REAXYSFILESUB

Subject Coverage

- Organic and inorganic chemistry
- Chemical data
- Electrochemical behaviour
- Electrical and magnetic properties
- Identification of substance
- Materials composition data
- Multi-component systems
- Optical properties
- Patent specific data
- Pharmacological and ecological data
- Physical and mechanical properties
- Reactions
- Safety data
- Spectroscopic data
- State of aggregation
- Structure and energy parameter
- Thermodynamic properties
- Transport phenomena

File Type

Bibliographic

Access

The file is only available on STNext

Features

Alerts (SDIs)	Monthly, weekly, or with each update (2 updates per week) (every update is the default)		
CAS Registry Number® Identifiers	☑	SLART	☑
Keep & Share	☐	Structures	☑

Record Content

- Records contain reviewed and evaluated documents from Handbook of Organic Chemistry as published by Friedrich Beilstein as well as well as data from leading journals in organic and inorganic chemistry covering the period from 1771 to date.

File Size

- more than 34 million records (01/22)

Coverage

1771- present

Updates

Twice a week

Language

English

Database Producer

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Copyright Holder:

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CH-2000, Neuchâtel
Switzerland

Sources	• Chemistry Journals • Handbook of Organic Chemistry (published by F. Beilstein)
User Aids	• Online Helps (HELP DIRECTORY lists all help messages available) • STNGUIDE
Cluster	• CASRNS • STRUCTURE STN Database Cluster information: http://www.stn-international.com/en/customersupport/customer-support#cluster+%7C+subjects+%7C+features
Related Databases	REAXYSFILEBIB

Search and Display Field Codes

Fields that allow left truncation are indicated by an asterisk (*).

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index* (contains single terms from Chemical Name (CN) and Chemical Name Segment (CNS))	/BI	S (AQUA? TOX?)/BI	CN,CNS
Accession Number	/AN	S 1915876/AN	AN
All Accession Numbers	/ALLAN	S 1915876/ALLAN	AN,CMAN, COMPAN
Alternate InChi Key	/AINCHI	S KWEZFXJCZZEGTG-JGRHXJNXBK/AINCHI	AINCHI
CAS Registry Number	/RN	S 100-03-8/RN	RN
Chemical Name *	/CN	S CHOLESTEROL/CN	CN
Chemical Name Segment*	/CNS	S CHOLESTERYL/CNS	CN
Component Molecular Accession Number	/CMAN	S 5811/CMAN	CMAN
Component Molecular Formula	/CMF	S C6 H13 N/CMF	CMF
Composition Accession Number	/COMPAN	S 8181997/COMPAN	COMPAN
Composition Conventration	/COMPC	S B WEIGHT PERCENT/COMPC	COMPC
Composition Name	/COMPN	S CHROMIUM COMPN	COMPN
Count of Referenced Markush Structures	/MARKREF.CNT	S 10/MARKREF.CNT	MARKREF.CNT
Element Count, Substance	/ELC.SUB	S 5/ELC.SUB	MF
Element Symbol	/ELS	S CI/ELS	MF
Element Symbol, Count	/ELS.CNT	S 5/ELS.CNT	MF
Element Symbol, SUB	/ELS.SUB	S CI/ELS.SUB	MF
Entry Date **(1)**	/ED	S L1 ED=JAN 2019	ED
Field Availability	/FA	S KW/FA	FA
Formula Weight **(1)**	/FW (or /MW)	S 3000<FW	FW
InChi Key	/INCHI	S KWEZFXJCZZEGTG-JGRHXJNXSA-N/INCHI	INCHI
Linearized Structure Formula	/LSF	S CH2O(1+)/LSF	LSF
Molecular Formula	/MF	S C4H9N5. H2O4S//MF	MF
Number of Components **(1)**	/NC	S 9/NC	NC
Periodic Group	/PG	S (A3 AND A6)/PG	MF
Reference Count **(1)**	/REC	S REC>=15	REC
Substance Descriptor	/SD	S ISOCYCLIC/SD	SD
Update Date **(1)**	/UP	S L1 AND UP=JAN 2019	UP

(1) Numeric search field that may be searched using numeric operators or ranges.

STRUCTURE SEARCHING
Structure Search Terms

Terms	Search Examples
L-numbers of structures built using the STRUCTURE command or uploaded from STN Express (Boolean logic allowed between the L-numbers)	SEARCH L1 FAM SAM SEA L1 AND L2 SSS FUL
L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L3 OR L4 SSS SAM
L-number of a structure built using the STRUCTURE command or uploaded from STN Express combined with L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L1 AND L2 NOT L3

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Substructure (default)	Search for substances which match the query. Substitution is allowed at all open positions. Additional components may be retrieved	SSS	SEARCH L1 SSS FUL S L2 OR L3 SSS SAM S L7 SSS RAN
Closed Substructure	Search for substances which match the query exactly. Substitution is allowed at positions opened by CONNECT. Additional components may be retrieved.	CSS	SEARCH L1 CSS FUL S L2 OR L3 CSS S L4 NOT L5 CSS RAN
Family	Search for substances which match the query exactly. Additional components may be retrieved.	FAM	S L6 FAM SAM
Exact	Search for substances which match the query exactly.	EXA	SEA L5 EXA FUL

Scopes of Structure Searches

Type	Definition	Search Code	Search Examples
Sample (default)	Search a fixed 5% of the file	SAM	SEARCH L3 EXA SAM S L6 NOT L7 SSS SAM
Full	Search 100% of the file.	FUL	S L5 OR L8 SSS FUL

DISPLAY and PRINT Formats

All predefined formats are listed in a hierarchical order, whereby the indented subformats are included in the previous format.

Format	Content	Examples
AINCHI	Alternate InChi Key	D AINCHI
ALLAN	All Accession Numbers	D ALLAN
AN	Accession Number	D AN
CMAN	Component Molecular Accession Number	D CMAN
CMF	Component Molecular Formula	D CMF
CN	Chemical Name	D CN
COMPAN	Composition Accession Number	D COMPAN
COMPN	Composition Conventration	D COMPN
ED	Entry Date	D ED
FW	Formula Weight	D FW
INCHI	InChi Key	D INCHI
LSF	Linearized Structure Formula	D LSF
MARKREF.CNT	Count of Referenced Markush Structures	D MARKREF.CNT
MF	Molecular Formula	D MF
MW	Molecular Weight	D MW
PG	Periodic Group	D PG
REC (RE,CNT)	Reference Count	D REC
RN	CAS Registry Number	D RN
SD	Substance Descriptor	D SD
STR	Structure	D STR
UP	Update Date	D UP
ALL (FULL)	AN, CN, SD, COMPAN, COMPN, COMPC, MF, CMF, LSF, INCHI, AINCHI, MW, MARKREF.CNT, REC, ED, UP, STR	D ALL
IDE	AN, CN, SD, COMPAN, COMPN, COMPC, MF, LCMF, LSF, INCHI, AINCHI, MW, MARKREF.CNT, REC, ED, UP, STR	D IDE
SCAN	CN, MF, SD, STR (random display, no answer number)	D SCAN
SAM, SAMPLE	AN, CN, MF, SD, STR	
HIT	All fields containing hit terms	D HIT
HIT IDE	Complete IDE with HIT	D HIT IDE

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Accession Number	AN	Y	Y
Chemical Name	CN	Y	N
Molecular Weight	MW	N	Y
Number of Components	NC	N	Y
Reference Count	RE (RE.CNT)	N	Y
CAS Registry Number	RN	Y	N
Substance Descriptor	SD	Y	N

(1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set,e.g., SEL HIT RN.

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SAMPLE Records

Display ALL

```
AN      37367   REAXYSFILESUB
RN      1361-02-0
CN      vilmorrianine D; sachaconitine; sachaconite; (16(i)S)-20-ethyl-13B1;
        ,16-dimethoxy-4-methyl-aconitane-8,143B1; -diol; (16(i)S)-20-Aethyl-13B1;
        ,16-dimethoxy-4-methyl-aconitan-8,143B1; -diol
SD      heterocyclic
MF      C23 H37 N O4
LSF     C23H37NO4
INCHI   NGWMZXLZSGJSRI-JPAZAREGSA-N
AINCHI NGWMZXLZSGJSRI-JPAZAREGBF
MW      391.551
MARKREF.CNT 0
REC     7
ED      Entered STN: 13 Jul 2020
        Last updated on STN: 13 Jul 2020
STR
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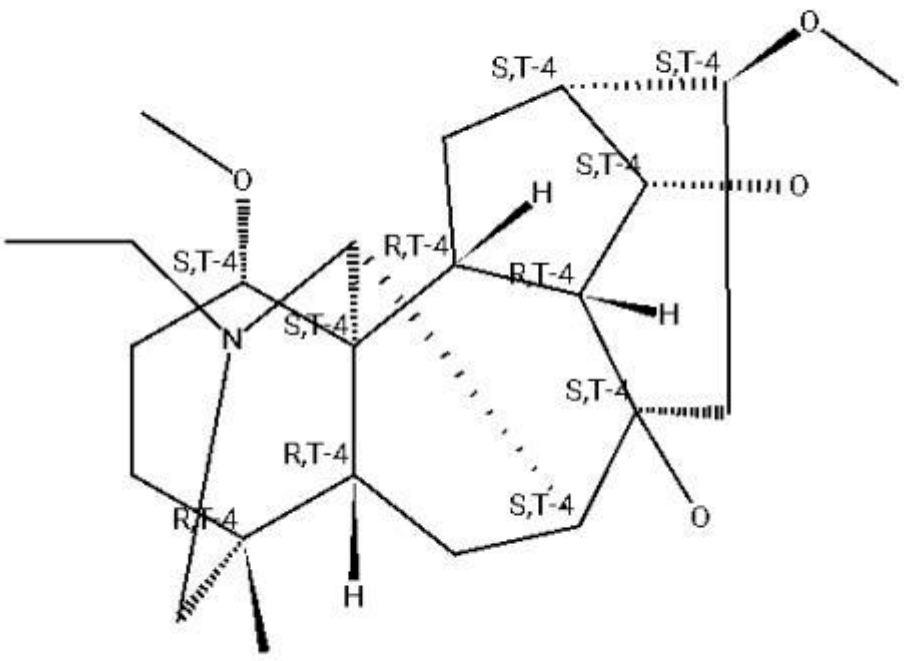

D BIB HITSTR (crossover from REAXYSFILESUB to REAXYSFILEBIB)

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ANSWER 2 OF 1479 REAXYSFILEBIB COPYRIGHT 2020 ELSEVIER INC. on STN.
AN     79742241   REAXYSFILEBIB
TI     DISCOVERY OF NOVEL ANTI-INFECTIVES FOR GRAM NEGATIVE PATHOGENS
IN     BULTERYS, Philip; MILLER, Jeffery F.; DAMOISEAUX, Robert D.; FRENCH, Christopher T.
PA     THE REGENTS OF THE UNIVERSITY OF CALIFORNIA; BULTERYS, Philip; MILLER, Jeffery F.;
       DAMOISEAUX, Robert D.; FRENCH, Christopher T.

PI     PATENT NO.           KIND  DATE       APPLICATION NO.          DATE
       -------------------  ----  --------   -----------------------  --------
       WO 2020072976 *      A1    20200409   WO 2019-US54824          20191004

       * = indexed patent
PRAI   US 2018-62741393         20181004 (62)
DT     Patent
LA     English
ED     Entered STN: 7 Jul 2020
       Last updated on STN: 7 Jul 2020

       HIT structure(s)
AN     33662   REAXYSFILESUB
CN     5-fluorouridine; 5-fluoro-uridine; 1-((2R,3R,4S,5R)-3,4-dihydroxy-5-
(hydroxymethyl)-
       tetrahydrofuran-2-yl)-5-fluoropyrimidine-2,4(1H,3H)-dione;
       1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-
fluoropyrimidine-
       2,4(1H,3H)-dione; 2'-deoxy-5-fluorouridine; fluorouridine; 5-fluorouracil
SD     heterocyclic
MF     C9 H11 F N2 O6
STR
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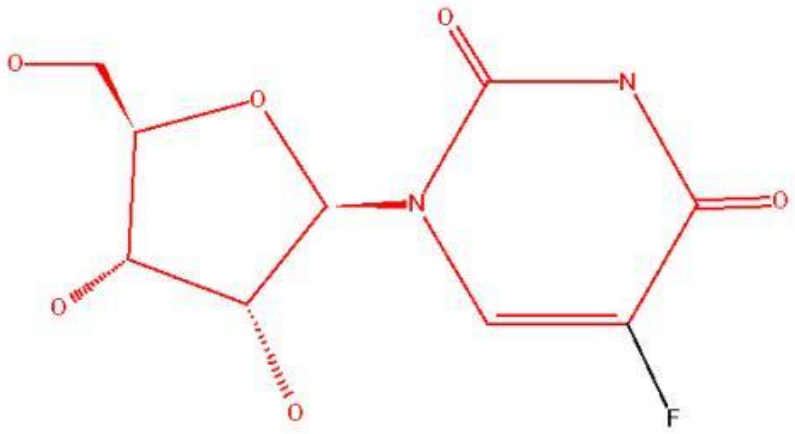


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       HIT structure(s)
AN     53321   REAXYSFILESUB
CN     5-fluorouridine 5'-monophosphate; 5-fluorouridine-5'-monophosphate;
       5-fluoro-5'-monophosphate uridine; 5-fluorouridine 5'-monophosphate; fluorouridine
       monophosphate; 5-FdUMP; [6-(1)H]-5-FUMP; Phosphoric acid
       mono-[(2R,3S,4R,5R)-5-(5-fluoro-2,4-dioxo-3,4-dihydro-2H-pyrimidin-1-yl)-3,4-
dihydroxy-
       tetrahydro-furan-2-ylmethyl] ester
SD     heterocyclic
MF     C9 H12 F N2 O9 P
STR
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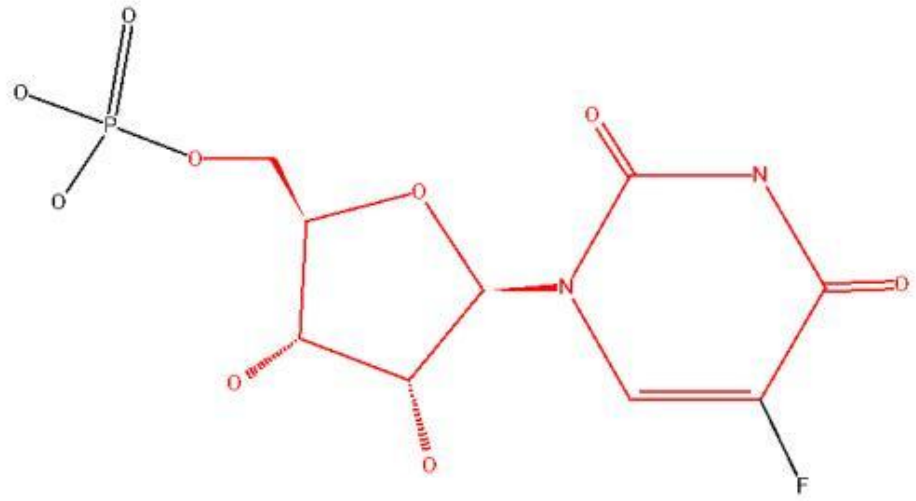
REAXYSFILESUB



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