

REAXYSFILESUB

Subject Coverage	<ul style="list-style-type: none"> • 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 STNnext			
Features	Alerts (SDIs)	Will be available soon		
	CAS Registry Number® Identifiers	<input checked="" type="checkbox"/>	Page Images	<input type="checkbox"/>
	Keep & Share	<input type="checkbox"/>	SLART	<input checked="" type="checkbox"/>
	Learning Database	<input type="checkbox"/>	Structures	<input checked="" type="checkbox"/>
Record Content	<ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • more than 30.5 million records (02/21) 			
Coverage	1771- present			
Updates	Twice a week			
Language	English			
Database Producer	Elsevier Information Systems GmbH Theodor-Heuss-Allee 108 60486 Frankfurt am Main Germany Phone: +49 69 5050 4252 Fax: +49 69 5050 4254		Copyright Holder: Elsevier Properties SA Espace de l'Europe 3 CH-2000, Neuchâtel Switzerland	

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**Database
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E-mail: helpdesk@fiz-karlsruhe.de

Sources

- Chemistry Journals
 - Handbook of Organic Chemistry (published by F. Beilstein)
-

User Aids

- Online Helps (HELP DIRECTORY lists all help messages available)
 - STNGUIDE
-

Cluster

STN Database Cluster information will be available soon.

**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 Concentration	/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	/ELC	S 5/CL	MF
Element Count, Substance	/ELC.SUB	S 5/ELC.SUB	MF
Element Symbol	/ELS	S C25/ELS	MF
Element Symbol, Count	/ELS.CNT	S C25/ELS	MF
Element Symbol, SUB	/ELS.SUB	S C25/ELS	MF
Entry Date (1)	/ED	S L1 ED=JAN 2019	ED
Field Availability	/FA	S KW/FA	FA
Formula Weight (1)	/FW	S 3000<FW	FW
InChi Key	(or /MW) /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 ALLAN AN CMAN CMF CN COMPAN COMPN ED FW INCHI LSF MARKREF.CNT MF MW PG REC (RE,CNT) RN SD STR UP	Alternate InChi Key All Accession Numbers Accession Number Component Molecular Accession Number Component Molecular Formula Chemical Name Composition Accession Number Composition Concentration Entry Date Formula Weight InChi Key Linearized Structure Formula Count of Referenced Markush Structures Molecular Formula Molecular Weight Periodic Group Reference Count CAS Registry Number Substance Descriptor Structure Update Date	D AINCHI D ALLAN D AN D CMAN D CMF D CN D COMPAN D COMPN D ED D FW D INCHI D LSF D MARKREF.CNT D MF D MW D PG D REC D RN D SD D STR D UP
ALL (FULL) IDE SCAN TRIAL (TRI, SAMPLE, SAM, FREE) HIT HIT IDE	AN, CN, SD, COMPAN, COMPN, COMPC, MF, CMF, LSF, INCHI, AINCHI, MW, MARKREF.CNT, REC, ED, UP, STR AN, CN, SD, COMPAN, COMPN, COMPC, MF, LCMF, LSF, INCHI, AINCHI, MW, MARKREF.CNT, REC, ED, UP, STR CN, MF, SD, STR (random display, no answer number) AN, CN, MF, SD, STR All fields containing hit terms Complete IDE with HIT	D ALL D IDE D SCAN D 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.

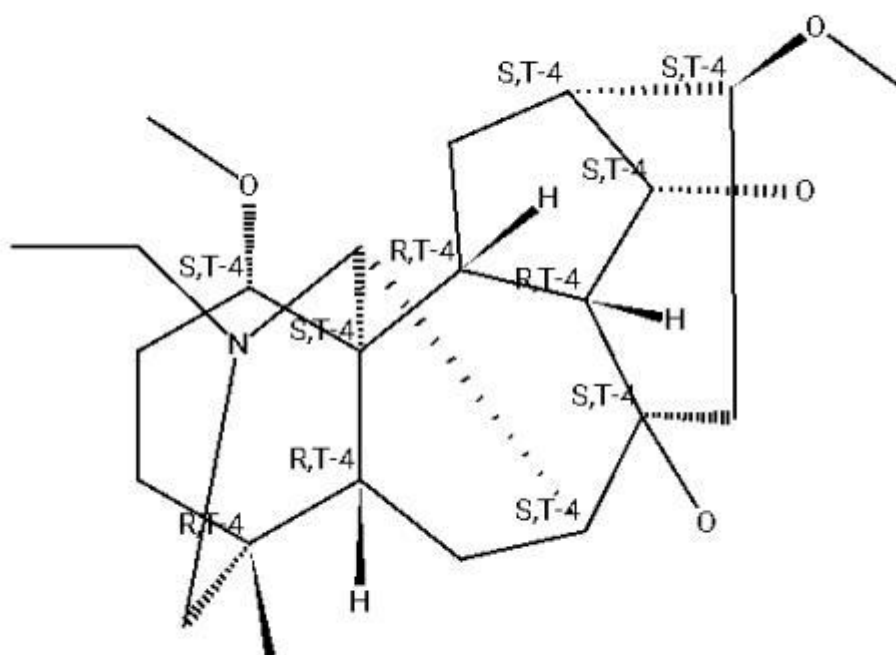
6

REAXYSFILESUB

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



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.

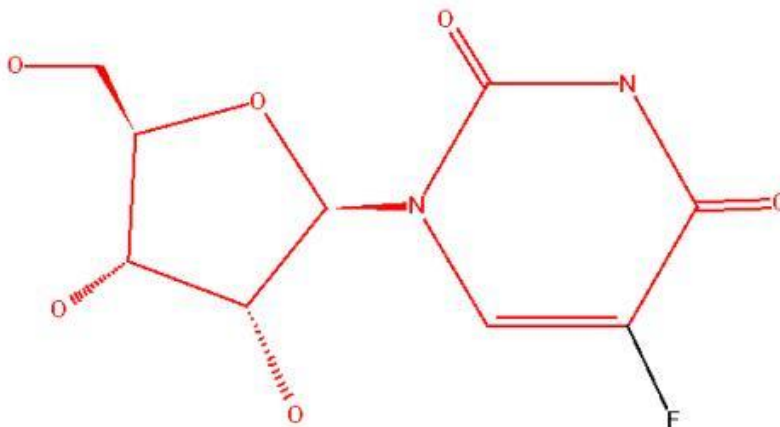
PI	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	WO 2020072976 *	A1	20200409	WO 2019-US54824	20191004

* = 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

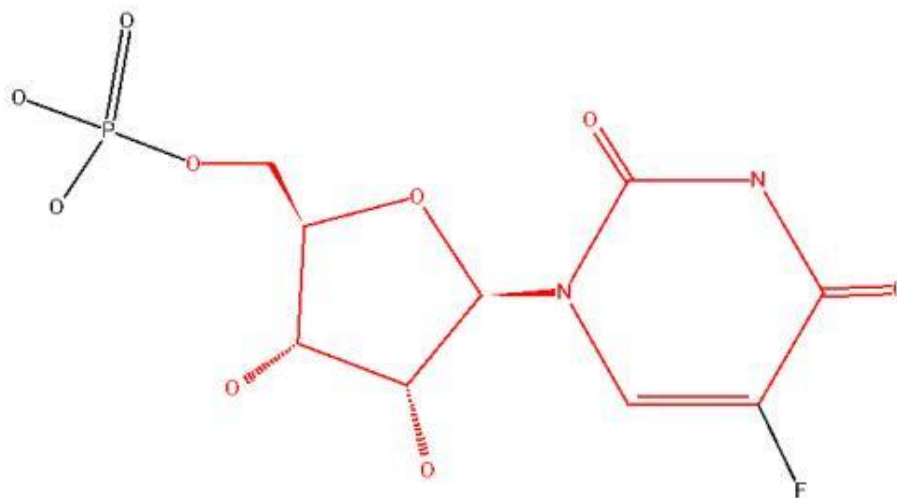
HIT structure(s)

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-
dihydroxy-
tetrahydro-furan-2-ylmethyl] ester
SD heterocyclic
MF C9 H12 F N2 O9 P
STR



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