Amino Acids and Peptides

Edited by

J. S. Davies

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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 or molecular formula index.

Indexes

There are three 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 or derivatives in Hill convention order; and a CAS registry number index listing all CAS number included in the *Sourcebook* in serial order. 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 three 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 particular 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 1972–6 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 Name Index.

3. Toxicity and Hazard Information

Toxicity and hazard information is highlighted by the sign ▷ which also appears in the indexes.

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

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

The hazard/toxicity information provided contains in many cases RTECS numbers which provide access to the database Registry of Toxic Effects of Chemical Substances which is obtainable in printed, microfiche and online versions from US Government sources.

4. 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 mnemonic 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.

5. 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

Preface

This is one of the first volumes 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. Each individual entry has, however, been reviewed and if necessary updated, and a considerable number (about 300) of totally new entries have been added.

The resulting coverage of entries in this sourcebook is as follows: The important protein aminoacids have extensive entries containing many derivatives. Certain important *N*-protected derivatives of these aminoacids (*N*-*tert*-butyloxycarbonyl, *N*-benzyloxycarbonyl and *N*-fluorenylmethylenoxycarbonyl) have their own individual entries. Virtually every known rare aminoacid has been included as well as many metabolic intermediates. Nearly all known dipeptides are represented; for higher peptides and proteins the selection of compounds has been on the basis of biological or pharmaceutical importance, with a strong bias in favour of compounds of which the structure is fully known. There is extensive coverage of peptide alkaloids and of peptide antibiotics including β-lactams.

With a work of this kind, some omissions are inevitable, but it is hoped that nearly all 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.

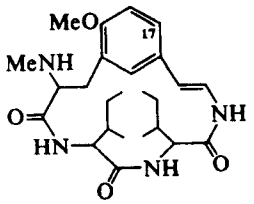
J.S. Davies

A

Abyssenine *B* **A-00001**

15-Methoxy-12-(methylamino)-6,9-bis(1-methylpropyl)-4,7,10-triazabicyclo[12.3.1]octadeca-1(18)-,2,14,16-tetraene-5,8,11-trione, 9CI

[54519-15-2]



$C_{25}H_{38}N_4O_4$ M 458.600

Alkaloid from the bark of *Zizyphus abyssinica* and *Z. mucronata* and from the stem bark of *Z. oenoplia*. Needles (MeOH/pet. ether). Mp 229-30°. $[\alpha]_D^{20}$ +151° (c, 0.16 in $CHCl_3$).

N-*Ac:* $[\alpha]_D^{20}$ −167° (c, 0.1 in $CHCl_3$)

N-*Me, dihydro:* $[\alpha]_D^{20}$ −75° (c, 0.15 in $CHCl_3$).

N-*De-Me:* [55857-03-9]. *Absyssenine* C. Alkaloid from the bark of *Z absyssinica* and from bark and leaves of *Z. mucronata*. Amorph. $[\alpha]_D^{20}$ +144° (c, 0.12 in $CHCl_3$), −15° (c, 0.13 in MeOH).

Tschesche, R. *et al*, *Justus Liebigs Ann. Chem.*, 1974, 1915 (*isol, uv, ir, pmr, ms, struct*)
Tschesche, R. *et al*, *Phytochemistry*, 19974, **13**, 2328 (*occur*)
Cassels, B.K. *et al*, *Tetrahedron*, 1974, **30**, 2461 (*isol*)

4-Acetamido-2-butenoic acid **A-00002**

4-(Acetylamino)-2-butenoic acid, 9CI

[64120-63-4]

$$HOOCCH{=}CHCH_2NHAc$$

$C_6H_9NO_3$ M 143.142

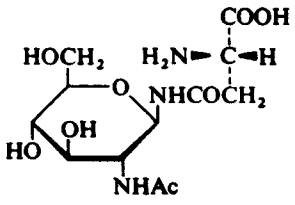
Metab. of *Fusarium graminearum*. Cryst. (MeOH/$CHCl_3$). Mp 140°.

Vesonder, R.F. *et al*, *Phytochemistry*, 1977, **16**, 1296 (*isol*)

***N*-(2-Acetamido-2-deoxy-β-D-glucopyranosyl)-L-asparagine**, 9CI **A-00003**

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

[2776-93-4]



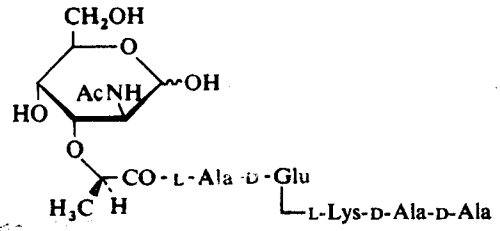
$C_{12}H_{21}N_3O_8$ M 335.313

Found in hydrolysates of glycopeptides/glycoproteins. Needles (EtOH). Mp 255-8° dec. $[\alpha]_D^{22}$ +23.6° (c, 1 in H_2O).

Hydrate: Plates (EtOH aq.). Mp 215-22° 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*)

***N*$^{\alpha}$-[2-(2-Acetamido-3-*O*-D-glucosyl)-D-propionyl-L-alanyl-D-γ-glutamyl]-L-lysyl-D-alanyl-D-alanine** **A-00004**



$C_{31}H_{53}N_7O_{15}$ M 763.798

Cell wall precursor in *Staphylococcus aureus*. Amorph. solid. Mp 148-50° dec. $[\alpha]_D^{25}$ +4° (c, 0.9 in H_2O).

Lanzilotti, A.E. *et al*, *J. Am. Chem. Soc.*, 1964, **86**, 1880 (*synth*)

***S*-Acetamidomethylcysteine** **A-00005**

S-[(*Acetylamino*)*methyl*]*cysteine*, 9CI

[19647-70-2]

$$AcNHCH_2SCH_2CH(NH_2)COOH$$

$C_6H_{12}N_2O_3S$ M 192.232

(S)-form

L-form

Useful *S*-protected deriv. of L-cysteine. $[\alpha]_D^{25}$ −42.5° (c, 1 in H_2O). Stable to CF_3COOH, HBr/AcOH, HCl/EtOH, HF at 0°.

N-tert-*butyloxycarbonyl:* Mp 110-2°. $[\alpha]_D^{25}$ −35.5° (c, 1 in H_2O).

N-*Hydroxysuccinimide ester:* Mp 106-8°. $[\alpha]_D^{25}$ +43° (c, 1 in $CHCl_3$).

Veber, D.F. *et al*, *Tetrahedron Lett.*, 1968, 3057 (*synth*)
Fontana, A. *et al*, *J. Chem. Soc., Chem. Commun.*, 1975, 976 (*use*)
Tomatis, R. *et al*, *Int. J. Pept. Protein Res.*, 1976, **8**, 65, 79, 87.

5-Acetamido-4-oxo-5-hexenamide, 8CI **A-00006**

5-(Acetylamino)-4-oxo-5-hexenamide, 9CI. *Primocarcin*

[3750-26-3]

$$H_2C{=}C(NHAc)COCH_2CH_2CONH_2$$

$C_8H_{12}N_2O_3$ M 184.194

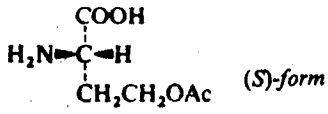
Isol. from *Nocardia fukaya*. Antitumour and antimicrobial antibiotic. Needles (MeOH). Mp 130-1°.

▷MP6475000.

Nagatsu, J. *et al*, *J. Antibiot., Ser. A*, 1962, **15**, 75, 77, 80 (*isol, struct*)
Bowman, R.E. *et al*, *Tetrahedron Lett.*, 1964, 1897 (*synth*)
Bowman, R.E. *et al*, *J. Chem. Soc.*, 1965, 470 (*synth, ir, uv*)

4-Acetoxy-2-aminobutanoic acid A-00007

O-Acetylhomoserine. Homoserine acetate



(*S*)-*form*

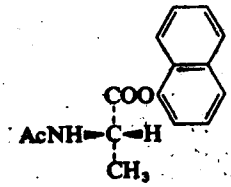
$C_6H_{11}NO_4$ M 161.157

(*S*)-*form* [7540-67-2]
Found in *Pisum sativum* (pea). Mp 200°. $[\alpha]_D^{20}$ +4.5° (c, 4 in H_2O), +3.9° (c, 16.8 in H_2O).

(±)-*form* [6232-10-6]
Found in *P. sativum*. Plates (EtOH). Mp 183-5°.

Grobbelaar, N. *et al*, *Nature (London)*, 1958, **182**, 1358
de Wald, H.A. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 4367.
Grobbelaar, N. *et al*, *Phytochemistry*, 1969, **8**, 553.

N-Acetylalanine 1-naphthyl ester A-00008



$C_{15}H_{15}NO_3$ M 257.288

(*S*)-*form* [69975-68-4]
L-form
Chromogenic substrate for histochemical demonstration of ester proteases. Cryst. (Et_2O). Mp 105°.

Schaller, E. *et al*, *Anal. Biochem.*, 1979, **93**, 251 (*synth, ms*)

N-Acetylcystathionine A-00009

S-(*2-Acetamido-2-carboxyethyl*)*homocysteine*. S-(β-N-*Acetyl-β-carboxyethyl*)*homocysteine*

$HOOCCH(NH_2)CH_2CH_2SCH_2CH(NHAc)COOH$

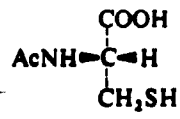
$C_9H_{16}N_2O_5S$ M 264.296

(*S*)-*form* [20619-80-1]
L-form
Urinary amino acid in congenital cystathioninuria.

Perry, T.L. *et al*, *Nature (London)*, 1968, **219**, 178 (*synth*)

N-Acetylcysteine, BAN, USAN A-00010

[616-91-1]



$C_5H_9NO_3S$ M 163.191

▶HA1660000.

(*R*)-*form*
L-form. Airbron. Mucomyst. Respaire
Mucolytic agent. Cryst. (H_2O). Mp 109-10°. $[\alpha]_D$ +5° (c, 3 in H_2O).

(±)-*form*
Cryst. (EtOH). Mp 124.5-125.5°.

Smith, H.A. *et al*, *J. Org. Chem.*, 1961, **26**, 820 (*synth*)
U.S.P., 3 184 505, (*1965*); *CA*, **63**, 7107 (*synth*)
Ohta, G. *et al*, *Chem. Pharm. Bull.*, 1967, **15**, 644 (*synth*)
Martin, T.A. *et al*, *J. Med. Chem.*, 1968, **11**, 625 (*synth*)
Suzuki, N. *et al*, *Bull. Chem. Soc. Jpn.*, 1976, **49**, 3155 (*synth*)

N-Acetylglycine, 9CI A-00011

Acetylaminoacetic acid. Aceturic acid. Acetylglycocoll. Acetamidoacetic acid

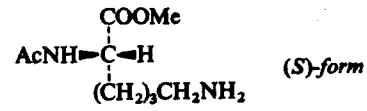
[543-24-8]

$AcNHCH_2COOH$

$C_4H_7NO_3$ M 117.104
Cryst. (H_2O). Mp 206°. pK_a 3.64 (25°).
Me ester: Mp 58-9°. Bp_{712} 254°.
Et ester: Leaflets (Et_2O). Mp 48°. Bp_{712} 260°, Bp_{14} 145°.
Benzyl ester: Mp 51°. Bp_1 175-80°.
Amide: Plates (H_2O). Sol. H_2O, EtOH, insol. Et_2O. Mp 137°.

Org. Synth., Coll. Vol., **2**, 11.
Davies, J.B. *et al*, *J. Chem. Soc., Perkin Trans. 2*, 1973, 1651 (*conformn*)
Mackay, M.F., *Cryst. Struct. Commun.*, 1975, **4**, 225 (*cryst, struct*)
Newmark, R.A. *et al*, *J. Magn. Reson.*, 1976, **21**, 1 (*cmr*)

N^2-Acetyllysine methyl ester, 9CI A-00012



(*S*)-*form*

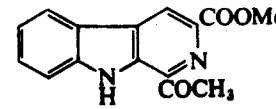
$C_9H_{18}N_2O_3$ M 202.253

(*R*)-*form*
D-form
B,HCl: [20911-99-3]. $[\alpha]_D^{25}$ +22.2° (c, 2.04 in H_2O). Hygroscopic.

(*S*)-*form* [6072-02-2]
L-form
Trypsin substrate. pK_a 10.8.
4-Methylsulphonylanilide; B,HBr: [58045-11-7]. Cryst. + $1H_2O$. Mp 109-11°. $[\alpha]_D^{25}$ −16.9° (c, 0.4 in MeOH).
4-Acetylanilide; B,HBr: [58045-12-8]. Cryst. + $1H_2O$. Mp 177-8°. $[\alpha]_D^{25}$ −21.7° (c, 0.4 in MeOH).

Sherry, S. *et al*, *J. Lab. Clin. Med.*, 1964, **64**, 145 (*synth*)
Sanborn, B.M. *et al*, *Biochemistry*, 1968, **7**, 3616 (*synth*)
Gupta-Bhaya, P., *Biopolymers*, 1975, **14**, 1143 (*pmr*)

1-Acetyl-3-methoxycarbonyl-β-carboline A-00013



$C_{15}H_{12}N_2O_3$ M 268.271
Alkaloid from *Vestia lycioides*. Mp 234-6°.

Faini, F. *et al*, *Phytochemistry*, 1978, **17**, 338 (*isol, uv, ir, pmr, ms, struct, synth*)

N-Acetylphenylalanylphenylalaninol A-00014

α-(*Acetylamino*)-N-[*1-(hydroxymethyl)-2-phenylethyl*]*benzenepropanamide*, 9CI

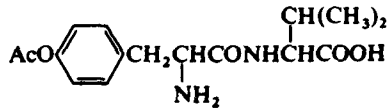
$PhCH_2CH(NHAc)CONHCH(CH_2OH)CH_2Ph$

$C_{20}H_{24}N_2O_3$ M 340.421

L-L-form [57449-34-0]
Metab. of *Emericellopsis salmosynnemata*. Needles (EtOH). $[\alpha]_D^{25}$ −40° (c, 1 in EtOH).

Argoudelis, A.D. *et al*, *J. Antibiot.*, 1975, **28**, 733.

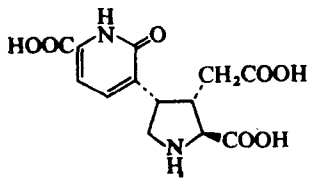
O-Acetyltyrosylvaline A-00015



$C_{16}H_{22}N_2O_5$ M 322.360
Peptide from pig neurohypophysis.
Penders, T.J. *et al*, *Experientia*, 1966, **22**, 722 (*isol, struct*)

Acromelic acid *A* A-00016

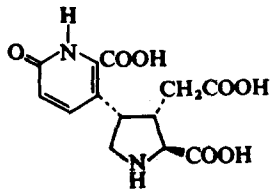
[86630-09-3]



$C_{13}H_{14}N_2O_7$ M 310.263
Isol. from the poisonous fungus *Clitocybe acromegala*.
Konno, K. *et al*, *Tetrahedron Lett.*, 1983, **24**, 939.

Acromelic acid *B* A-00017

[86630-10-6]



Relative configuration

$C_{13}H_{14}N_2O_7$ M 310.263
Isol. from the poisonous fungus *Clitocybe acromegala*.
Konno, K. *et al*, *Tetrahedron Lett.*, 1983, **24**, 939.

Actinine A-00018

*3-Carboxy-*N,N,N*-trimethyl-1-propanaminium hydroxide inner salt*, 9CI. *Tri-*N*-methyl-*γ*-butyrobetaine. 4-Aminobutanoic acid betaine.* γ*-Butyrobetaine*

[407-64-7]

$Me_3N^{\oplus}CH_2CH_2CH_2COO^{\ominus}$

$C_7H_{15}NO_2$ M 145.201
Inner salt. Occurs in the sea-rose *Actinia equina*, in muscles of various snakes and in urine in cases of pernicious anaemia. Isol. from brain tissue. Biosynthetic intermed. in synth. of Carnitine. Plates + $3H_2O$ ($EtOH/Et_2O$ aq.). Sol. EtOH. Dec. at 220°.

▷BP3930000.

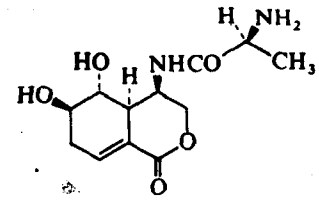
B,HCl: Mp 203°, 214-9°.

Engeland, R., *Ber.*, 1921, **54**, 2212 (*derivs*)
Linneweh, W., *Z. Physiol. Chem.*, 1928, **175**, 95; **176**, 220; 1929, **181**, 48; **182**, 9 (*isol*)
Hosein, E.A. *et al*, *Nature (London)*, 1960, **187**, 321 (*isol*)
Cox, R.A. *et al*, *Biochem. J.*, 1973, **136**, 1083 (*biosynth*)
Anderson, L. *et al*, *Synthesis*, 1981, 468 (*synth*)

Actinobolin A-00019

Actinovorin

[24397-89-5]



$C_{13}H_{20}N_2O_6$ M 300.311
From *Streptomyces griseoviridus* var. *atrofaciens*. Broad spectrum antibiotic. Amorph. powder. Sol. H_2O, EtOH. $[\alpha]_D^{28}$ +59° (c, 0.5 in pH 7 phosphate butter). pK_{a1} 7.5, pK_{a2} 8.8. Unstable in alk. soln.

▷NQ7800000.

B_2,H_2SO_4: [18802-17-0]. Cryst. (EtOH aq.). $[\alpha]_D^{22}$ +54.5° (c, 1 in H_2O).

Ac: Cryst. (EtOH). Mp 263-6° dec. (part. melts at 130° then resolidifies). $[\alpha]_D^{26}$ +58° (c, 1 in H_2O).

N-*Ac:* Needles (EtOH). Mp 254-5°. $[\alpha]_D^{26}$ +30.0° (c, 3.8 in H_2O).

Struck, R.F. *et al*, *Tetrahedron Lett.*, 1967, 1589 (*struct*)
Monk, M.E. *et al*, *J. Am. Chem. Soc.*, 1968, **90**, 1087.
Antosz, F.J. *et al*, *J. Am. Chem. Soc.*, 1970, **92**, 4933 (*abs config*)
Wetherington, J.B. *et al*, *Acta Crystallogr., Sect. B*, 1975, **31**, 501 (*cryst struct*)
v. Dreele, R.B., *Acta Crystallogr., Sect. B*, 1976, **32**, 2853 (*cryst struct*)

Actinocarcin A-00020

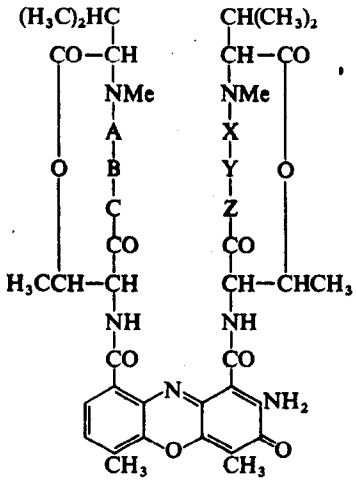
[54990-35-1]
M ca. 11,000
Large peptide. Isol. from *Streptomyces* sp. 3654-JT_1 resembling *S. cinnamomens*. Shows antitumour activity, inhibits the growth of Ehrlich ascites carcinoma. Fluffy solid. $[\alpha]_D^{20}$ −23.4° (c, 1 in H_2O).

Kihara, T. *et al*, *J. Antibiot.*, 1974, **27**, 994; 1976, **29**, 428 (*isol*)

Actinomycin C_2 A-00021

2^A-D-Alloisoleucineactinomycin D, *9Cl. Actinomycin VI*

[2612-14-8]



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

$C_{63}H_{88}N_{12}O_{16}$ M 1269.459

Isol. from *Actinomyces* sp. Biol props. virtually identical with Actinomycin *D*. Red pyramids or prisms (EtOH). Mp 237-9°. $[\alpha]_D$ −325° (c, 0.23 in MeOH).

▷AU1490000.

Brockmann, H. *et al*, *Naturwissenschaften*, 1952, **39**, 429 (*isol*)
Brockmann, H. *et al Tetrahedron Lett.*, 1964, 3517 (*synth*)
Conti, F. *et al*, *Nature (London)*, 1970, **227**, 1239 (*conformn, pmr*)
Lackner, H., *Chem. Ber.*, 1970, **103**, 2476 (*synth, nmr, ms*)
Lackner, H., *Tetrahedron Lett.*, 1970 2807 (*conformn, pmr*)
Meienhofer, J., *J. Am. Chem. Soc.*, 1970, **92**, 3771 (*synth*)

Actinomycin C_{2a} A-00022

2^B-D-Alloisoleucineactinomycin D, *9Cl*

[17914-41-9]

As Actinomycin C_2, A-00021 with

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

$C_{63}H_{88}N_{12}O_{16}$ M 1269.459

Isol. from *Actinomyces* sp. Biol. props. appear to be similar to those of Actinomycin C_2. Mp 233-5°. $[\alpha]_D^{18}$ −297° (c, 0.267 in MeOH).

Brockmann, H. *et al*, *Naturwissenschaften*, 1960, **47**, 15 (*isol, struct*)
Brockmann, H. *et al*, *Chem. Ber*, 1968, **101**, 1312, 2231 (*synth, uv, nmr*)

Actinomycin C_3 A-00023

2^A-D-Alloisoleucine-2^B-D-alloisoleucineactinomycin D, *9Cl. Actinomycin VII*

[6156-47-4]

As Actinomycin C_2, A-00021 with

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

$C_{64}H_{90}N_{12}O_{16}$ M 1283.486

Isol from *Actinomyces* sp. Similar biol. activity to Actinomycin *D*. Red hexagonal bipyramids (EtOAc). Mp 235° dec. $[\alpha]_D^{17}$ −328° (c, 0.5 in EtOH).

▷AU1577500.

Brockmann, H. *et al*, *Angew. Chem.*, 1956, **68**, 70 (*isol, struct*)
Bachmann, H.G. *et al*, *Nature (London)*, 1964, **201**, 261 (*cryst struct*)
Brockmann, H. *et al*, *Chem. Ber.*, 1967, **100**, 353; 1968, **101**, 1312, 2231 (*synth, uv, nmr*)

Actinomycin *D*, 9Cl, 8Cl A-00024

Actinomycin C_1. *Dactinomycin*

[50-76-0]

As Actinomycin C_2, A-00021 with

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

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

Isol. from *Actinomyces* spp. Antibiotic active against gram-positive bacteria and tumours. Red rhomboids $+3H_2O$ (EtOH). Mp 241.5-243° dec. $[\alpha]_D^{28}$ −315° (c, 0.25 in MeOH).

▷AU1575000.

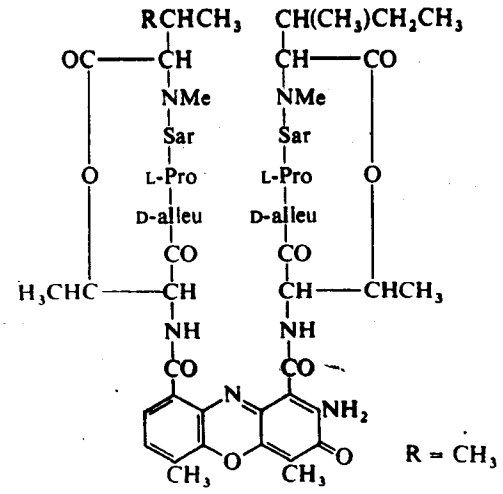
Di-Me ester; B,HCl: Mp 251-3°. $[\alpha]_D^{20}$ −130° ($CHCl_3$)

▷Exp. carcinogen and teratogen

Bullock, E. *et al*, *J. Chem. Soc.*, 1957, 3280 (*struct, uv*)
Brockmann, H. *et al*, *Naturwissenschaften*, 1964, **51**, 382, 384 (*synth*)
Meienhofer, J., *J Am. Chem. Soc.*, 1970, **92**, 3771 (*synth*)
Lackner, H., *Chem. Ber.*, 1971, **104**, 3653 (*synth, ir, ms, nmr*)
Lackner, H., *Tetrahedron Lett.*, 1971, 2221 (*struct, pmr, conformn*)
Hollstein, U. *et al*, *J. Am. Chem. Soc.*, 1974, **96**, 8036 (*cmr, struct*)
Nakajima, K. *et al*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 3237 (*synth*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th Ed., Van Nostrand-Reinhold, 1979, 343.

Actinomycin E_1 A-00025

[1402-41-1]



$C_{64}H_{96}N_{12}O_{16}$ M 1289.533

Obt. when DL-isoleucine is included in the medium in which *Streptomyces antibioticus* is grown. Shows antibacterial and antitumour activity.

▷AU1631000.

Günther, H. *et al*, *Naturwissenschaften*, 1956, **43**, 131 (*isol*)
Brockmann, H. *et al*, *Angew. Chem.*, 1960, **72**, 939 (*rev, struct*)
Kuznetsova, V.S. *et al*, *Antibiotiki* (*Moscow*), 1971, **16**, 18; *CA*, **74**, 75151 (*biosynth*)

Actinomycin E_2 A-00026

[1402-42-2]

As Actinomycin E_1, A-00025 with

R = CH_2CH_3

$C_{65}H_{98}N_{12}O_{16}$ M 1303.560

Obt. when DL-isoleucine is included in the medium in which *Streptomyces antibioticus* is grown. Shows antibacterial and antitumour activity.

▷AU1578500.

Günther, H. *et al*, *Naturwissenschaften*, 1956, **43**, 131 (*isol*)
Brockmann, H. *et al*, *Angew. Chem.*, 1960, **72**, 945 (*rev, struct*)
Kuznetsova, V.S. *et al*, *Antibiotiki* (*Moscow*), 1971, **16**, 18; *CA*, **74**, 75151 (*biosynth*)

Actinomycin F_1 A-00027

As Actinomycin C_2, A-00021 with

A = X = Sar
B = Y = Sar
C = D-Val
Z = D-alloisoleucine

$C_{58}H_{88}N_{12}O_{16}$ M 1209.404

Isol. from *Actinomyces* sp.

Günther, H. *et al*, *Naturwissenschaften*, 1956, **43**, 131 (*isol*)
Brockmann, H. *et al*, *Angew. Chem.*, 1960, **72**, 939 (*rev, struct*)

Actinomycin F_2 A-00028

As Actinomycin C_2, A-00021 with

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

$C_{60}H_{90}N_{12}O_{16}$ M 1235.442

Isol. from *Actinomyces* spp.

Günther, H. *et al*, *Naturwissenschaften*, 1956, **43**, 131 (*isol*)
Brockmann, H. *et al*, *Angew. Chem.*, 1960, **72**, 939 (*rev, struct*)

Actinomycin F_3 A-00029

[1402-46-6]

As Actinomycin C_2, A-00021 with

A = X = Sar
B = Y = Sar
C = Z = D-alloisoleucine

$C_{59}H_{90}N_{12}O_{16}$ M 1223.431

Isol. from *Actinomyces* spp.

▷AU1578000.

Günther, H. *et al*, *Naturwissenschaften*, 1956, **43**, 131 (*isol*)
Brockmann, H. *et al*, *Angew. Chem.*, 1960, **72**, 939 (*rev, struct*)

Actinomycin F_4 A-00030

As Actinomycin C_2, A-00021 with

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

$C_{61}H_{92}N_{12}O_{16}$ M 1249.469

Isol. from *Actinomyces* sp.

Günther, H. *et al*, *Naturwissenschaften*, 1956, **43**, 131 (*isol*)
Brockmann, H. *et al*, *Angew. Chem.*, 1960, **72**, 939 (*rev, struct*)

Actinomycin F_8 A-00031

3^A-(N-*Methylglycine*)-3^B-(N-*methylglycine*)*actinomycin* D, *9CI*. *Actinomycin II*. A_{II}

[2646-41-5]

As Actinomycin C_2, A-00021 with

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

$C_{57}H_{86}N_{12}O_{16}$ M 1195.377

Prod. by *Streptomyces antibioticus*. Plates (Me_2CO/CS_2). Mp 215-6°. $[\alpha]_D^{17}$ −157° (c, 0.24 in $CHCl_3$).

▷AU1620000.

Johnson, A.W. *et al*, *Biochem. J.*, 1959, **73**, 535 (*isol, struct*)
Brockmann, H. *et al*, *Angew. Chem.*, 1960, **72**, 939 (*rev, struct*)
Goss, W.A. *et al*, *Antibiot. Chemother.* (*Washington, D.C.*), 1960, **10**, 221 (*biosynth*)
Devan, M.L. *et al*, *Antibiotiki* (*Moscow*), 1974, **19**, 1023; *CA*, **82**, 94446

Actinomycin F_9 A-00032

Actinomycin III. A_{III}. *Actinomycin* X_{O_7}

As Actinomycin C_2, A-00021 with

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

$C_{60}H_{84}N_{12}O_{16}$ M 1229.394

Prod. by *Streptomyces antibioticus*. Prisms. Mp 237-8°. $[\alpha]_D^{19}$ −205° (c, 0.22 in $CHCl_3$).

Johnson, A.W. *et al*, *Biochem. J.*, 1959, **73**, 535 (*isol, struct*)
Brockmann, H. *et al*, *Angew. Chem.*, 1960, **72**, 939 (*rev, struct*)

Actinomycin K_{1c} A-00033

3^A(*or* 3^B)-(cis-*4-Methyl-L-proline*)*actinomycin* D, *9CI*

[64078-99-5]

As Actinomycin C_2, A-00021 with

A = X = Sar
B = Pro
Y = *cis*-4-Me-L-Pro
C = Z = D-Val

$C_{63}H_{90}N_{12}O_{16}$ M 1271.475

Isol. from *Streptomyces parvulus*. Antibiotic.

Katz, E. *et al*, *Antimicrob. Agents Chemother.*, 1977, **11**, 1056 (*isol*)

Actinomycin K_{1t} A-00034

3^A(*or* 3^B)-(trans-*4-Methyl-L-proline*)*actinomycin* D, *9CI*

[64091-35-6]

As Actinomycin C_2, A-00021 with

A = X = Sar
B = Pro
Y = *trans*-4-Me-L-Pro
C = Z = D-Val

$C_{63}H_{88}N_{12}O_{16}$ M 1269.459

Isol. from *Streptomyces parvulus*. Shows antibiotic props.

Katz, E. *et al*, *Antimicrob. Agents Chemother.*, 1977, **11**, 1056 (*isol*)

Actinomycin K_{2c} A-00035

3^A-(cis-4-Methyl-L-proline)-3^B-(cis-4-methyl-L-proline)actinomycin D, *9CI*

[64085-85-4]

As Actinomycin C_2, A-00021 with

A = X = Sar
B = Y = *cis*-4-Me-L-Pro
C = Z = D-Val

$C_{64}H_{90}N_{12}O_{16}$ M 1283.486

Isol. from *Streptomyces parvulus*. Antibiotic.

Katz, E. *et al*, *Antimicrob. Agents Chemother.*, 1977, **11**, 1056 (*isol*)

Actinomycin K_{2t} A-00036

3^A-(trans-4-Methyl-L-proline)-3^B-(trans-4-methyl-L-proline)actinomycin D, *9CI*

[64161-90-6]

As Actinomycin C_2, A-00021 with

A = X = Sar
B = Y = *trans*-4-Me-L-Pro
C = Z = D-Val

$C_{64}H_{90}N_{12}O_{16}$ M 1283.486

Isol. from *Streptomyces parvulus*. Antibiotic.

Katz, E. *et al*, *Antimicrob. Agents Chemother.*, 1977, **11**, 1056 (*isol*)

Actinomycin $X_{O\beta}$ A-00037

Actinomycin I

[1402-60-4]

As Actinomycin C_2, A-00021 with

A = X = Sar
B = L-Pro
Y = L-4-Hydroxyproline
C = Z = D-Val

$C_{62}H_{88}N_{12}O_{17}$ M 1273.447

Isol. from *Actinomyces* sp. Yellow ($CHCl_3$/pet. ether). Mp 245-7°. $[\alpha]_D^{22}$ −308° (c, 0.2 in MeOH).

Mono-Ac: Mp 242-3°. $[\alpha]_D^{21}$ −283° (c, 0.2 in MeOH).

Monohexadecanoyl: Mp 200-1°. $[\alpha]_D^{22}$ −238° (c, 0.2 in MeOH).

Brockmann, H. *et al*, *Chem. Ber.*, 1959, **92**, 1249; 1960, **93**, 2971 (*isol, struct*)

Brockmann, H. *et al*, *Naturwissenschaften*, 1960, **47**, 62 (*struct*)

Devan, M.L. *et al*, *Antibiotiki* (*Moscow*), 1974, **19**, 1023

Actinomycin $X_{O\delta}$ A-00038

As Actinomycin C_2, A-00021 with

A = X = Sar
B = L-Pro
Y = L-*allo*-4-Hydroxyproline
C = Z = D-Val

$C_{62}H_{88}N_{12}O_{17}$ M 1273.447

Semisynthetic antibiotic produced by redn. of Actinomycin X_2, A-00040. Red prisms ($CHCl_3$/pet. ether). Mp 245-6°. $[\alpha]_D^{20}$ −297° (c, 0.2 in MeOH).

Mono-Ac: Mp 249-50°. $[\alpha]_D^{18}$ −310° (c, 0.2 in MeOH).

Monohexadecanoyl: Mp 200-1°. $[\alpha]_D^{21}$ −256° (c, 0.2 in MeOH).

Brockmann, H. *et al*, *Chem. Ber.*, 1960, **93**, 2971 (*isol, struct*)

Actinomycin X_{1a} A-00039

As Actinomycin C_2, A-00021 with

A = X = Sar
B = Sar
Y = L-4-Oxoproline
C = Z = D-Val

$C_{60}H_{82}N_{12}O_{17}$ M 1243.378

Minor antibiotic from *Streptomyces* sp. Red cryst. Mp 246-7° dec. $[\alpha]_D^{22}$ −418° (c, 0.10 in Me_2CO).

Brockmann, H. *et al*, *Chem. Ber.*, 1954, **87**, 1036; 1960, **93**, 2971 (*isol, struct*)

Actinomycin X_2 A-00040

Actinomycin V

[1402-61-5]

As Actinomycin C_2, A-00021 with

A = X = Sar
B = L-Pro
Y = L-4-Oxoproline
C = Z = D-Val

$C_{62}H_{86}N_{12}O_{17}$ M 1271.432

Isol. from *Streptomyces* spp. Cryst. (pet. ether). Mp 249.5-250.5°. $[\alpha]_D^{24}$ −359° (c, 0.2 in MeOH). Redn. affords Actinomycin *D*, A-00024.

▷AU2010000.

Brockmann, H. *et al*, *Chem. Ber.*, 1960, **93**, 2971 (*isol, struct*)

Brockmann, H. *et al*, *Naturwissenchaften*, 1960, **47**, 62 (*struct*)

Actinomycin Pip 1α A-00041

As Actinomycin C_2, A-00021 with

A = X = Sar
B,Y = L-4-Oxopipecolic acid and L-Pipecolic acid
C = Z = D-Val

$C_{64}H_{90}N_{12}O_{17}$ M 1299.485

Isol. from *Streptomyces antibioticus* when grown with L-Pipecolic acid in the culture medium. Mp 232-5°. $[\alpha]_D$ −100° (c, 0.3 in MeOH).

Formica, J.V. *et al*, *J. Bacteriol.*, 1968, **95**, 2139 (*isol*)

Formica, J.V. *et al*, *J. Biol. Chem.*, 1973, **248**, 2066 (*struct*)

Actinomycin Pip 1β A-00042

As Actinomycin C_2, A-00021 with

A = X = Sar
B,Y = L-Pro and L-Pipecolic acid

C = Z = D-Val

$C_{63}H_{88}N_{12}O_{16}$ M 1269.459
Isol. from *Streptomyces antibioticus* grown in culture medium containing L-Pipecolic acid. Mp 230-2°. $[\alpha]_D$ −241° (c, 0.3 in MeOH).

Formica, J.V. *et al*, *J. Bacteriol.*, 1968, **95**, 2139 (*isol*)
Formica, J.V. *et al*, *J. Biol. Chem.*, 1973, **248**, 2066 (*struct*)

Actinomycin Pip 2 A-00043

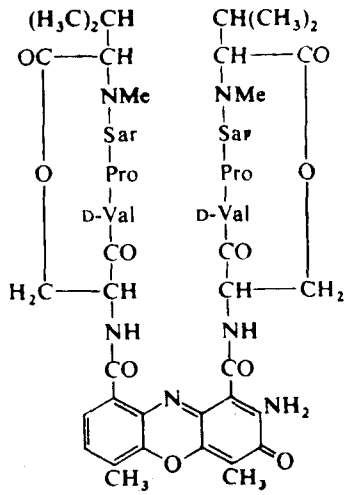
As Actinomycin C_2, A-00021 with

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

$C_{64}H_{90}N_{12}O_{16}$ M 1283.486
Obt. from *Streptomyces antibioticus* grown in culture medium contg. L-Pipecolic acid. Mp 218-20°. $[\alpha]_D$ −56° (c, 0.3 in MeOH).

Formica, J.V. *et al*, *J. Bacteriol.*, 1968, **95**, 2139 (*isol*)
Formica, J.V. *et al*, *J. Biol. Chem.*, 1973, **248**, 2066 (*struct*)

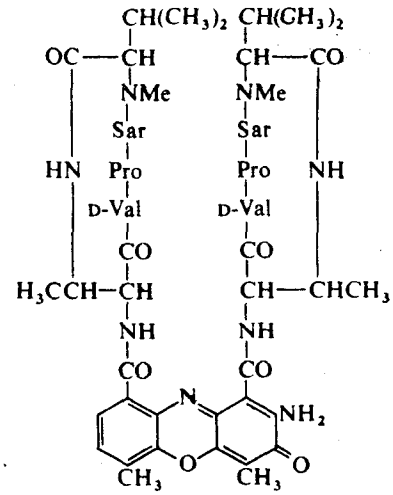
Actinomycin (Ser-D-Val-Pro-Sar-MeVal) A-00044



$C_{60}H_{82}N_{12}O_{16}$ M 1227.379
Synthetic actinomycin. Antibiotic. Red cryst. (EtOAc/C_6H_6). Mp 269-73° dec. $[\alpha]_D^{21}$ −435° (c, 0.25 in MeOH).

Brockmann, H. *et al*, *Tetrahedron Lett.*, 1964, 3523 (*synth*)

Actinomycin (Dbu-D-Val-Pro-Sar-MeVal) A-00045

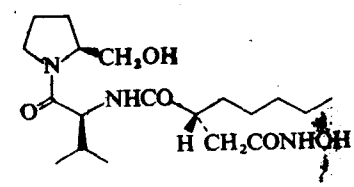


$C_{62}H_{88}N_{14}O_{14}$ M 1253.463
Totally synthetic antibiotic. Shows moderate antibacterial and antitumour activity.

Atherton, E. *et al*, *J. Med. Chem.*, 1973, **16**, 355 (*synth*)

Actinonin A-00046

[13434-13-4]



$C_{19}H_{35}N_3O_5$ M 385.503
Peptide-type antibiotic. Isol. from *Streptomyces roseoposullatus*. Shows broad spectrum activity. Microprisms (MeOH/Et_2O). Mp 148°. $[\alpha]_D^{22}$ −48° (c, 1.0 in MeOH). pK_a 9.32.

▷RG9900700.

Gordon, J.J. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1975, 819 (*struct*)
Anderson, N.M. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1975, 825, 852 (*synth, ms*)
Broughton, B.J. *et al*, *J. Chem. Soc., Perkin Trans. 1*, 1975, 857 (*props*)

Actinotiocin A-00047

[39454-49-4]

Struct. unknown

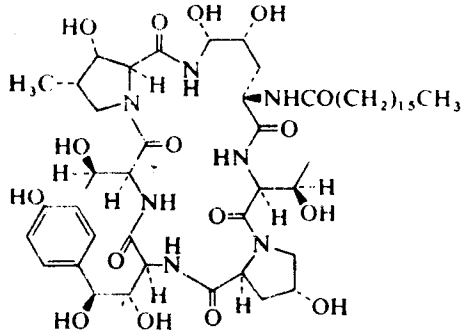
$C_{69}H_{53}N_{13}O_{10}S_5$ M 1144.339
Peptide-type antibiotic. Isol. from *Actinomadura purilla*. Active against gram-positive bacteria and mycobacteria. Mp 247-9°. $[\alpha]_D^{20}$ +164° (c, 0.77 in dioxan).

▷AU2363000.

Tamura, A. *et al*, *J. Antibiot.*, 1973, **26**, 343 (*isol*)
Japan. Pat., 78 18 596, (*1978*); *CA*, **89**, 145011b (*isol*)

Aculeacin *A* **A-00048**

[58814-86-1]



$C_{51}H_{83}N_7O_{16}$ M 1050.254

Cyclic peptide antibiotic. Isol. from *Aspergillus aculeatus*. Active against fungi and yeasts. Amorph. powder. Mp 162-6°. $[\alpha]_D^{24}$ −54° (c, 1 in MeOH).

▷AU2980000.

Mizuno, K. *et al*, *J. Antibiot.*, 1977, **30**, 297 (*isol, props*)
Satoi, S. *et al*, *J. Antibiot.*, 1977, **30**, 303 (*struct*)
Can. Pat., 1 041 446, (*1978*); *CA*, **90**, 101942x (*manuf*)

Aculeacin *B* **A-00049**

[58814-87-2]

Isol. from *Aspergillus aculeatus*. Antibiotic. Amorph. powder. Mp 148-51°. $[\alpha]_D^{24}$ −45° (c, 1 in MeOH).

▷AU3030000.

Japan. Pat., 76 98 387, (*1976*); *CA*, **86**, 15206w (*isol*)
Mizuno, K. *et al*, *J. Antibiot.*, 1977, **30**, 297 (*isol, props*)
Can. Pat., 1 041 446, (*1978*); *CA*, **90**, 101942x (*manuf*)

Aculeacin *C* **A-00050**

[58814-88-3]

Isol. from *Aspergillus aculeatus*. Antibiotic. Amorph. powder. Mp 164-8°. $[\alpha]_D^{24}$ −47.5° (c, 1 in MeOH).

▷AU3050000.

Japan. Pat., 76 98 387, (*1976*); *CA*, **86**, 15206w (*isol*)
Mizuno, K. *et al*, *J. Antibiot.*, 1977, **30**, 297 (*isol, props*)
Satoi, S. *et al*, *J. Antibiot.*, 1977, **30**, 303 (*props*)
Can. Pat., 1 041 446, (*1978*); *CA*, **90**, 101942s (*manuf*)

Aculeacin *D* **A-00051**

[58814-89-4]

Isol. from *Aspergillus aculeatus*. Antibiotic. Mp 159-62°. $[\alpha]_D^{24}$ −46° (c, 1 in MeOH).

▷AU3070000.

Japan. Pat., 76 98 387, (*1976*); *CA*, **86**, 15206w (*isol*)
Mizuno, K. *et al*, *J. Antibiot.*, 1977, **30**, 297 (*isol, props*)
Satoi, S. *et al*, *J. Antibiot.*, 1977, **30**, 303 (*props*)
Can. Pat., 1 041 446, (*1978*); *CA*, **90**, 101942x (*manuf*)

Aculeacin *E* **A-00052**

[58814-90-7]

Isol. from *Aspergillus aculeatus*. Antibiotic. Amorph. powder. Mp 186-91°. $[\alpha]_D^{24}$ −66° (c, 1 in MeOH).

Japan. Pat., 76 95 387, (*1976*); *CA*, **86**, 15206w (*isol*)
Mizuno, K. *et al*, *J. Antibiot.*, 1977, **30**, 297 (*isol, props*)
Satoi, S. *et al*, *J. Antibiot.*, 1977, **30**, 303 (*props*)
Can. Pat., 1 041 446, (*1978*); *CA*, **90**, 101942x (*manuf*)

Aculeacin *F* **A-00053**

[58814-91-8]

Isol. from *Aspergillus aculeatus*. Amorph. powder. Mp 163-7°. $[\alpha]_D^{24}$ −55° (c, 1 in MeOH).

Japan. Pat., 76 98 387, (*1976*); *CA*, **86**, 15206w (*isol*)
Mizuno, K. *et al*, *J. Antibiot.*, 1977, **30**, 297 (*isol, props*)
Satoi, S. *et al*, *J. Antibiot.*, 1977, **30**, 303 (*props*)
Can. Pat., 1 041 446, (*1978*); *CA*, **90**, 101942x (*manuf*)

Aculeacin *G* **A-00054**

[58814-92-9]

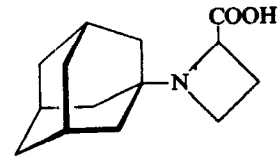
Isol. from *Aspergillus aculeatus*. Antibiotic. Mp 166-70°. $[\alpha]_D^{24}$ −52° (c, 1 in MeOH).

Japan. Pat., 76 98 387, (*1976*); *CA*, **86**, 15206w (*isol*)
Mizuno, K. *et al*, *J. Antibiot.*, 1977, **30**, 297 (*isol, props*)
Satoi, S. *et al*, *J. Antibiot.*, 1977, **30**, 303 (*props*)
Can. Pat., 1 041 446, (*1978*); *CA*, **90**, 101942x (*manuf*)

1-(1-Adamantyl)-2-azetidinecarboxylic acid **A-00055**

1-Tricyclo[3.3.1.1^{3,7}]dec-1-yl-2-azetidinecarboxylic acid, *9CI*. *Carmantadine*, *USAN*

[38081-67-3]



$C_{14}H_{21}NO_2$ M 235.325

(±)-*form*

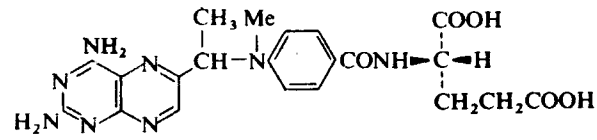
Antiparkinsonian drug.

Ger. Pat., 2 156 499, (*1972*); *CA*, **77**, 88330f (*synth, pharmacol*)

Adenopterin **A-00056**

N-[4-[[1-(2,4-Diamino-6-pteridinyl)ethyl]methylamino]benzoyl]-L-glutamic acid, *9CI*. *4-Amino-9,10-dimethylpteroylglutamic acid*

[25663-23-4]



$C_{21}H_{24}N_8O_5$ M 468.471

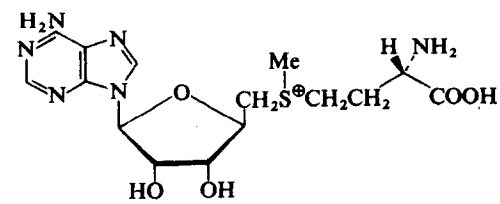
Folic acid antagonist. Yellow-orange microcryst. ppt.

Hultquist, M.E. *et al*, *J. Am. Chem. Soc.*, 1949, **71**, 619 (*synth*)

***S*-Adenosylmethionine** **A-00057**

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.

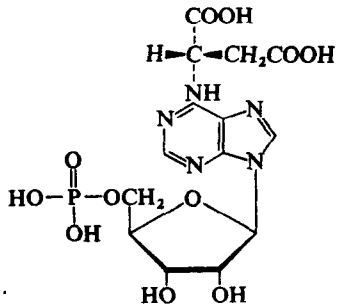
▷AU7334000.

Cantoni, G.L., *J. Am. Chem. Soc.*, 1952, **74**, 2942 (*isol*)
Baddiley, J. *et al*, *J. Chem. Soc.*, 1953, 2662 (*struct*)
Cantoni, G.L., *J. Biol. Chem.*, 1953, **204**, 403 (*struct*)
Baddiley, J. *et al*, *J. Chem. Soc.*, 1954, 4280; 1955, 1085 (*synth*)
de la Haba, G. *et al*, *J. Am. Chem. Soc.*, 1959, **81**, 3975 (*synth, resoln*)
Follmann, H. *et al*, *Eur. J. Biochem.*, 1975, **58**, 31 (*uv, cd*)
Cornforth, J.W. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 7292 (*abs config*)
Minch, M.J. *et al*, *J. Am. Chem. Soc.*, 1981, **103**, 6015 (*nmr*)

Adenylosuccinic acid A-00058

N-[9-(5-O-*Phosphono*-β-D-*ribofuranosyl*)-9H-*purin*-6-*yl*]-L-*aspartic acid*, 9CI. N-(9-β-D-*Ribofuranosyl*-9H-*purin*-6-*yl*)-L-*aspartic acid* 5'-(*dihydrogen phosphate*), 8CI

[19046-78-7]



$C_{14}H_{18}N_5O_{11}P$ M 463.297

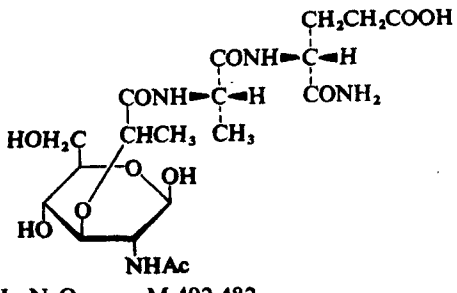
Found with adenosinesuccinic acid in the mycelium of *Penicillium chrysogenum* and in *Fusarium nivale*. Intermed. in the formn. of adenylic acid. $[\alpha]_D^{25}$ −3.4° (c, 1.04 in H_2O at pH 7). The diastereoisomer from D-aspartic acid has $[\alpha]_D^{25}$ −77.3° (c, 1.15 in H_2O at pH 7).

Lieberman, I., *J. Biol. Chem.*, 1956, **223**, 327.
Ballio, A. *et al*, *Arch. Biochem. Biophys.*, 1963, **101**, 311.
Mansurova, S.E. *et al*, *Biokhimiya*, 1966, **31**, 1057.
Ballio, A. *et al*, *Ann. Ist. Super. Sanita*, 1967, **3**, 149; *CA*, **68**, 59824d (*synth*)
Van der Weyden, M.B. *et al*, *J. Biol. Chem.*, 1974, **249**, 7282.

Adjuvant peptide A-00059

N^2-[N-(N-*Acetylmuramoyl*)-L-*alanyl*-D-α-*glutamine*, 9CI. N-*Acetylmuramyl*-L-*alanyl*-D-*isoglutamine*. *Muramyl dipeptide*. *MDP*

[53678-77-6]



$C_{19}H_{32}N_4O_{11}$ M 492.482

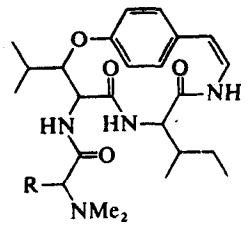
Identified as the minimum structural constit. of the mycobacterial cell wall component of Freund's complete adjuvant which is necessary for adjuvant activity. It and many of its analogues have been investigated as adjuvants in the immunisation of animals. $[\alpha]_D^{25}$ +44° (c, 1 in AcOH).

Lefrancier, P. *et al*, *Int. J. Pept. Protein Res.*, 1977, **9**, 249; 1978, **11**, 289 (*synth*)
Nebelin, E. *et al*, *FEBS Lett*, 1979, **107**, 254 (*ms*)
Lefrancier, P., *Fortschr. Chem. Org. Naturst.*, 1981, **40**, 1 (*rev*)
Chapman, B.E. *et al*, *Aust. J. Chem.*, 1982, **35**, 489 (*pmr*)

Adouétine X A-00060

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

[19542-37-1]



R = $CH_2CH(CH_3)_2$

$C_{28}H_{44}N_4O_4$ M 500.680

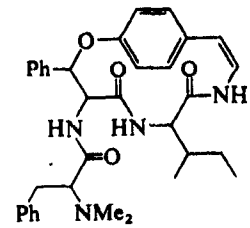
Alkaloid from *Waltheria americana*, the root bark of *Ceanothus americanus* and *Zizyphus jujuba*, and the leaves of *Alphitonia macrocarpa*. Needles (MeOH or CH_2Cl_2/EtOAc). Mp 279-280.5°. $[\alpha]_D^{25}$ −370° (c, 0.205 in $CHCl_3$).

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

Adouétine Y A-00061

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

[19542-38-2]



$C_{34}H_{40}N_4O_4$ M 568.714

Alkaloid from *Waltheria americana* and the root bark of *Ceanothus americanus*. Cryst. (MeOH or $CHCl_3$/Et_2O). Mp 292°. $[\alpha]_D$ −230° ($CHCl_3$/MeOH 9:1).

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

Adouétine Y' A-00062

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

[19542-39-3]
As Adouétine *X*, A-00060 with

$$R = —CH_2Ph$$

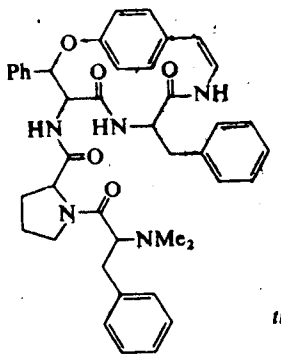
$C_{31}H_{42}N_4O_4$ M 534.697
Alkaloid from *Waltheria americana*, the leaves of *Myrianthus arboreus* and *Melochia corchorifolia*, the roots of *Discaria longispina* and the root bark of *Ceanothus sanguineus*. Mp 289-290.5°, 295-7°, 302° dec. $[\alpha]_D$ −294°, −305°, −390° ($CHCl_3$).

N-De-Me: [73045-49-5]. *N-Demethyladouétine Y'. 5-sec-Butyl-8-N-(N-methylphenylalanyl)-9-isopropylphencyclopeptine.* Alkaloid from the root bark of *C. sanguineus*. Mp 229°. Opt. rotn. not recorded.

Marchand, J. *et al*, *Ann. Pharm. Fr.*, 1968, **26**, 771; *CA*, **71**, 42203q (*isol*)
Pais, M. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 1145 (*uv, ir, pmr, ms, struct*)
Tschesche, R. *et al*, *Tetrahedron Lett.*, 1968, 3817 (*isol, ms*)
Merkuza, V.M. *et al*, *Phytochemistry*, 1974, **13**, 1279 (*ir, ms*)
Lagarias, J.C. *et al*, *J. Nat. Prod.*, 1979, **42**, 663 (*isol, ms, deriv*)

Adouétine *Z* A-00063

N,N-Dimethyl-L-phenylalanyl-N-[5,8-dioxo-3-phenyl-7-(phenylmethyl)-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]-L-prolinamide, *9CI. N-Methylferetine*
[19542-40-6]



trans-form

$C_{42}H_{45}N_5O_5$ M 699.848
Isol. as a mixt. of *E*- and *Z*-isomers. Alkaloid from *Waltheria americana*, and from the leaves of *Feretia apodanthera* and *Melochia pyramidata*. Cryst. (cyclohexane). Mp 135-40°, 140-5°. $[\alpha]_D$ −184° (c, 1 in $CHCl_3$).

▷TW3577000.

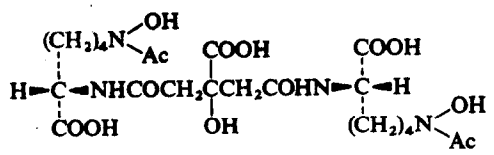
Dihydro: Cryst. (Me_2CO/hexane). Mp 221°. $[\alpha]_D$ −87° ($CHCl_3$).

N-De-Me: [56031-09-5]. *Feretine. N-Demethyladouétine Z.* Alkaloid from the leaves of *F. apodanthera*. Cryst. (cyclohexane). Mp 123°. $[\alpha]_D$ −139° (c, 1 in $CHCl_3$).

Pais, M. *et al*, *Ann. Pharm. Fr.*, 1963, **21**, 139 (*isol, ir, pmr*)
Pais, M. *et al*, *Bull. Soc. Chim. Fr.*, 1968, 1145 (*uv, ir, pmr, ms, struct*)
Bailleul, F. *et al*, *C.R. Hebd. Seances Acad. Sci.*, 1974, **279**, 949 (*uv, ir, pmr, ms; Feretine*)
Medina, E. *et al*, *Justus Liebigs Ann. Chem.*, 1981, 538 (*isol, ir, cmr, ms*)

Aerobactin A-00064

3,12,21-Trihydroxy-2,10,14,22-tetraoxo-3,9,15,21-tetraazatricosane-8,12,16-tricarboxylic acid, *9CI. $N^2,N^{2'}$-(3-Carboxy-3-hydroxyglutaroyl)bis[N^6-acetyl-N^6-hydroxylysine]*, *8CI*
[26198-65-2]

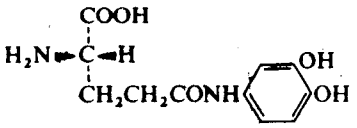


$C_{22}H_{36}N_4O_{13}$ M 564.545
Isol. from cultures of *Aerobacter aerogenes* 62-1. Microbial iron chelator. Hygroscopic sl. off-white powder. $[\alpha]_D^{22}$ −10.8° (c, 1.7 in H_2O).

Gibson, F. *et al*, *Biochim. Biophys. Acta*, 1969, **192**, 175 (*isol*)
Maurer, P.J. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 3096 (*synth*)

Agaridoxin A-00065

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

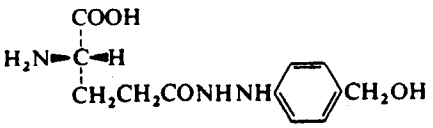


$C_{11}H_{14}N_2O_5$ M 254.242
(S)-form
L-form
Constit. of *Agaricus campestris*. Grey-white powder (MeOH aq.). Darkens in air. Mp 220-1°.

Szent-Gyorgyi, A., *J. Org. Chem.*, 1976, **41**, 1603 (*synth*)

Agaritine A-00066

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



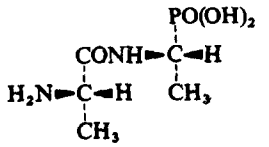
$C_{12}H_{17}N_3O_4$ M 267.284
▷MA1284000.
(S)-form
L-form
Constit. of some members of the family *Agaricaceae*, notably *Agaricus bisporus*. Cryst. (EtOH/butanol). Mp 205-9°. $[\alpha]_D^{25}$ +7° (c, 0.8 in H_2O). pK_{a1} 3.4, pK_{a2} 8.86 (H_2O).

Daniels, E.G. *et al*, *J. Org. Chem.*, 1962, **23**, 3229 (*isol, synth*)
Levenberg, B., *J. Biol. Chem.*, 1964, **239**, 2267 (*isol, struct*)

Alafosfalin A-00067

[1-[2-Amino-1-oxopropyl)amino)ethyl]phosphonic acid, 9CI. 1-(Alaninamido)ethylphosphonic acid

[60668-24-8]



Absolute configuration

$C_5H_{13}N_2O_4P$ M 196.142

Antibiotic.

Ger. Pat., 2 602 193, (*1976*); *CA*, **85**, 143525r (*synth*)
Belg. Pat., 844 377, (*1977*); *CA*, **88**, 7368b (*synth*)
Allen, J.G. *et al*, *Nature (London)*, 1978, **272**, 56 (*use*)
Ger. Pat., 2 730 549, (*1978*); *CA*, **88**, 191494p (*use*)
Atherton, F.R. *et al*, *Antimicrob. Agents Chemother.*, 1979, **15**, 677 (*synth, use*)
Hahn, F.E., *Naturwissenschaften*, 1981, **68**, 90 (*rev, bibl*)

Alamethicin A-00068

[27061-78-5]

Ac-Aib-Pro-Aib-Ala-Aib-Ala-Gln-Aib-Val-Aib-Gly-Leu-Aib-Pro-Val-Aib-Aib-Glu(OH)-Gln-Phol

$C_{92}H_{150}N_{22}O_{25}$ M 1964.329

Struct. shown is that of Alamethicin I. Alamethicin II is closely related with Aib replacing Ala in one residue.

Alamethicin I [59588-86-2]

Alamethicin F30

Peptide antibiot. from *Trichoderma viridis* which has the ability to transport cations through biological and artifical lipid membranes. Like Gramicidin *A* it functions by forming pores or channels in the membrane. Causes haemolysis of erythrocytes. Cryst. (MeOH). Mp 259-60°, 275-9°. $[\alpha]_D^{22}$ −45° (c, 1.2 in EtOH). pK_a 6.04 (EtOH aq.). There is also a minor component, Alamethicin F50.

▷AY1900000.

Ac: [64918-47-4]. Cryst. ($MeOH/Et_2O$). Mp 175-80°.

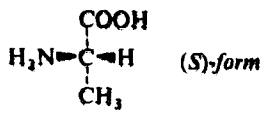
Me ester: [64918-62-3]. Cryst. ($CHCl_3/Et_2O$). Mp 240-2°, 275-6°.

Me ester, Ac: [64936-53-4]. Cryst. (MeOH aq.). Mp 145-50°.

Ovchinnikov, Y.A. *et al*, *J. Gen. Chem. USSR (Engl. Transl.)*, 1971, **41**, 2105 (*isol, ms*)
Burgess, A.W. *et al*, *Biopolymers*, 1973, **12**, 2691 (*conformn*)
Martin, D.R. *et al*, *Biochem. Soc. Trans.*, 1975, **3**, 166 (*use*)
Martin, D.R. *et al*, *Biochem. J.*, 1976, **153**, 181 (*pmr*)
Pandey, R.C. *et al*, *J. Am. Chem. Soc.*, 1977, **99**, 8469 (*struct, uv, ir, cmr, ms, bibl*)
Rinehart, K.L. *et al*, *Nature (London)*, 1977, **269**, 832 (*ms*)
Nagaraf, R. *et al*, *Acc. Chem. Res.*, 1981, **14**, 356 (*rev*)
Chait, B.T. *et al*, *J. Am. Chem. Soc.*, 1982, **104**, 5157 (*ms*)

Alanine A-00069

2-Aminopropanoic acid, 9CI. α-Alanine



(S)-form

$C_3H_7NO_2$ M 89.094

(R)-form [338-69-2]

D-form

Occurs in the cell walls of bacteria and in some higher plants. Prisms (EtOH aq.). Sol. hot H_2O. Mp 295-7° dec. $[\alpha]_D^{25}$ −1.8° (c, 1 in H_2O), −14.6° (c, 1 in 5M HCl).

B,HCl: Sol. H_2O. $[\alpha]_D^{20}$ −10.3° (H_2O).

Et ester: Needles (EtOH aq.). Mp 104-5°. $[\alpha]_D^{20}$ +6.91° (EtOH).

Benzyl ester; B,HCl: Mp 139-40°. $[\alpha]_D^{25}$ +10.5° (c, 2 in 0.1M HCl).

Benzyl ester, p-toluenesulphonate salt: Mp 113-4°. $[\alpha]_D^{27}$ +6.9° (c, 2 in H_2O).

N-*Benzoyl:* Mp 151°. $[\alpha]_D$ −37.3° (c, 0.8 in KOH).

N-*Ac:* Mp 125°. $[\alpha]_D$ +66.5° (c, 2 in H_2O).

(S)-form [56-41-7]

L-form

Obt. from hydrolysates of many proteins. Insol. EtOH, sl. sol. H_2O. Mp 297° dec. $[\alpha]_D$ +14.6° (c, 1 in 5M HCl), +1.8° (c, 1 in H_2O). *N*-Protected derivs. useful in peptide systems synth. have been listed alphabetically elsewhere.

B,HCl: Mp 204°. $[\alpha]_D^{20}$ +10.4° (H_2O).

Me ester; B,HCl: Mp 154-5° (109-10°).

Et ester; B,HCl: Mp 76°. $[\alpha]_D^{25}$ −11.4° (c, 2 in 5M HCl).

Benzyl ester; B,HCl: Mp 140°. $[\alpha]_D^{25}$ −10.9° (c, 2 in 0.1M HCl).

Benzyl ester, p-toluenesulphonate salt: Mp 114°. $[\alpha]_D^{13}$ −6.8° (c, 2 in H_2O).

N-*Ac:* Mp 125°. $[\alpha]_D$ −66.2° (c, 2 in H_2O).

N-*Benzoyl:* Mp 152-4°. $[\alpha]_D^{20}$ +37.1° (c, 0.7 in KOH).

N-*2,4-Dinitrophenyl:* Yellow plates (Et_2O/pet. ether). Mp 177°.

N-(*2-Hydroxyethyl*): [24560-77-8]. Prod. by the seaweed *Petalonia jascia*.

Amide: Prisms ($CHCl_3$). Mp 72°. Hygroscopic.

(±)-form [302-72-7]

Needles or prisms. Spar. sol. H_2O, insol. Et_2O. Mp 295° dec. pK_{a1} 2.35 (COOH), pK_{a2} 9.69 (NH_2).

Me ester: Bp_{15} 38-42°.

Me ester; B,HCl: Mp 158°.

Et ester: Bp_{11} 48°.

Et ester; B,HCl: Mp 64-8° (86-7° and 129°).

N-*Ac:* Mp 137-8°.

N-*Benzoyl:* Mp 165-6°.

N-*Et, Et ester:* Bp_{11} 48°.

N-*Di-Et, Et ester:* Bp_{13} 74°.

N-*Di-Et, nitrile:* Bp_{15} 66°.

Amide: Mp 62°.

Amide; B,HCl: Mp 170°.

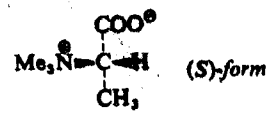
Nitrile; B,HCl: Mp 115-7° (132-8° dec.).

Biochem. Prep., 1949, **1**, 9.
Greenstein, J.P. *et al*, *Chemistry of the Amino Acids*, 1961, Wiley, N.Y., Vol. 3, 1819 (*rev*)
Org. Synth., Coll. Vol., **1**, 20 (*synth*)
Kost, A.N. *et al*, *Chem. Ind. (London)*, 1966, 1496 (*synth*)
Cavanaugh, J.R., *J. Am. Chem. Soc.*, 1967, **89**, 1558 (*pmr*)
Lehmann, M.S. *et al*, *J. Am. Chem. Soc.*, 1972, **94**, 2657 (*cryst struct*)
Okawara, T. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 869 (*synth*)
Kiyooka, S. *et al*, *Bull. Chem. Soc. Jpn.*, 1976, **49**, 1897 (*synth*)
Krapcho, A. *et al*, *Tetrahedron Lett.*, 1976, 2205 (*synth*)

Alanine trimethylbetaine A-00070

1-Carboxy-N,N,N-trimethylethanaminium hydroxide inner salt, 9CI. Alaninebetaine. β-Homobetaine. Methylbetaine

[6458-06-6]



(S)-form

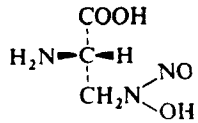
$C_6H_{13}NO_2$ M 131.174

(S)-form [17087-29-5]
Isol. from wood of *Limonium vulgare*. Mp 202-4°. $[\alpha]_D$ −19.5° (2M HCl).

Fischer, E., *Per.*, 1907, **40**, 5000 (*synth*)
Gacek, M. *et al*, *Acta Chem. Scand., Ser. B*, 1975, **29**, 206 (*synth*)
Larker, F. *et al*, *Phytochemistry*, 1975, **14**, 205 (*isol*)

Alanosine A-00071

3-(Hydroxynitrosoamino)alanine, 9CI. *2-Amino-3-(N-hydroxy-N-nitrosoamino)propionic acid*
[16931-22-9]



(S)-form
Absolute configuration

$C_3H_7N_3O_4$ M 149.106

(S)-form
L-form
From *Streptomyces alanosinicus*. Antibiotic with antiviral and antitumour activity. Cryst. $[\alpha]_D^{25}$ −37.8° (c, 0.5 in H_2O).

(±)-form
Cryst. (H_2O). Mp 190° dec.

Murthy, Y.K.S. *et al*, *Nature (London)*, 1966, **211**, 1198 (*isol*)
Lancini, G.C. *et al*, *Tetrahedron Lett.*, 1966, 1769 (*synth, struct*)
Isowa, Y. *et al*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 1847 (*synth*)

Alanylalanine A-00072

$H_3CCH(NH_2)CONHCH(CH_3)COOH$

$C_6H_{12}N_2O_3$ M 160.172

D-D-form [923-16-0]
$[\alpha]_D^{25}$ +21.3° (c, 2 in H_2O), $[\alpha]_D^{24}$ +37.9° (c, 2 in 0.5N HCl).

D-L-form [1115-78-2]
Mp 269-70° dec. $[\alpha]_D^{20}$ −68.5°.

L-D-form [3695-80-5]
Mp 275-6°. $[\alpha]_D^{25}$ +67.2° (c, 2 in 6N HCl).

L-L-form [1948-31-8]
Prisms. Mp 298°. $[\alpha]_D^{25}$ −38.3° (c, 2 in 6N HCl).
Me ester: Mp 126-8°. $[\alpha]_D^{25}$ −35.9° (c, 1.0 in EtOH).
N-Benzyloxycarbonyl, tert-butyl ester: Mp 70-1°. $[\alpha]_D^{20}$ −46.8° (c, 1.0 in EtOH), $[\alpha]_D^{20}$ −54.1° (c, 2.0 in MeOH).

Fischer, E. *et al*, *Ber.*, 1906, **39**, 3981 (*synth*)
Green, B. *et al*, *J. Chem. Soc. (C)*, 1969, 401 (*synth*)
Mitin, Yu.V. *et al*, *Tetrahedron Lett.*, 1969, 5267 (*synth*)

Alanylalanylalanine A-00073

$H_2NCH(CH_3)CONHCH(CH_3)CONH(CH_3)COOH$

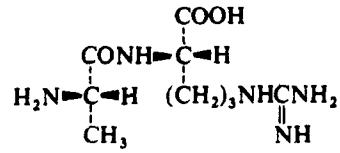
$C_9H_{17}N_3O_4$ M 231.251

N-Ac, Me ester: [26910-17-8]. Substrate for elastase. Mp 254-5°. $[\alpha]_D^{20}$ −147.5° (c, 1.0 in H_2O).
N-Ac, Et ester: Cryst. (trifluoroethanol/hexane). Mp 246-7°.
N-Ac, p-Nitroanilide: Specific substrate for elastase.

Goodman, M. *et al*, *Biopolymers*, 1966, **4**, 275 (*synth*)
Gertler, A. *et al*, *Can. J. Biochem.*, 1970, **48**, 384 (*synth*)
Feinstein, G. *et al*, *Biochem. Biophys. Res. Commun.*, 1973, **50**, 1020 (*synth, use*)
Thomson, A. *et al*, *Eur. J. Biochem.*, 1973, **38**, 1 (*synth, use*)

Alanylarginine A-00074

N^2-*Alanylarginine*, 9CI
[16709-12-9]



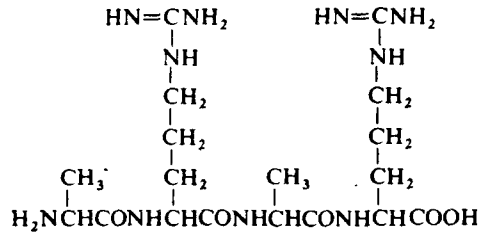
$C_9H_{19}N_5O_3$ M 245.281

L-L-form
B,AcOH: Cryst. (EtOH aq.). Mp 168-9°. $[\alpha]_D^{22}$ +9° (H_2O).
Benzyl ester, N^{α}-Benzyloxycarbonyl, N^{ϵ}-nitro: Cryst. (EtOH aq.). Mp 150-1°. $[\alpha]_D^{22}$ −13.3° (MeOH).
N^{α}-Benzyloxycarbonyl,N^{ϵ}-nitro: Cryst. (EtOH aq.). Mp 172-3°. $[\alpha]_D^{22}$ −10° (MeOH).

Hofmann, K. *et al*, *J. Am. Chem. Soc.*, 1956, **78**, 238 (*synth*)
Harris, G. *et al*, *J. Chem. Soc.*, 1961, 2053.

L-Alanyl-L-arginyl-L-alanyl-L-arginine A-00075

Antibiotic Ro 22-5417. Ro 22-5417

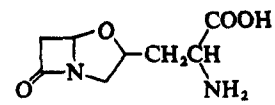


$C_{18}H_{36}N_{10}O_5$ M 472.546
B,2AcOH: Plates (EtOH aq.). Mp 240° dec. $[\alpha]_D^{22}$ +8.2° (H_2O).
N^{α}-Benzyloxycarbonyl-di-N^{ϵ}-nitro, benzyl ester: Plates (EtOH aq.). Mp 196-7°. $[\alpha]_D^{22}$ −7.3° (MeOH).

Harris, G. *et al*, *J. Chem. Soc.*, 1963, 5552.

2-Alanylclavam A-00076

α-Amino-7-oxo-4-oxa-1-azabicyclo[3.2.0]heptane-3-propanoic acid, 9CI. Ro *22-5417. Antibiotic Ro 22-5417*
[74758-63-7]



$C_8H_{12}N_2O_4$ M 200.194
β-Lactam antibiotic. From *Streptomyces clavuligerus*. Active against *Bacillus* spp. grown on minimal agar. Sol. H_2O. Mp 247-65° dec. $[\alpha]_D^{25}$ −137.6° (c, 0.7 in H_2O).

U.S.P., 4 202 819, (*1980*); *CA*, **93**, 130567

N-Alanylglutamic acid, 9CI A-00077

$H_3CCH(NH_2)CONHCH(COOH)CH_2CH_2COOH$

$C_8H_{14}N_2O_5$ M 218.209

D-L-form
$[\alpha]_D^{23}$ −32.9° (c, 1-2 in 0.5M HCl).
L-D-form [16809-27-1]
$[\alpha]_D^{23}$ +32.4° (c, 1-2 in 0.5M HCl).
L-L-form [13187-90-1]
Mp 92-8°. $[\alpha]_D^{24}$ −40.0° (c, 0.5 in MeOH).
Boc-Ala-Glu-(OBu^t)$_2$: Mp 87-9°. $[\alpha]_D^{25}$ −27.0° (c, 1.2 in MeOH).
DL-L-form [16371-85-0]
$[\alpha]_D^{25}$ −17.3° (H_2O).

Sachs, H. *et al*, *J. Am. Chem. Soc.*, 1953, **75**, 4608 (*synth*)
Chaturvedi, N.C. *et al*, *J. Med. Chem.*, 1966, **9**, 971 (*synth*)
Harnden, M.R., *J. Chem. Soc.* (*C*), 1967, 2341 (*synth*)
Gray, C.J. *et al*, *Tetrahedron Lett.*, 1969, 2647 (*synth*)
Suzuki, K. *et al*, *Chem. Pharm. Bull.*, 1977, **25**, 2613 (*synth*)

Alanylglycine A-00078

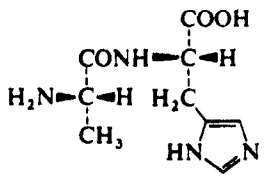
$H_3CCH(NH_2)CONHCH_2COOH$

$C_5H_{10}N_2O_3$ M 146.146

(R)-form [3997-90-8]
D-form
Cryst. (EtOH aq.). Mp 233-5°. $[\alpha]_D^{20}$ −46.6° (c, 1.02 in H_2O).
(S)-form [687-69-4]
L-form
Cryst. (EtOH aq.). Mp 230-231.5° dec. $[\alpha]_D^{21}$ +50.9° (c, 2.0 in H_2O).
N-*Benyloxycarbonyl:* Cryst. (H_2O). Mp 134-5°. $[\alpha]_D^{23}$ −17.3° (c, 2.0 in EtOH).
N-*Benzyloxycarbonyl Et ester:* Cryst. (EtOAc/cyclohexane). Mp 88-89.5°. $[\alpha]_D^{19}$ −18.3° (c, 2.0 in EtOH).
(±)-form [1188-01-8]
B,HCl: Mp 65-8°.

Losse, G. *et al*, *Chem. Ber.*, 1957, **90**, 1279.
Losse, G. *et al*, *Justus Liebigs Ann. Chem.*, 1960, **636**, 140.
Stewart, F.H.C., *Aust. J. Chem.*, 1966, **19**, 1067 (*synth*)
Stewart, F.H.C., *Aust. J. Chem.*, 1968, **21**, 2543.

N-Alanylhistidine, 9CI A-00079



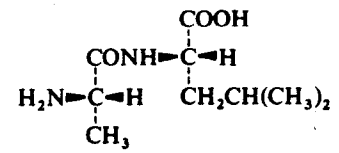
$C_9H_{14}N_4O_3$ M 226.235

L-L-form [3253-17-6]
Mp 157°. $[\alpha]_D^{27}$ +27.0° (H_2O).
N-*Benzyloxycarbonyl:* Cryst. (H_2O). Mp 131°.
DL-DL-form
Cryst. ($EtOH/Et_2O$). Mp 198-202° dec.

Hunt, M. *et al*, *J. Biol. Chem.*, 1938, **124**, 699 (*synth*)
Losse, G. *et al*, *Chem. Ber.*, 1961, **94**, 2768 (*synth*)

Alanylleucine A-00080

N-*Alanylleucine*, 9CI



L-L-*form*

$C_9H_{18}N_2O_3$ M 202.253

D-D-form
Cryst. + $1H_2O$. Mp 254-5° dec.
L-L-form [3303-34-2]
Leaflets (EtOH). Mp 254-7° dec. $[\alpha]_D^{20}$ −19.9° (c, 2.0 in H_2O).
N-*Benzyloxycarbonyl:* Oil.
N-*Benzyloxycarbonyl, Et ester:* Cryst. (EtOH aq.). Mp 52°. $[\alpha]_D^{25}$ +37.3° (c, 2.0 in EtOH).
N-*Piperidinooxycarbonyl:* Cryst. ($CHCl_3$/EtOAc/pet. ether). Mp 160-2°. $[\alpha]_D^{20}$ +13.2°.
N-*Piperidinooxycarbonyl, Me ester:* Cryst. (EtOAc/pet. ether). Mp 143-7° dec. $[\alpha]_D^{20}$ +10°.
DL-DL-form [1999-42-4]
Mp 240°.
B,HCl: Mp 178-81°.

Smith, C.S. *et al*, *J. Am. Chem. Soc.*, 1941, **63**, 2605 (*synth*)
Losse, G. *et al*, *Justus Liebigs Ann. Chem.*, 1960, **636**, 140 (*synth*)
Hirschmann, R. *et al*, *J. Org. Chem.*, 1967, **32**, 3421 (*synth*)
Stevenson, D. *et al*, *J. Chem. Soc.*, 1969, 2389 (*synth*)

N^2-Alanyllysine A-00081

$H_3CCH(NH_2)CONHCH(COOH)(CH_2)_4NH_2$

$C_9H_{19}N_3O_3$ M 217.267

D-L-form [65882-14-6]
$[\alpha]_D^{22}$ −27.1° (c, 1 in 0.5N HCl).
B,AcOH: Cryst. (MeOH/EtOH). Mp 219-21°. $[\alpha]_D^{22}$ −17.6° (c, 1 in H_2O).
Z-Ala-Z-Lys-OH: Mp 162°.
Z-Ala-Z-Lys-OMe: Mp 130°.
L-D-form [65882-13-5]
$[\alpha]_D^{22}$ +19.3° (c, 1 in 0.5N HCl).
B,AcOH: Cryst. (MeOH/EtOH). Mp 219-21°. $[\alpha]_D^{22}$ +16.7° (c, 1 in H_2O).
Z-Ala-Z-Lys-OMe: Mp 128°.
Z-Ala-Z-Lys-NHNH$_2$: Mp 190-1°.
L-L-form [6366-77-4]
$[\alpha]_D^{22}$ −7.1° (c, 1 in 0.5N HCl).
B,AcOH: Cryst. (MeOH/EtOH). $[\alpha]_D^{22}$ +9.1° (c, 1 in H_2O).
Z-Ala-Z-Lys-OH: Mp 134°.
Z-Ala-Z-Lys-OMe: Mp 90°.

Erlanger, B.F. *et al*, *J. Am. Chem. Soc.*, 1950, **72**, 3314; 1951, **73**, 4025 (*synth*)
Padayatty, J.D. *et al*, *J. Org. Chem.*, 1966, **31**, 1934 (*synth*)
Sakarellos, C. *et al*, *Bull. Soc. Chim. Fr.*, 1976, 781 (*synth*)
Herrmann, V. *et al*, *Hoppe-Seyler's Z. Physiol. Chem.*, 1978, **359**, 47 (*synth*)

N-Alanylphenylalanine A-00082

$H_3CCH(NH_2)CONHCH(COOH)CH_2Ph$

$C_{12}H_{16}N_2O_3$ M 236.270

L-L-form [3061-90-3]
$[\alpha]_D^{25}$ +17° (c, 1 in 1N HCl).
Z-Ala-Phe-OMe: Cryst. (EtOAc/pet. ether). Mp 99-100°. $[\alpha]_D^{22}$ −9.3° (c, 1 in EtOH).