. Confign. not confirmed.

Fr. Pat., 2 532 950, (*1984*); *CA*, **101**, 37205 (*isol*)

Acovenose A-00031

6-Deoxy-3-O-methyltalose



D-form

$C_7H_{14}O_5$ M 178.185

D-form [51795-06-3]

Constit. of the lipopolysaccharides of *Rhodopseudomonas palustris*. Syrup. $[\alpha]_D^{25}$ +16.5° (H_2O).

L-form [642-33-1]

Occurs in Acovenoside *A* and in *Mycobacterium avium*. Syrup. $Bp_{0.01}$ 85°. $[\alpha]_D^{25}$ −14.2° (c, 1.2 in H_2O).

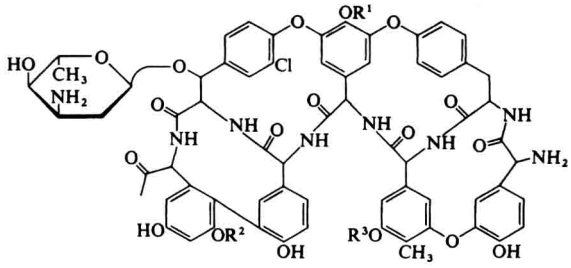
1,4-Onolactone: 6-Deoxy-3-O-methyl-L-talono-1,4-lactone. Mp 167-168°. $[\alpha]_D^{26}$ +32.6° (c, 0.3 in MeOH).

Euw, J.V. *et al*, *Helv. Chim. Acta*, 1950, **33**, 485 (*isol*)
Reichstein, T. *et al*, *Adv. Carbohydr. Chem.*, 1962, **17**, 65 (*rev*)
Kapur, B.M. *et al*, *Helv. Chim. Acta*, 1968, **51**, 89 (*synth*)
Weckesser, J. *et al*, *Biochem. J.*, 1973, **135**, 293 (*synth*)

Actaplanin A-00032

A 4696. Antibiotic A 4696

[37305-75-2]



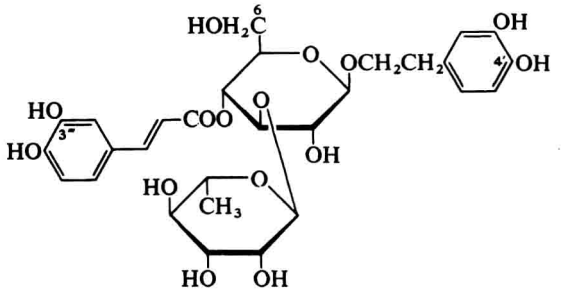
Actaplanin	R^1	R^2	R^3
A	mannosylglucose	mannose	mannose
B_1	rhamnosylglucose	mannose	mannose
B_2	glucose	mannose	mannose
B_3	mannosylglucose	mannose	H
C_1	rhamnosylglucose	mannose	H
G	glucose	mannose	H

Glycopeptide antibiotic complex. Isol. from *Actinoplanes missouriensis*. Active against gram-positive bacteria. Shows growth-promoting activity for chickens and swine.

Actaplanin A [88357-81-7]
Actaplanin B_1 [88357-82-8]
A 4696B_1. Antibiotic A 4696B_1
Actaplanin B_2 [88357-83-9]
A 4696B_2. Antibiotic A 4696B_2
Actaplanin B_3 [88357-84-0]
A 4696B_3. Antibiotic A 4696B_3
Actaplanin C_1 [88357-85-1]
Actaphanin C_{1a}. A 4696C_{1a}. Antibiotic A 4696C_{1a}
Acteplanin C_3 [88357-88-4]
A 4696C_3. Antibiotic A 4696C_3
Actaplanin G [83381-73-1]

U.S.P., 3 952 095, (*1976*); *CA*, **85**, 19065 (*isol*)
Eur. Pat. Appl., 55 071, (*1982*); *CA*, **97**, 180142 (*isol*)
Debono, M. *et al*, *J. Antibiot.*, 1984, **37**, 85 (*isol*)
Hunt, A.H. *et al*, *J. Org. Chem.*, 1984, **49**, 635, 641 (*pmr, struct*)

Acteoside A-00033



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

Glycoside from *Leucosceptrum japonicum* and other plants.

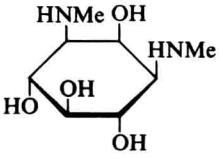
3‴-Me ether: Leucosceptoside A. Isol. from *L. japonicum*. Amorph. powder.
4′,3‴-Di-Me ether: Martynoside. Glycoside from *Martynia louisiana* and *L. japonicum*.
6-O-Apiofuranoside: Leucosceptoside B. From *L. japonicum*.
3‴-Me ether, 6′-O-β-D-apioside: Leucosceptoside B. From *L. japonicum*. Amorph. powder. $[\alpha]_D^{19}$ −81.8° (c, 3.43 in MeOH).

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

Actinamine A-00034

*1,3-Dideoxy-1,3-*N,N-*bis*(*methylamino*)-myo-*inositol*

[6216-38-2]



$C_8H_{18}N_2O_4$ M 206.241

Component of spectinomycin (Actinospectacin). Mp 135-136°. Opt. inactive (*meso*-).

B,2HCl: Mp >300°.

Di-N-*Ac:* Mp 255-256° dec.

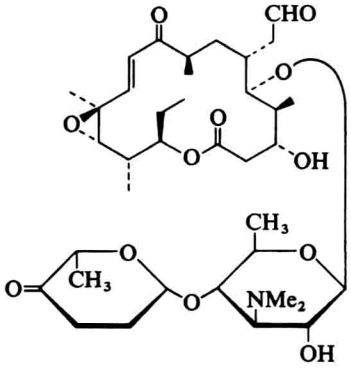
N,N,O,O,O,O-*Hexa-Ac:* Mp 205-206°.

Johnson, A.L. *et al*, *J. Org. Chem.*, 1963, **28**, 300.

Hanessian, S. *et al*, *J. Am. Chem. Soc.*, 1979, **79**, 5839.

Acumycin A-00035

[25999-30-8]



Absolute configuration

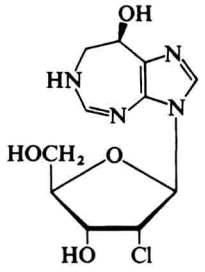
$C_{37}H_{59}NO_{12}$ M 709.873

Macrolide antibiotic. Isol. from *Streptomyces griseoflavus*. Prisms (EtOAc). Mp 230-233°.

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

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

Adechlorin A-00037



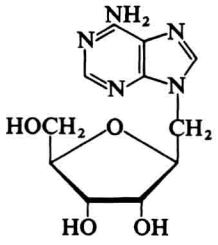
$C_{11}H_{15}ClN_4O_4$ M 302.717

Proposed struct. shown. Nucleoside-type antibiotic. Isol. from *Actinomadura* sp. OMR-37. Adenosine deaminase inhibitor. Needles (H_2O). Mp 125-131°. $[\alpha]_D^{20}$ +21° (c, 1 in H_2O).

Omura, S. *et al*, *J. Antibiot.*, 1985, **38**, 1008 (*isol*, *uv*, *ir*, *pmr*, *cmr*)

1-(9-Adeninyl)-2,5-anhydro-1-deoxyallitol A-00038

*1-(6-Amino-9*H*-purin-9-yl)-2,5-anhydro-1-deoxyallitol*, *9CI*, *8CI*



$C_{11}H_{15}N_5O_4$ M 281.271

D-form [29868-39-1]

Mp 206°. $[\alpha]_D^{24}$ +15.7° (c, 1.07 in 50% EtOH aq.). λ_{max} 261 (ε 14 600) (H_2O), 258 (14 300) (pH 1), 261 nm (14 600) (pH 13).

2′,3′-O-(*Ethoxyethylidene*): Syrup. λ_{max} 257 (pH 1), 260 nm (pH 7, 13).

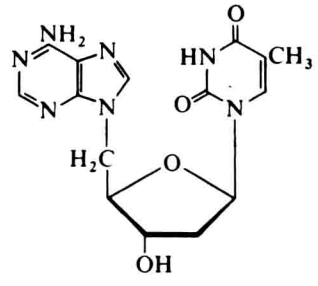
Montgomery, J.A. *et al*, *J. Heterocycl. Chem.*, 1970, **7**, 443 (*synth*)

Farkas, J., *Collect. Czech. Chem. Commun.*, 1971, **36**, 3043 (*synth*)

5′-(9-Adeninyl)-5′-deoxythymidine A-00039

*1-[5′-(6-Amino-9*H*-purin-9-yl)-2′,5′-dideoxy-β-D-*erythro-*pentofuranosyl]thymine*, *8CI*

[28220-19-1]



$C_{15}H_{17}N_7O_4$ M 359.344

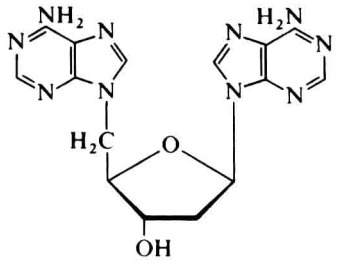
Mp 239-240° (monohydrate). λ_{max} 257 (ε 19 840) (H_2O), 260 (18 700) (0.1N HCl), 260 nm (18 200) (0.1N NaOH).

Fecher, R. *et al*, *Carbohydr. Res.*, 1970, **13**, 105.

Fecher, R. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 1400 (*synth*, *pmr*, *cd*)

5′-(9-Adeninyl)-2′,5′-dideoxyribofuranosyladenine **A-00040**

9-[5-(6-Amino-9H-purin-9-yl)-2,5-dideoxy-erythro-*pentofuranosyl]adenine, 8CI*



$C_{15}H_{16}N_{10}O_2$ M 368.357

β-D-form [28220-20-4]

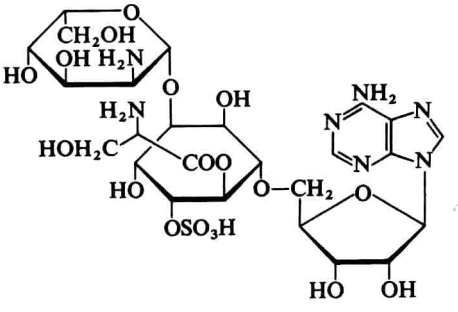
Mp 305-306°. λ_{max} 256 nm (ε 24 900) (H_2O).

Fecher, R. *et al*, *Carbohydr. Res.*, 1970, **13**, 105 (*synth*)
Fecher, R. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 1400 (*synth, pmr, cd*)

Adenomycin **A-00041**

C19-97 Substance. Antibiotic C19-97

[70535-13-6]



$C_{25}H_{39}N_7O_{18}S$ M 757.679

Nucleoside antibiotic. Isol. from *Streptomyces griseoflavus* C19-97. Active against gram-positive and -negative bacteria and tumours. Mp 165-168° dec. $[\alpha]_D^{22.5}$ +10.5° (c, 2 in H_2O). λ_{max} 260 nm.

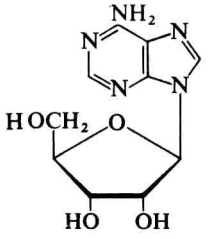
B,2HCl: Powder. Mp 210-220°. $[\alpha]_D^{25}$ +14° (c, 1 in H_2O).

Japan. Pat., 79 14 595, (*1979*); *CA*, **91**, 37478 (*isol*)
Ogita, T. *et al*, *Tetrahedron Lett.*, 1980, **21**, 3203 (*struct*)
Otake, N. *et al*, *J. Antibiot.*, 1981, **34**, 130 (*spectra*)

Adenosine, 9CI, 8CI **A-00042**

9-β-D-Ribofuranosyl-9H-purin-6-amine, 9CI. 9-β-D-Ribofuranosyladenine, 8CI. 6-Amino-9-β-D-ribofuranosyl-9H-purine

[58-61-7]



$C_{10}H_{13}N_5O_4$ M 267.244

Widely distributed in nature. One of the four principal nucleosides of nucleic acid. Mp 234-236°. $[\alpha]_D^{11}$ −61.7° (c, 0.7 in H_2O). λ_{max} 259 nm (ε 15 400) (H_2O, pH 7).

▷AU7175000.

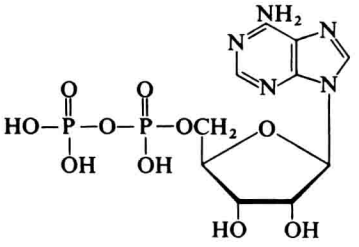
6N,6N-Di-Me: see N-Dimethyladenosine, D-00249
6N-(Dimethylallyl): see N-(3-Methyl-2-butenyl)-adenosine, M-00105
2-Me: see 2-Methyladenosine, M-00064
6N-Trityl: Mp 153-156°.
6N-(p-Anisoyl): Mp 155-156°. λ_{max} 292 nm (ε 28 400) (95% EtOH).
2-Fluoro: see 2-Fluoroadenosine, F-00009
8-Fluoro: see 8-Fluoroadenosine, F-00010
2′,3′-O-Isopropylidene: [362-75-4]. *2′,3′-O-Isopropylideneadenosine.* Mp 220°.
3′-Ac: [6554-21-8]. Mp 180-181°. λ_{max} 260 nm (ε 14 130) (95% EtOH aq.).
5′-Ac: [2140-25-2]. Mp 143°.
5′-Pivaloyl: Mp 162-163°. λ_{max} 260 nm (ε 13 180) (95% EtOH aq.).
5′-Tosyl: [5135-30-8]. Mp 151-153°.
3′,5′-Di-Ac: Mp 175-176°.
3′,5′-Dibenzoyl: Mp 193-194°.
2′,3′,5′-Tribenzoyl: Glass. $[\alpha]_D^{22}$ −71° (c, 1.0 in $CHCl_3$). λ_{max} 258 (ε 20 500), 231 nm (47 100) (EtOH).
6N,2′,3′,5′-Tetrabenzoyl: Glass. $[\alpha]_D^{22}$ −94° (c, 1.0 in $CHCl_3$). λ_{max} 279 (ε 22 400), 230 nm (49 200) (EtOH).
3′-Benzoyl, 2′-methoxytetrahydropyranyl: Mp 233-235°. λ_{max} 259 (ε 17 000), 234 nm (16 300) (95% EtOH).
2′-Phosphate: see 2′-Adenylic acid, A-00053
3′-Phosphate: see 3′-Adenylic acid, A-00054
5′-Phosphate: see Adenylic acid, A-00052
2′,5′-Diphosphate: see Adenosine 2′,5′-diphosphate, A-00044
3′,5′-Diphosphate: see Adenosine 3′,5′-diphosphate, A-00045
5′-Diphosphate: see Adenosine diphosphate, A-00043
5′-Triphosphate: see Adenosine triphosphate, A-00048
2′,3′-Cyclic monophosphate, Na salt: [37063-35-7]. Hydrate. Mp 241-243° dec.
3′,5′-Cyclic monophosphate: see Cyclic AMP, C-00099
2′-Me: see 2′-O-Methyladenosine, M-00066
2′-C-Me: see 2′-C-Methyladenosine, M-00065
3′-C-Me: see 3′-C-Methyladenosine, M-00067
5′-Trityl: Mp 259°. $[\alpha]_D^{20}$ −8.8° ($CHCl_3$).
6N,5′-Ditrityl: [31085-55-9]. Mp 215-216°.
6N,2′,5′-Tritrityl: [31085-56-0]. Mp 153-157°.
6N,3′,5′-Tritrityl: [31085-57-1]. Mp 155-158°.
N-(o-*Methylbenzyl):* [23707-33-7]. N-[(2-*Methylphenyl)methyl]adenosine, 9CI. Metrifudil, INN.* Coronary vasodilator. Mp 157-158°.

Davoll, J. *et al*, *J. Chem. Soc.*, 1948, 967 (*synth*)
Formageot, H.P.M. *et al*, *Tetrahedron*, 1967, **23**, 2315.
South African Pat., 6 707 414, (*1968*); *CA*, **70**, 115505f (*Metrifudil*)
Blank, H.U. *et al*, *Justus Liebigs Ann. Chem.*, 1970, **742**, 34.
Shikata, K. *et al*, *Acta Crystallogr., Sect. B*, 1973, **29**, 31 (*cryst struct*)
Sarma, R.H. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 7337 (*pmr, conformn*)
Earl, R.A. *et al*, *J. Org. Chem.*, 1975, **40**, 1822 (*cmr*)
Reese, C.B. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1975, 934.
Ishido, Y. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1977, 657.

Adenosine diphosphate A-00043

Adenosine 5′-(trihydrogen diphosphate), 9CI. Adenosine 5′-pyrophosphate. ADP

[58-64-0]



$C_{10}H_{15}N_5O_{10}P_2$ M 427.204

Formed from ATP in the muscle by the enzyme adenosinetriphosphatase. λ_{max} 259 nm (ϵ 15 400) (H_2O).

▷AU7467000.

Acridine salt: Mp 215° dec.

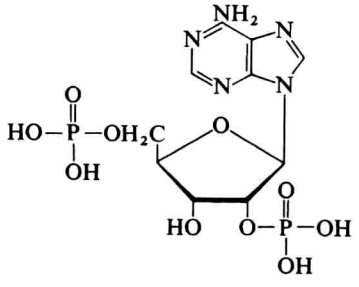
6N-Benzoyl, tri-Na salt: λ_{max} 281 nm (ϵ 19 400) (H_2O).

Baddiley, J. *et al*, *J. Chem. Soc.*, 1947, 648.
Biochem. Prep., 1949, **1**, 1.
Chambers, R.W. *et al*, *J. Am. Chem. Soc.*, 1960, **82**, 970 (*synth*)
Wieland, T. *et al*, *Chem. Ber.*, 1968, **107**, 3031 (*synth*)
Sarma, R.H. *et al*, *J. Chem. Soc., Chem. Commun.*, 1973, 140 (*pmr, nmr*)
Hampton, A. *et al*, *Biochemistry*, 1975, **14**, 5438.

Adenosine 2′,5′-diphosphate A-00044

2′-Adenylic acid 5′-(dihydrogen phosphate), 9CI. Adenosine 2′,5′-bis(phosphate), 8CI

[3805-37-6]



$C_{10}H_{15}N_5O_{10}P_2$ M 427.204

Component of coenzyme II. Amorph. powder.

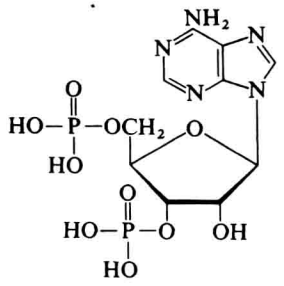
Di-Ca salt: Octahydrate. λ_{max} 258 nm (ϵ 14 250) (H_2O).

Wang, T.P. *et al*, *J. Biol. Chem.*, 1954, **206**, 299.
Baddiley, J. *et al*, *J. Chem. Soc.*, 1958, 1000 (*synth*)
Japan. Pat., 536, (*1967*); *CA*, **66**, 64391y (*synth*)
Takaku, H. *et al*, *Chem. Pharm. Bull.*, 1973, **21**, 1844 (*synth*)
Roeder, S.B.W., *Physiol. Chem. Phys.*, 1975, **7**, 115 (*cmr*)

Adenosine 3′,5′-diphosphate A-00045

3′-Adenylic acid 5′-(dihydrogen phosphate), 9CI. Adenosine 3′,5′-bis(phosphate), 8CI

[1053-73-2]



$C_{10}H_{15}N_5O_{10}P_2$ M 427.204

Component of coenzyme *A*. Amorph. powder.

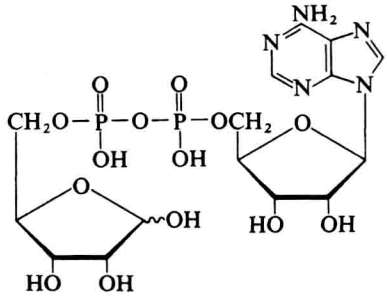
Ca salt: Pentahydrate. λ_{max} 258 nm (ϵ 14 050) (H_2O).

Wang, T.P. *et al*, *J. Biol. Chem.*, 1954, **206**, 299.
Baddiley, J. *et al*, *J. Chem. Soc.*, 1958, 1000 (*synth*)
Takaku, H. *et al*, *Chem. Pharm. Bull.*, 1973, **21**, 1844 (*synth*)
Lee, C. *et al*, *FEBS Lett.*, 1974, **43**, 271; *CA*, **82**, 12479u (*pmr*)
Roeder, S.B.W., *Physiol. Chem. Phys.*, 1975, **7**, 115 (*cmr*)

Adenosine diphosphate ribose A-00046

Adenosine 5′-(trihydrogen diphosphate) 5′→5-ester with D-ribose, 9CI. ADPR

[20762-30-5]



$C_{15}H_{23}N_5O_{14}P_2$ M 559.319

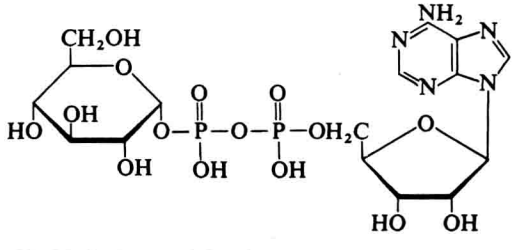
Prod. of enzymic or chemical hydrol. of diphosphopyridine nucleotide. Inhibits coenzyme action of diphosphopyridine nucleotide.

Rosenberg, S. *et al*, *J. Biol. Chem.*, 1954, **211**, 763 (*isol*)
Blumenstein, M. *et al*, *Biochemistry*, 1972, **11**, 1643 (*cmr, nmr*)
Sarma, R.H. *et al*, *J. Am. Chem. Soc.*, 1973, **95**, 7470 (*conformn, pmr*)
Abdallah, M.A. *et al*, *Eur. J. Biochem.*, 1975, **50**, 475 (*cryst struct*)

Adenosine 5′-diphosphoglucose A-00047

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

[2140-58-1]



$C_{16}H_{25}N_5O_{15}P_2$ M 589.346

Present in ripening cereal grains. Glucose donor in glycogen synth., sucrose synth. and glucoside formn. λ_{max} 257 nm (pH 2).

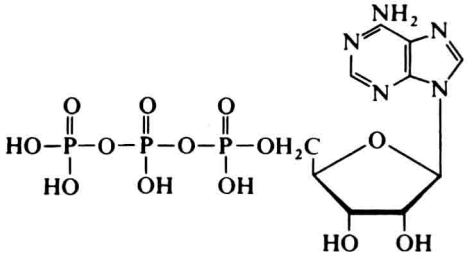
Di-K salt: λ_{max} 259 nm (ϵ 15 400) (H_2O).

Roseman, S. *et al*, *J. Am. Chem. Soc.*, 1961, **83**, 659.
Murata, T. *et al*, *Arch. Biochem. Biophys.*, 1964, **106**, 371 (*isol, synth*)
Krauss, G. *et al*, *J. Chromatogr.*, 1973, **76**, 248 (*chromatog*)
Sarma, R.H. *et al*, *FEBS Lett.*, 1973, **36**, 157 (*nmr*)
Lee, C.H. *et al*, *Biochemistry*, 1976, **15**, 697 (*conformn, pmr*)

Adenosine triphosphate A-00048

Adenosine 5′-(tetrahydrogen triphosphate), 9CI, 8CI. ATP

[56-65-5]



$C_{10}H_{16}N_5O_{13}P_3$ M 507.183

Isol. from muscle extracts. Mammalian skeletal muscle at rest contains 0.3-0.4 g of ATP/100 g. Important metabolic coenzyme. Mp 143-145° dec. $[\alpha]_D^{22}$ −26.7° (c, 3.1 in H_2O). λ_{max} 259 nm (ϵ 15 400) (H_2O).

▷AU7416000.

Di-Na salt: Trinosin. Adetphos. Inhibits enzymatic browning of apples, potatoes etc. Mp 188-190° dec. (hydrate).

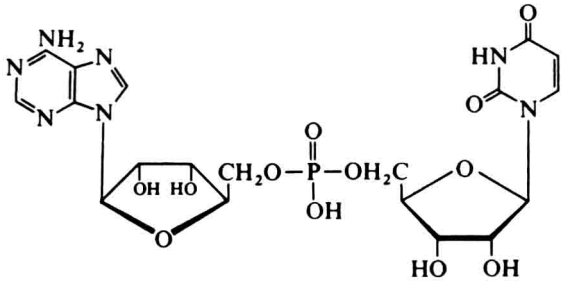
Triacridine salt: Mp 208-209° dec.

6N-Benzoyl, tetra-Na salt: λ_{max} 281 nm (ϵ 19 400) (H_2O).

Baddiley, J. *et al*, *J. Chem. Soc.*, 1949, 582 (*synth*)
Biochem. Prep., 1949, **1**, 5 (*isol*)
Michelson, A.M., *The Chemistry of Nucleosides and Nucleotides*, 1963, Academic Press, N.Y. and London, 153 (*rev*)
Feldman, I. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 7329 (*pmr*)
Dorman, D.E. *et al*, *Proc. Natl. Acad. Sci. U.S.A.*, 1970, **65**, 19 (*cmr*)
Kennard, O. *et al*, *Nature (London)*, 1970, **225**, 333 (*cryst struct*)
Hampton, A. *et al*, *Biochemistry*, 1975, **14**, 5438.

Adenosine 5′-uridine 5′-phosphate A-00049

Uridylyl-(5′,5′)-adenosine



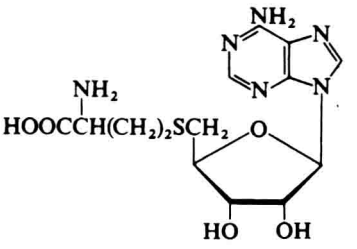
$C_{19}H_{24}N_7O_{12}P$ M 573.412

Amorph. hygroscopic powder. Dec. at 180-200° without melting. λ_{max} 259.5 (ϵ 21 300) (0.01N H_2SO_4), 260.5 nm (20 300) (0.01N NaOH).

Elmore, D.T. *et al*, *J. Chem. Soc.*, 1952, 3681 (*synth*)
Michelson, A.M., *CA*, 1962, **56**, 14622b.

S-Adenosylhomocysteine A-00050

5′-S-(3-Amino-3-carboxypropyl)-5′-thioadenosine, 9CI, 8CI. SAH



$C_{14}H_{20}N_6O_5S$ M 384.409

***L*-form** [979-92-0]

L-SAH

Methyl transferase inhibitor. Mp 210-211° dec. $[\alpha]_D^{23}$ +44.5° (c, 0.1 in 0.05N HCl). λ_{max} 260 nm (H_2O).

Picrate: Mp 170° dec.

6N-Me: Mp 208-210°.

de la Haba, G. *et al*, *J. Biol. Chem.*, 1959, **234**, 603 (*synth*)
Duerre, J.A., *Arch. Biochem. Biophys.*, 1962, **96**, 70.
Follmann, H. *et al*, *Eur. J. Biochem.*, 1974, **47**, 187 (*conformn, pmr*)
Borchardt, R.T. *et al*, *J. Org. Chem.*, 1976, **41**, 565 (*synth*)
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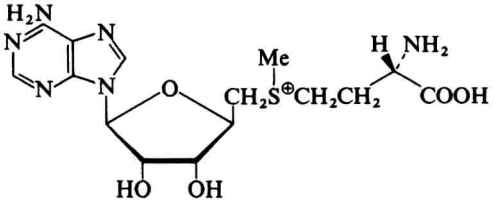
S-Adenosylmethionine A-00051

S-5′-[(3-Amino-3-carboxypropyl)methylsulfonio]-5′-deoxyadenosine hydroxide, inner salt, 9CI

[29908-03-0]



$C_{15}H_{23}N_6O_5S$ M 399.444

Metab. intermed. which functions as the principle biological donor of methyl groups, as the source of the propylamine moieties of spermidine and spermine, and as the regulator of a variety of enzymatic reactions.

▷AU7334000.

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