THOMSON REUTERS

303

Chapman and Hall Chemical Database

FILE DESCRIPTION

The **Chapman & Hall Chemical Database** (CHCD), formerly HEILBRON, the chemical properties database, represents the complete text of several chemical dictionaries from Chapman and Hall. CHCD is a source database of chemical identification, physical-chemical properties, use, hazard, and key reference data to the world's more important chemical substances, as selected by a panel of experts. CHCD provides chemical substance identification through searching physical and/or chemical properties, compound variants, derivative names, synonyms, CAS® Registry numbers, molecular formulae and molecular weight, biological source statements, use/importance data, melting point, freezing point, boiling point, solubility, relative density, optical rotation, and dissociation constants, as well as providing suppliers and toxicity data.

SUBJECT COVERAGE

- Fundamental acyclic, alicyclic, aromatic and heterocyclic organic compounds.
- Comprehensive coverage for natural products including alkaloids, amino acids, antibiotics, carbohydrates, flavonoids, lichen acids, lignans, nucleosides, peptides, steroids, tannins, and terpenoids.
- Pharmaceuticals including marketed drugs and compounds in clinical trials.
- Pharmaceuticals including marketed drugs and compounds in clinical trials.
- Analytical reagents: biological status, extractants, indicators, nmr shift reagents, resolving agents.
- Industrial chemicals, synthetic reagents and laboratory solvents.
- A wide range of inorganic and organometallic compounds, covering coordination complexes and cluster compounds.
- Compounds with unusual structural, physical or chemical properties.

SOURCES

CHCD is the online version of the database used to produce the *Dictionary of Organic Compounds* - 5th Edition, (DOC 5) and the *Dictionary of Organometallic Compounds* (DMC) and supplements. The contents of the database are prepared from the primary and secondary chemical literature under the supervision of a panel of subject experts. Material from the following source books is also included: *Carbohydrates*, *Amino Acids and Peptides*, the *Dictionary of Antibiotics and Related Compounds*, and the *Dictionary of Organophosphorus Compounds*.

DIALOG FILE DATA

Inclusive Dates:

Latest editions of printed counterparts (which include citations from chemical literature to the present, with many pre-1967 citations)

Update Frequency: Irregular

File Size: 442,257 records as of May 1997

CONTACT

The Chapman and Hall Chemical Database is produced by Chapman & Hall/ CRC (UK). Questions concerning file content should be directed to:

Dr. Fiona Macdonald
Managing Editor, Chapman & Hall/CRC
23 Blades Court, Deodar Road
London SW15 2NU
United Kingdom
Phone: +44 (0) 208 875 4375
Fax: +44 (0) 208 871 3443
E-Mail: fmacdonald@crcpress.com

FORMAT 5 AND 9 FULL RECORD

```
                DIALOG(R)File 303:Chapman & Hall Chemical Database
                (c) 1995 Chapman & Hall. All rts. reserv.

/MAIN           00007992
SF=             Subfile: Dictionary of Natural Products, 1994
                CHCD Acc. No: A-01440V0
AA=             Unique Key: 00019586- -00
/NA, NA=, /DE, /CN, CN=
                CHCD NAME: 4-Amino-3-isoxazolidinone
/SY, SY=, /DE, /NA, NA=
                Synonyms:  Cycloserine  ;  Cyclomycin;  Closina;  Micoserina;
                     Farmiserina; Orientomycin; Oxymycin; Antibiotic 106-7;
                     Antibiotic 5915; Antibiotic 8217;  Antibiotic  17452;
                     Antibiotic  E  733A;  Antibiotic  I 1431; Antibiotic  K 300;
                     Antibiotic NJ 21; Antibiotic PA 94;
/TX             Compound Type:  Drug - Antibacterial agents;  Drugs - Antibiotics;
                     Drugs - Tuberculostatic agents
RN=             CAS Registry No: 4834-58-6
                Additional CAS Reg. No: 339-72-0
MF=             Molecular Formula: C3H6N2O2
MW=             Molecular Wt: 102.093
                Unique Key: 00019586-A-00
/VAR            VARIANT: 4-Amino-3-isoxazolidinone\(R)-form
                     Compound  Type:  Selected  General Organics - Miscellaneous
                     modified aminoacids;  Natural  Products - Miscellaneous
                     modified aminoacids; Natural Products - Isoazole alkaloids
                       Hazard: CNS adverse effects reported when used
                       therapeutically. LD50 (mus, orl) 5290 mg/kg
                     Source:  Prod.  by  Streptomyces garyphalus, Streptomyces
                     orchidaceus, Streptomyces lavendulae and Streptomyces
                     nagasakiensis
                     Use/Importance: Shows antibiotic activity primarily against
                     mycobacteria.
                     Tuberculostatic
                     Physical State: Cryst.
                     Miscellaneous: Of limited clinical use due to toxicity
                     CAS Registry No: 68-41-7
                     RTECS No.: NY2975000
                     Solubility: Sol. H2O, alkalis
                     Optical  Rotation: +116 deg at 23 deg C (c, 1.17 in H2O)
                     wavelength Na line
                     Melting Pt: Mp 155-156 deg C (dec.)
                Unique Key: 00019586-A-01
/DERIV          DERIVATIVE: 4-Amino-3-isoxazolidinone\(R)-form\N-Ac
                     Physical State: Needles
                     Molecular Formula: C5H8N2O3
                     Molecular Wt: 144.130
                     Melting Pt: Mp 179-180 deg C
                Unique Key: 00019586-A-02
/DERIV          DERIVATIVE: 4-Amino-3-isoxazolidinone\(R)-form\N N'-Di-Ac
                     Physical State: Chunky needles (Me2CO)
                     Molecular Formula: C7H10N2O4
                     Molecular Wt: 186.167
                     Melting Pt: Mp 121-122 deg C
                Unique Key: 00019586-B-00
/VAR            VARIANT: 4-Amino-3-isoxazolidinone\(S)-form
                     CAS Registry No: 339-72-0
                     Optical  Rotation:  -104  deg  at 20 deg C (c, 1 in H2O)
                     wavelength Na line
                     Melting Pt: Mp 146 deg C (dec.)
                Unique Key: 00019586-C-00
/VAR            VARIANT: 4-Amino-3-isoxazolidinone\(+/-)-form
                     CAS Registry No: 68-39-3
                     RTECS No.: NY2974900
                     Melting Pt: Mp 137-140 deg C
                References:
                     01 Aldrich Library of FT-IR Spectra, 1st edn. 810A (ir)
                     02 Aldrich Library of NMR Spectra, 2nd edn. 1 678B (nmr)
                     03 Harned  RL  et al., Antibiot. Chemother. (Washington, D.C.)
                     1955 5 204 (struct)
                     04A Stammer CH et al., J.A.C.S. 1955 77 2344, 2345, 2346
                     04B 1957 79 3236 (struct, synth, isol, resoln)
                     05 Neuhaus FC Antibiotics (N.Y.) 1967 1 40 (rev)
                     06 Milne GWA et al., Tetrahedron 1967 23 65 (nmr, ms)
                     07 Lamb JW Anal. Profiles Drug Subst. 1972 1 53 (rev, synth,
                     anal)
```

FORMAT 5 AND 9 FULL RECORD (cont'd)

```
                08 O'Brien P Met. Ions Biol. Syst. 1985 19 295 (rev, pharmacol)
               09  Negwer  M  Organic-Chemical  Drugs  and  their  Synonyms
                6th Ed., Akademie-Verlag, Berlin 1987 107 (synonyms)
                10 El-Obeid HA et al., Anal. Profiles Drug Subst. 1989 18 567
                (rev)
                11 Merck Index 11th edn. 1989 2758
                12  Martindale,  The  Extra  Pharmacopoeia  30th  edn.,
                Pharmaceutical Press, London 1993 156
                79  Lewis  RJ  Sax's  Dangerous Properties of Industrial
                Materials
                8th Ed., Van Nostrand-Reinhold 1992 CQH000
/DP, DP=        Data  Tags:  Cas  Registry  number;  Molecular  formula; Compound
                 Variants; Source;  Use/Importance;  Physical State; Solubility;
                Melting Point; Optical Rotation;  Miscellaneous Data;
                 Hazard/Toxicity Data; Rtecs Reference; Derivatives
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FORMAT 2, 3, 4 AND 7 INDIVIDUAL COMPOUND

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                DIALOG(R)File 303:Chapman & Hall Chemical Database
                (c) 1995 Chapman & Hall. All rts. reserv.

/VAR            00007993
SF=             Subfile: Dictionary of Natural Products  1994
AA=             Unique key: 00019586-A-00
/NA, NA=, /CN   VARIANT: 4-Amino-3-isoxazolidinone\(R)-form
RN=             CAS Registry No: 68-41-7
/TX             Compound   Type:  Selected  General Organics - Miscellaneous
                     modified aminoacids  Natural  Products - Miscellaneous
                     modified aminoacids Natural Products - Isoazole alkaloids
RR=             RTECS: NY2975000
/TX             Hazard:  CNS adverse effects reported when used therapeutically.
                     LD50 (mus, orl) 5290 mg/kg
/TX             Source:   Prod.  by  Streptomyces  garyphalus,  Streptomyces
                     orchidaceus, Streptomyces lavendulae and Streptomyces
                     nagasakiensis
/TX             Use/Importance:  Shows antibiotic activity primarily against
                     mycobacteria.
                     Tuberculostatic
PS=             Physical State: Cryst.
MP=             Melting Pt.: Mp 155-156 deg C (dec.)
SL=             Solubility: Sol. H2O, alkalis
OP=, OT=        Optical Rotation: +116 deg at 23 deg C (c, 1.17 in H2O)
                wavelength Na line
/TX             Miscellaneous: Of limited clinical use due to toxicity
/DP, DP=        Data  Tags: Compound Variants; Cas Registry number; Source;
                Use/Importance; Physical  State; Solubility; Melting Point; Optical
                Rotation; Miscellaneous Data; Hazard/Toxicity Data; Rtecs Reference
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Note: /MAIN, /DERIV, and /VAR search only the individual compound

File 303 Chapman and Hall Chemical Database

SEARCH OPTIONS

BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
—	—	All Basic Index Fields	Word	S AMINO(1W)ISOXAZOLIDINONE
/CN	CN	Main CHCD Substance Name, Variant Name(s), Derivative Name(s)[1,2,4]	Segment & Word & Phrase	S ONE/CN S AMINO(1W)ISOXAZOLIDINONE/CN S 4-AMINO-3-ISOXAZOLIDINONE/CN
/DE	DE	CHCD Name, Variant Name, Derivative Name, and Synonyms[1,2,4,5]	Segment & Word & Phrase	S ONE/DE S AMINO(1W)ISOXAZOLIDINONE/DE S 4-AMINO-3-ISOXAZOLIDINONE/DE
/DERIV	—	Derivative Substance Information[4]	Segment & Word & Phrase	S ONE/DERIV S AMINO(1W)ISOXAZOLIDINONE/NA,DERIV S 4-AMINO-3-ISOXAZOLIDINONE?/DERIV
/DP	DP	Data Present[1,4]	Word & Phrase	S BOILING(W)POINT/DP S BOILING POINT/DP
/EC	—	Element Count[4]	Word	S C3/EC
/MAIN	—	Main CHCD Substance Information[4]	Segment & Word & Phrase	S ONE/MAIN S AMINO(1W)ISOXAZOLIDINONE/MAIN,NA S 3-AMINO-3-ISOXAZOLIDINONE/MAIN
/NA	NA	CHCD Name, Variant Name, Derivative Name, and Synonyms[1,2,4]	Segment & Word & Phrase	S ONE/NA S AMINO(1W)ISOXAZOLIDINONE/NA S 4-AMINO-3-ISOXAZOLIDINONE/NA
/SY	SY	Synonyms[1,2,4]	Segment & Word & Phrase	S CYCLO/SY S ANTIBIOTIC(W)17452/SY S ANTIBIOTIC 17452/SY
/TX	TX	Text[3,4]	Word	S CNS(W)ADVERSE/TX
/VAR	—	Compound Variant Information[4]	Segment & Word & Phrase	S ONE/VAR S (ISOAZOLE(W)ALKALOIDS)/VAR,NA S 4-AMINO-3-ISOXAZOLIDINONE?/VAR

[1] Searchable in the Basic Index and in the Additional Indexes.

[2] All chemical names are indexed as complete phrases, individual words, and chemically significant segments of words. Use /FW to retrict retrieval to the complete term, e.g., S ETHANE/FW to only select ethane as a single word rather than as a segment of a larger chemical term, such as trichloroethane.

[3] The Text field includes Compound Type, Hazard Information, General Information, Source of Substance, Use/Importance, Miscellaneous,and Physical State.

[4] Terms can be qualified to any one of three levels using one of the following suffixes: /MAIN to restrict retrieval to the Main CHC substance information; /VAR to restrict retrieval to the Compound Variant substance information, and /DERIV to restrict retrieval to the Derivative substance information (e.g., MP=24/VAR retrieves compound variant substances with a melting point of 24).

[5] Also /DF.

ADDITIONAL INDEXES

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
AA=	AA	Unique ID	Phrase	S AA=00019586-A-00
—	AN	DIALOG Accession Number		
BP=	BP	Boiling Point (degrees Celsius)[4,6]	Numeric	S BP=120
BT=	BP	Boiling Point Text[4]	Word	S BT=2MM(F)BP=120
CN=	CN	Main CHCD Substance Information[1,4]	Phrase	S CN=4-AMINO-3-ISOXAZOLIDINONE
DP=	DP	Data Present	Phrase	S DP=BOILING POINT
EC=	—	Element Count[4]	Word	S EC=C0003
ME=	MF	Molecular Element[4]	Phrase	S ME=CHNO
MF=	MF	Molecular Formula[4]	Phrase	S MF=C3H6N2O2 S MF=C3H6N2O2/MAIN S MF=C5H8N2O3/DERIV S MF=C13H9NO/VAR
MP=	MP	Melting Point (degrees Celsius)[4,6]	Numeric	S MP=155
MW=	MW	Molecular Weight[4,6]	Numeric	S MW=102.093
NA=	NA	Chemical Name[1,4]	Phrase	S NA=CYCLOSERINE
OP=	OP	Optical Rotation (degrees)[4,6]	Numeric	S OP=116
OT=	OP	Optical Rotation Text[4]	Word	S OT=(NA(W)LINE)
PK=	PK	Dissociation Constant (pKa)[4,6]	Numeric	S PK=9.47
PS=	PS	Physical State[4]	Word	S PS=CRYST?
RN=	RN	CAS(R) Registry Number[4]	Phrase	S RN=4834-58-6 S RN=339-72-0/VAR S RN=23113-01-1/DERIV
RR=	RR	RTECS Reference[4]	Phrase	S RR=NY2975000
SF=	SF	Dictionary Name (Subfile)	Phrase	S SF=DICTIONARY OF NATURAL PRODUCTS
SG=	SG	Specific Gravity or Relative Density[4,6]	Numeric	S SG=1.10:1.25
SL=	SL	Solubility[4]	Word	S SL=(SOL(2W)ALKALIS)
ST=	SG	Specific Gravity Text	Word	S ST=(AT(W)20(W)DEG(W)C)
UD=	—	Update	Phrase	S UD=9999

[6] Numeric values can be entered in several different ways: directly as a number, i.e., S BP=100.0; in exponential notation, i.e., S BP=1E2. Letter abbreviations are also available: K for thousand, M for million, B for billion, e.g., S BP=0.5K:1.0K. To search a range of values, use a colon between starting and ending value, e.g., S BP=78:79 OR use numeric operators (>, <, >=, and <=), e.g., S 78<=BP<=79.

SPECIAL FEATURES

For command descriptions, enter HELP LIMIT, HELP SORT, HELP RANK, HELP MAP online.

LIMIT	/**DOC** -- Dictionary of Organic Compounds /**HZ** -- Hazard/Toxicity Data available /**NOHZ** -- Hazard/Toxicity Data unavailable	S S3/DOC S S4/HZ S S2/NOHZ
SORT	**AA, MF, RN**	SORT S1/ALL/RN,D PRINT S5/5/1-24/MF
RANK	All phrase- and numeric-indexed fields in the Additional Indexes can be ranked.	RANK NA RANK SF S4
MAP	RN, SY	MAP RN TEMP S2

PREDEFINED FORMAT OPTIONS

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1	--	DIALOG Accession Number
2	--	Individual Compound (Variant, Derivative, or Main Compound)
3	Medium	Individual Compound (Variant, Derivative, or Main Compound)
4	--	Individual Compound (Variant, Derivative, or Main Compound)
5	--	Full Record
6	Free	Compound Name, CAS Registry Number, Data Present
7	Long	Individual Compound (Variant, Derivative, or Main Compound)
8	Short	Compound Name, Synonyms, CAS Registry Number, Data Present, Subfile
9	Full	Full Record
K	--	KWIC (Key Word In Context) displays a window of text; may be used alone or with other formats

OTHER OUTPUT OPTIONS

For an explanation, enter HELP TYPE, HELP UDF, HELP TAG online.

USER DEFINED FORMATS	Display codes listed in the Search Options tables can be used to customize output.	TYPE S4/NA,DP/1-10
TAG	Output can be displayed with tags identifying each display field.	TYPE S3/5/1-10 TAG
DIRECT RECORD ACCESS	If the accession number of a specific record is known, it can be used to display the record directly.	TYPE 00007993/2 DISPLAY 00007993/NA,RN PRINT 00007993/9

FOR ONLINE HELP:

See HELP FIELDS 303 for searchable fields; HELP FORMAT 303 for output formats; HELP LIMIT 303 for limits; HELP RATES 303 for cost information; HELP SORT 303 for sorts.