

REAXYSFILESUB

Subject Coverage	Extensive chemistry content: All types organic and inorganic substances, including alloys, coordination compounds, minerals, mixtures, polymers, salts	
File Type	Structure	
Access	The file is only available on STNNext	
Features	Alerts (SDIs) Not available CAS Registry Number® Identifiers <input checked="" type="checkbox"/> SLART <input checked="" type="checkbox"/> Keep & Share <input type="checkbox"/> Structures <input checked="" type="checkbox"/>	
Record Content	Substance Identification (Chemical Names, Molecular Formula etc)	
File Size	More than 49 million records (08/23)	
Coverage	1771- present	
Updates	Twice a week	
Language	English	
Database Producer	Elsevier Information Systems GmbH Franklinstr. 61-63 60486 Frankfurt am Main Germany Phone: +49 69 5050 4242	Copyright Holder: Elsevier Properties SA Espace de l'Europe 3 CH-2000, Neuchâtel Switzerland
Sources	<ul style="list-style-type: none"> • More than 16,000 chemistry-related periodicals • Conference abstracts • Patent information from all major authorities 	
User Aids	<ul style="list-style-type: none"> • Online Helps (HELP DIRECTORY lists all help messages available) • STNGUIDE 	
Cluster	<ul style="list-style-type: none"> • CASRNS • STRUCTURE STN Database Cluster information: https://www.cas.org/support/training/stn/database-clusters	
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 CINNAMON? AND ACID S URIDIN? AND HYDROXY?/BI S URIDINE/BI	CN,CNS
Accession Number All Accession Numbers	/AN /ALLAN	S 1915876/AN S 1915876/ALLAN	AN 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 Concentration	/COMPC	S B WEIGHT PERCENT/COMPC	COMPC
Composition Name	/COMPN	S CHROMIUM/COMPN	COMPN
Count of Referenced Markush Structures (1)	/MARKREF.C NT	S 10/MARKREF.CNT	MARKREF.CNT
Element Count, Substance (1)	/ELC.SUB	S AU/ELS AND 5/ELC.SUB	MF
Element Symbol	/ELS	S CL/ELS	MF
Element Symbol, Count (1)	/ELS.CNT	S 5/ELS.CNT	MF
Entry Date (1)	/ED	S L1 AND ED=APR 2020	ED
Field Availability	/FA	S SD/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/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= APR 2020	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 Concentration	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).

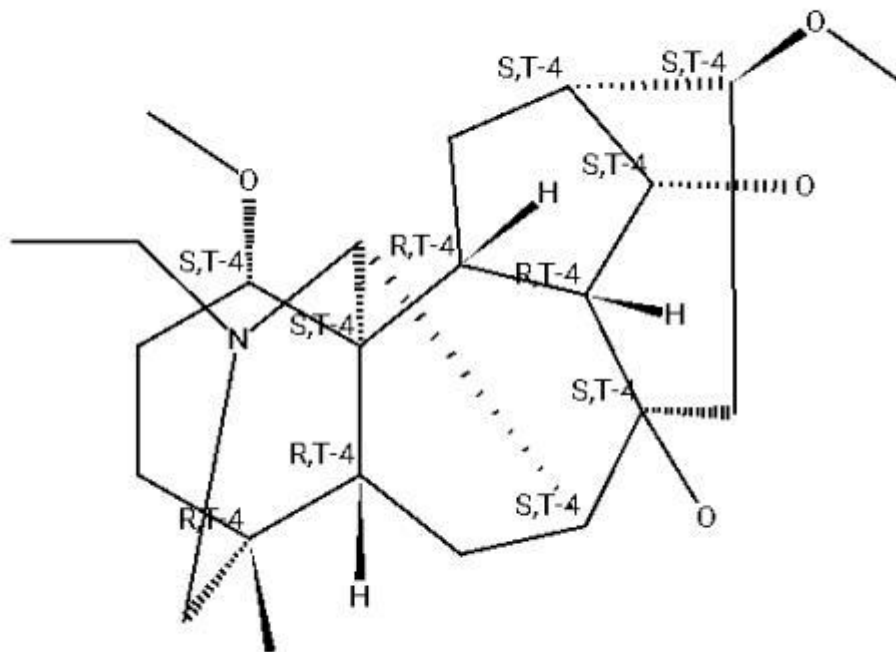
Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Accession Number	AN	Y	Y
Chemical Name	CN	Y	N
Molecular Weight	MW	N	Y
Number of Components	NC	N	Y
Reference Count	RE (RE.CNT)	N	Y
CAS Registry Number	RN	Y	N
Substance Descriptor	SD	Y	N

(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.

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



REAXYSFILESUB

D BIB HITSTR (crossover from REAXYSFILESUB to REAXYSFILEBIB)

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)

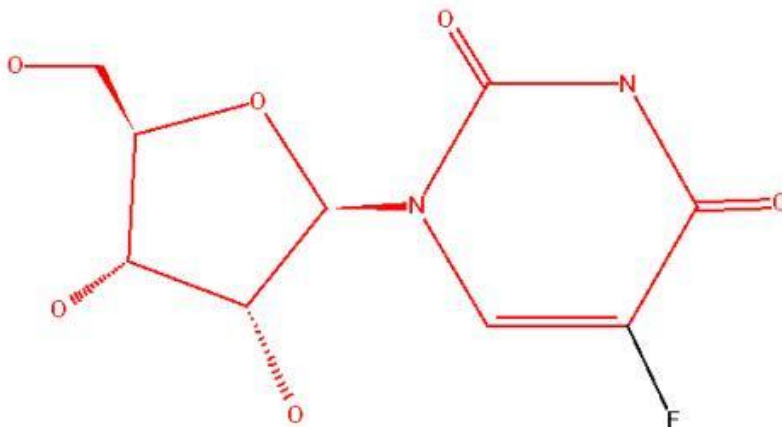
AN 33662 REAXYSFILESUB

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



HIT structure(s)

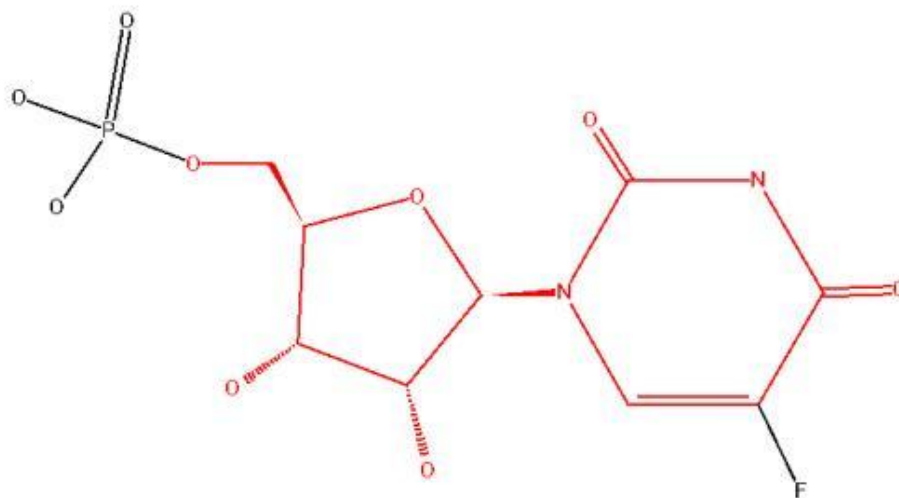
AN 53321 REAXYSFILESUB

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-
 dihydro-
 tetrahydro-furan-2-ylmethyl] ester

SD heterocyclic

MF C9 H12 F N2 O9 P

STR



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