



# REAXYSFILEBIB and REAXYSFILESUB on STNext



# Agenda

- Up-to-Date REAXYSFILE databases available on STNext
- REAXYSFILE Content and Coverage
- Structure information on STNext
- Crossfile search strategies in REAXYSFILE databases



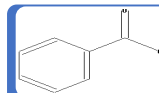
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# Up-to date ReaxysFile Databases on STNNext

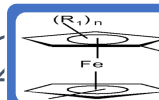
- REAXYSFILE**Sub**
  - **>34** million chemical substances (2/2021)
  - From 1771 to date
- REAXYSFILE**Bib**
  - **10.8** million bibliographic references (2/2021)
  - Patent and Nonpatent Literature records
  - Both databases are updated twice weekly



Organic



Inorganic



Organometallic

# Reaxysfile answers the following questions

- Does this compound exist?
  - the latest chemistry literature and patents
- What do we know about it?
- Is it involved in novel research?
  - Patent data from relevant offices, including Asia
- Who else is working on it?
  - Combined data in one substance record



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# Substances covered in REAXYSFILESub



- Substance records include data from different patents and non-patent sources
- All classes of substances including inorganic substances, coordination compounds, polymers, materials, enzymes etc.
  - (Bio)polymers and mixtures are included from 1995 onwards
  - Many polymers, enzymes, biosequences, alloys or mixtures are indexed without a topological structure (“substance image not available”)

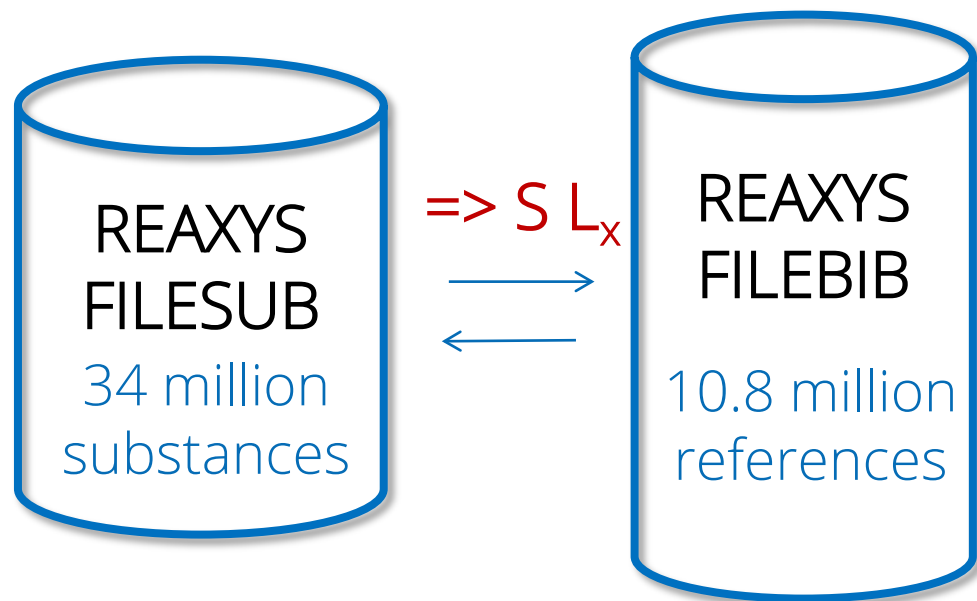
# Chemistry Patent Coverage in ReaxysFile Databases

- More than 2.1 million chemistry patent records (2/2021)
  - Substance data from >34 million substances
- Selected historical patent information from about 1803-1984
- 1984 – present: systematic patent coverage from 26 patent authorities:  
US, DE, FR, GB, JP, CH, SU, BE, NL, DD, ZA, AT, HU, CA, IT, PL, SE, RU, ES, NO, CZ, IN, DK, FI, IL, YU
- In-depth patent information for major patent authorities
  - English language patents from [US/EP/WO](#) from 1976
  - Asian patents of [JP/KR](#) from 2015 and [CN/TW](#) from 2016





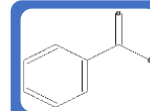
# ReaxysFile Databases on STNNext: Important Resource of Prior Art



- Powerful structure retrieval options including SAMPLE, FULL, BATCH
- Convenient crossfile searching from substances to biblio and vice versa
- Integrated display for bibliographic records including HIT structures
- Multifile searching with STN patent and bibliographic databases fully supported

# Up-to date ReaxysFile databases complement the chemistry portfolio of STN

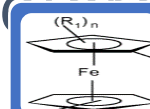
- REAXYSFILE**Sub** | > 34 M structures
  - From 1771 to date
  - Organic and inorganic chemical substances
- REAXYSFILE**Bib** | > 10.8 M bibliographic references
  - From 1771 to date
  - Bibliographic documents from handbooks of organic chemistry, chemistry journals and chemistry patents
  - Both databases are updated **twice weekly**



Organic



Inorganic



Organometallic

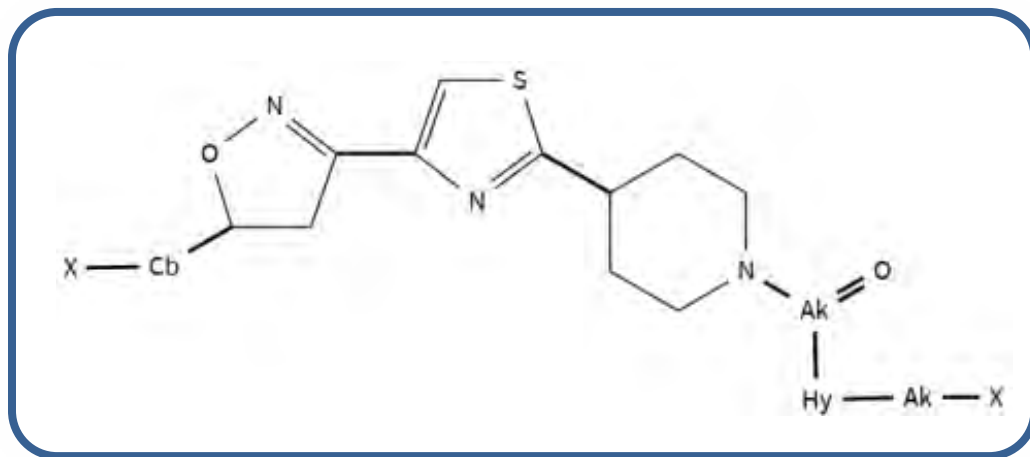


# Agenda

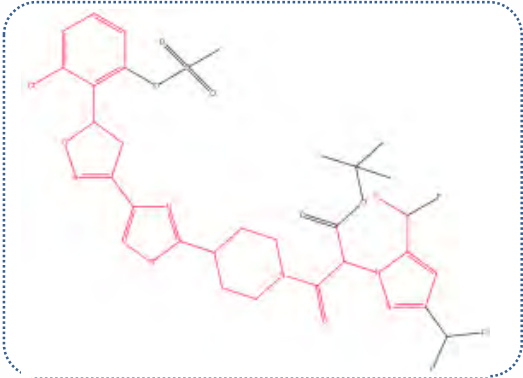
- Up-to-Date REAXYSFILE databases available on STNext
- REAXYSFILE Content and Coverage
- Structure information on STNext
- Crossfile search strategies in REAXYSFILE databases



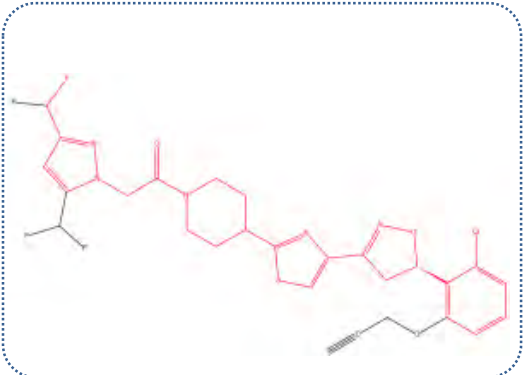
# Chemical structures in STNNext



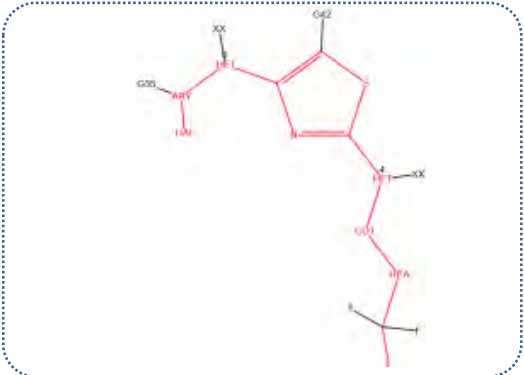
REAXYSFILESUB  
> 34 M structures



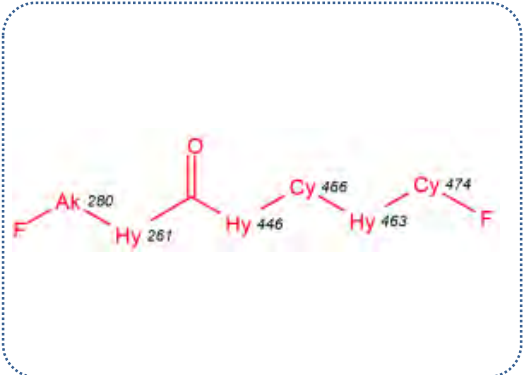
DCR: Derwent  
Chemistry Resource  
> 2.8 M structures



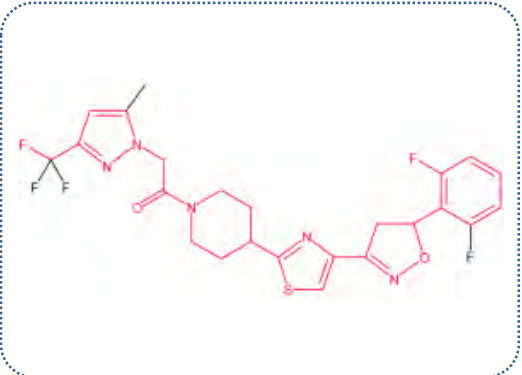
DWPIM  
> 2.3 M structures



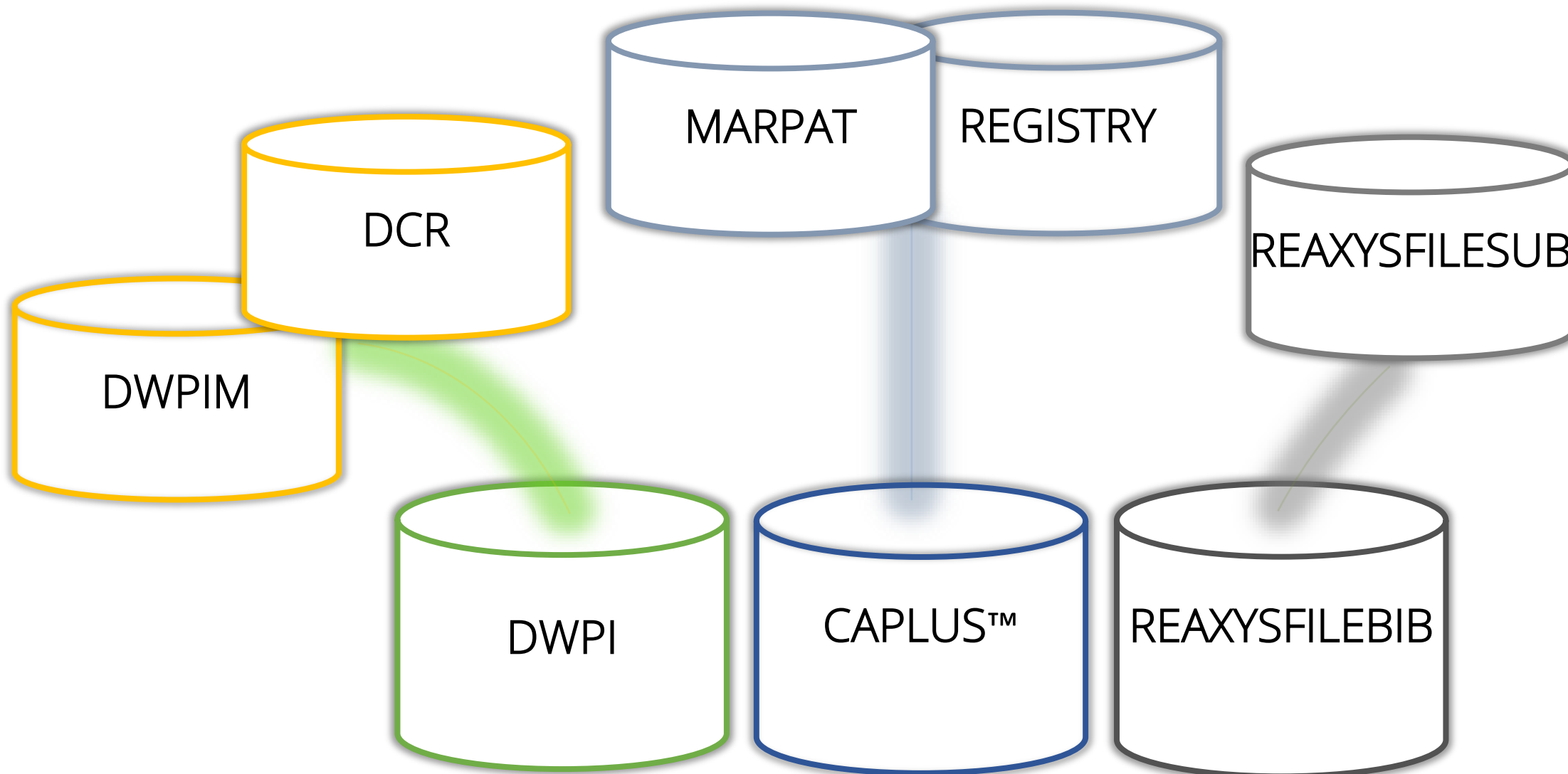
MARPAT®  
> 1.1 M structures



CAS Registry®  
> 159 M substances

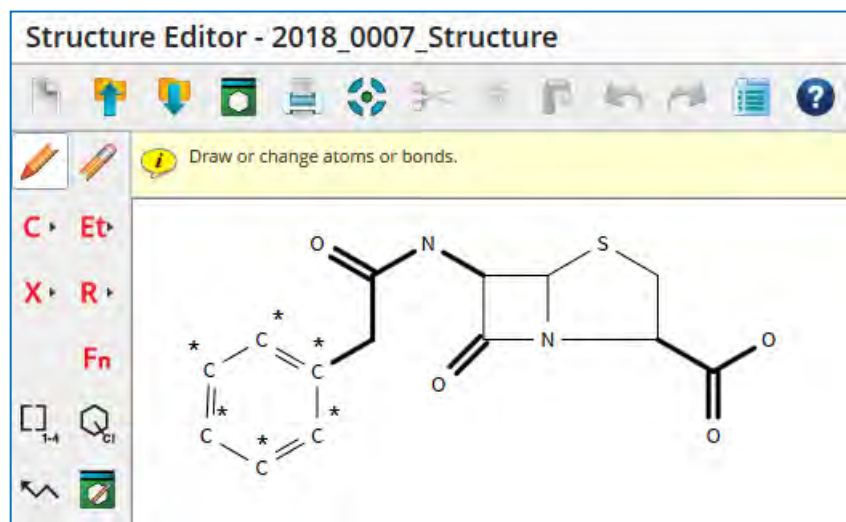


# Structure database interaction on STN





# REAXYSFILESUB Structure Searching and Crossover is Similar to DCR/DWPI and REGISTRY/CAplus



=> FILE REAXYSFILESUB

1

=>

Uploading structure file: 2018\_0006\_Structure  
L1 STRUCTURE UPLOADED

=> S L1 SSS FULL

100.0% PROCESSED 0 ITERATIONS 5122 ANSWERS  
L2 5122 SEA SSS FUL L3

=> FIL REAXYSFILEBIB

2

=> S L2

L3 7203 L5

=> D ALL HITSTR

3

1 REAXYSFILESUB structure search

2 Crossover to REAXYSFILEBIB

3 REAXYSFILEBIB display with HIT structures

# ReaxysFileSub and ReaxysFileBib Provide Unique Structure Information for Patents

*DWPI:* New benzylic compound having only one hydroxyl group substituted by organic group having specific aliphatic hydrocarbyl group, used for e.g. producing .....

Assignee (AJIN-C) Ajinomoto Co Inc

## Chemical Indexing:

Extended Patent Family			
US20110160433 A1 *		DWPI	20 specifics + 7 Markus
W02011078295 A1		REAXYSFILEBIB	43 specifics
EP2518041 A1		CAplus	76 specifics + 1 Markus
JP2011547615X		REAXYSFILEBIB	88 specifics
IN2012DN06545 A			
US8859732 B2		DWPI	1 specific + 1 Markush
US20140371424 A1			
US9206230 B2 *			

# HIT Structure Highlighting is Valuable to Assess Structure-based Results

=> D ALL HITSTR

L4 ANSWER 1 OF 7203 REAXYSFILEBI COPYRIGHT 2018 ELSEVIER INC. on STN.

AN 71263694 REAXYSFILEBI

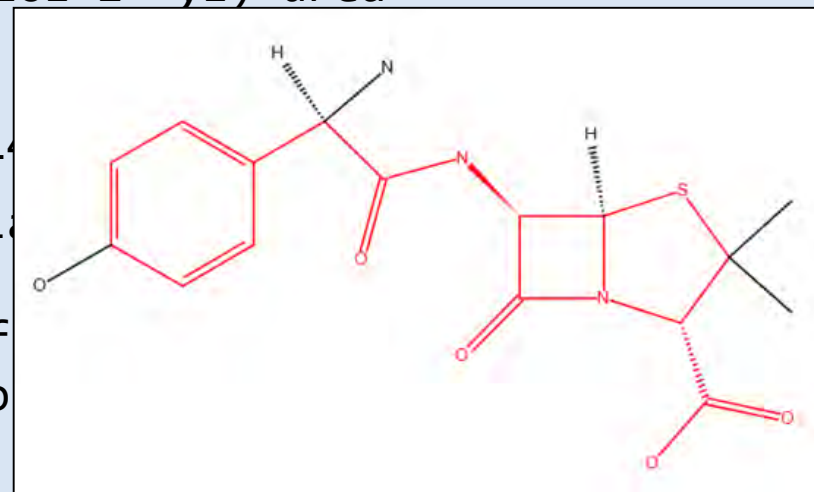
TI Crystal structure, spectral property, antimicrobial activity and DFT calculation of N-(coumarin-3-yl)-N'-(2-amino-5-phenyl-1,3,4-thiadiazol-2-yl) urea

AU Zhang; Zhang; Chen; Li; Chai

SO Journal of Molecular Structure (2017), Volume 114

AB N-(coumarin-3-yl)-N'-(2-amino-5-phenyl-1,3,4-thiadiazol-2-yl) urea and characterized by elemental analysis, IR, <sup>1</sup>H NMR, spectroscopy, as well as by single-crystal X-ray diffraction analyses have indicated that the crystal structure of the compound in dimethyl sulfoxide (DMSO) solvent ....

KW Author Keyword: DFT calculations; DMSO; Spectroscopic studies; Unsymmetrical urea  
...



# REAXYSFILESUB and REAXYSFILEBIB provide unique structure information for patents

DWPI title  
organic  
producing peptide  
or peptide

New benzylic compound having only one hydroxyl group substituted by group having specific aliphatic hydrocarbyl group, used for e.g. compound and in reagent for protecting carboxyl group of amino acid

Inventor  
Assignee

DWPI Family
US20110160433 A1
W02011078295 A1
EP2518041 A1
JP2011547615X
IN2012DN06545 A
US8859732 B2

• DWPI

• CAplus

• ReaxysFileBib

## Chemical Indexing:

20 specifics + 7 Markush

76 specifics + 1 Ma

88 specifics

# New Synergies for REAXYS Files in the STN Environment

## - Duplicate Removal Options for REAXYSFILEBIB -

### Non Patent Literature



Journal of Pharmaceutical and Biomedical Analysis

Volume 145, 25 October 2017, Pages 765-772

Development and validation of a GC-MS method for the determination of hydroxyzine and its active metabolite, cetirizine, in whole blood

CAPLUS  
 BIOSIS  
 EMBASE™  
 ESBIODBASE  
 MEDLINE®  
 REAXYSBIB

=> SET DUPORDER FILE

=> DUP REM L<sub>CAPLUS</sub> L<sub>REAXYSBIB</sub> L<sub>BIOMED</sub>

=> D ALL 1-

### Patents



=> FILE REAXYSFILEBIB

=> S L7 AND P/DT

REAXYSFILEBIB

L8 98 L4 AND patents

=> TRANSFER L4 PNK

CAPLUS/DWPI

L9 TRANSFER patents : 1286

TERMS

L10 216 L9

=> S L8 NOT L10

REAXYSFILEBIB patents,

L11 8 L6 unique



# New Synergies for REAXYS Files in the STN Environment

## - Patent Family Sorting for REAXYSFILEBIB -

### FSORT in REAXYSFILEBIB

=> FIL REAXYSFILESUB

=> S ZOLEDRONIC ACID/CN

L1 5 ZOLEDRONIC ACID/CN

=> FIL REAXYSFILEBIB

=> S L1 AND P/DT

L2 121 L1 AND P/DT

=> FSORT L2

L3 121 FSO L13

3 Multi-record Families	Answers 1-6
Family 1	Answers 1-2
Family 2	Answers 3-4
Family 3	Answers 5-6
115 Individual Records	Answers 7-121
0 Non-patent Records	

FSORT can also be used for a multifile answer set of REAXYS-FILEBIB and CAPLUS/DWPI results

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- REAXYSFILE Content and Coverage
- Structure information on STNext
- Crossfile search strategies in REAXYSFILE databases



# Crossfile Search strategies in REAXYSFILESUB/BIB

- Starting in REAXYSFILESUB
  - Draw a structure, if needed, in the STN Structure Editor
  - Use the structure or other non-structure substance information to retrieve substance answer set
  - Cross-file search substance sets in REAXYSFILEBIB to retrieve references
- Starting in REAXYSFILEBIB
  - Use keywords, descriptive data, or other concepts to search for classes of substances, novel types of substances, or substances lacking well-defined structures
  - Cross-file search answer sets in REAXYSFILESUB to find all indexed substances in the bibliographic references

# Structure drawing

Structure Editor

130018-77-8

Draw or change atoms or bonds. Shortcut Keys

The screenshot shows a chemical structure editor window. The main canvas displays a chemical structure consisting of a piperazine ring connected to a cyclohexane ring, which is further connected to a chlorocyclohexane ring. The interface includes a toolbar at the top with various drawing tools, a command line at the bottom left with the letter 'C' entered, and a properties panel on the right side. The properties panel is titled 'Attribute Values' and contains several sections: 'Bond Type' (Chain, Ring, Ring / Chain), 'Bond Value' (Exact, Normalized, Exact / Normalized), 'Node Type' (Chain, Ring, Ring / Chain), 'Generic Definition' (Saturated / Unsaturated, Linear / Branched, Monocyclic / Polycyclic, 1 hetero atom / 2+ hetero atoms, 1-6 carbons / 7+ carbons), 'Match Level' (Atom, Class, Any), 'Element Count Level' (Limited, Unlimited), and 'Other Node Attributes' (Mass, Valency, Hydrogen Count, Non-Hydrogen Count, Element Count).

Use the text-to-structure tool to create a preliminary structure

Modify the structure as desired to meet search requirements – flatten stereo bonds, set bonds to unspecified order, etc.

# Structure drawing

The screenshot displays the 'Structure Editor' software interface. At the top, there is a title bar with the text 'Structure Editor'. Below it is a toolbar with various icons for file operations and editing. A search bar contains the text '130018-77-8'. The main workspace shows a chemical structure of a complex molecule with a central nitrogen atom connected to a piperazine ring, a cyclohexane ring, and a chlorocyclohexane ring. The interface includes a left sidebar with drawing tools, a top status bar with the text 'Draw or change atoms or bonds.', and a bottom toolbar with buttons for 'Upload', 'Save', 'Save As', and 'Cancel'. A text input field at the bottom left contains the letter 'C'. The right sidebar contains a panel titled 'Attribute Values' with various settings for bond type, bond value, node type, generic definition, match level, and element count.

Use the text-to-structure tool to create a preliminary structure

Modify the structure as desired to meet search requirements – flatten stereo bonds, set bonds to unspecified order, etc.

Use "Save As" to specify the structure's file name.



# Multiple fields are available for searching chemical information in REAXYSFILESUB without a structure

- Chemical names
- Chemical name segment
- Molecular formula
- Component molecular formula
- Element count
- Element symbol
- Substance descriptor
- INCHI key

/CN

/CNS

/MF

/CMF

/ELC

/ELS

/SD

/INCHI



# Other ways of searching substances

=> E ARTEMISIN/CN

E1 1 ARTEMISIIFOLIN-6-0-03C/CN  
E2 1 ARTEMISIIFOLIN-PYRAZOLIN/CN  
E3 5 --> ARTEMISIN/CN  
E4 1 ARTEMISIN ALCOHOL/CN  
E5 1 ARTEMISIN-(SUP)18(/SUP)02/CN  
...

=> S C21H25CLN203/MF

L6 398 C21H25CLN203/MF

=> S AL/ELS AND CU/ELS AND ZN/ELS

105210 AL/ELS  
265793 CU/ELS  
145181 ZN/ELS  
L7 212 AL/ELS AND CU/ELS AND ZN/ELS

Additional approaches to searching for substances in REAXYSFILESUB include chemical name (/CN), molecular formula (/MF), elemental composition, and others.

# Upload structure

My Files Sarah S

Structures (15) Sort: Date Modified: Newest

Move to Folder Search Files by Name Import Biosequence Import Structure

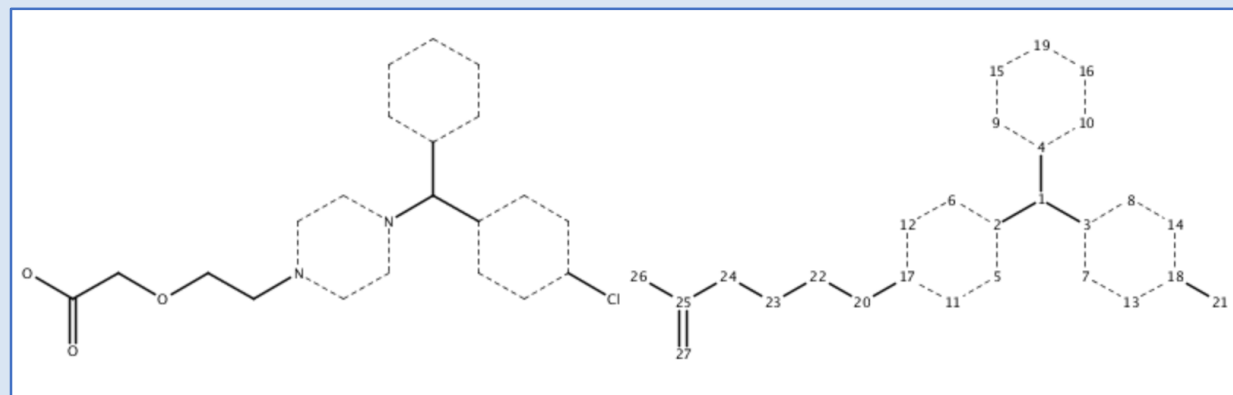
levocetirizine flat 2021 Feb 9 1:37 PM Edit Upload ...

=> FILE REAXYSFILESUB

=>

Uploading structure file: levocetirizine

L1 STRUCTURE UPLOADED



# Run the structure search in REAXYSFILESUB

=> S L1 SSS FULL

FULL SEARCH INITIATED 19:48:57

FULL SCREEN SEARCH COMPLETED - 33741168 TO ITERATE

100.0% PROCESSED 33741168 ITERATIONS

156 ANSWERS

SEARCH TIME: 00.00.07

L2 156 SEA SSS FUL L1

156 structures in the file  
match our query as searched

# Crossover to REAXYSFILEBIB and search structure

=> FILE REAXYSFILEBIB

=> S L2

L3            2425 L2

=> S L3 AND PATENT/DT

1803909 PATENT/DT

L4            192 L3 AND PATENT/DT

=> S L4 AND PY>=2010

6953222 PY>=2010

L5            123 L4 AND PY>=2010

Enter REAXYSFILEBIB and search the  
structure answer set from  
REAXYSFILESUB

Refine larger answer sets  
according to search requirements  
– document type, publication  
date, keywords, etc.



# Use D SCAN to preview results; refine further as

=> D SCAN

L5 123 ANSWERS REAXYSFILEBI COPYRIGHT 2021 ELSEVIER INC. on STN.

TI POLYMORPHIC FORMS OF DIHYDROCHLORIDE SALTS OF CETIRIZINE AND PROCESSES  
FOR PREPARATION THEREOF

DT Patent

IPC C07D0295-00; C07D0295-08; A61K0031-495

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L5 123 ANSWERS REAXYSFILEBI COPYRIGHT 2021 ELSEVIER INC. on STN.

TI Levocetirizine hydrochloride compound and preparation method thereof (by  
machine translation)

DT Patent

IPC C07D0295-088; A61P0029-00; A61P0037-08

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

# DISPLAY Records

=> D L5 1- BIB ABS

L5 ANSWER 5 OF 123 REAXYSFILEBI COPYRIGHT 2021 ELSEVIER INC. on STN.

AN 79517394 REAXYSFILEBI

TI Preparation method of levocetirizine (by machine translation)

PA Hunan Jiu Dian Hongyang Pharmaceutical Co., Ltd.; Tan Junhua; Hu Kuang

PI	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
	CN 110950821 *	A	20200403	CN 2020-10114345	20200225
	CN 110950821	B	20200515	CN 2020-10114345	20200225

\* = indexed patent

PRAI CN 2020-10114345 20200225

ED Entered STN: 18 Nov 2020

Last updated on STN: 19 Jan 2021

AN 79517394 REAXYSFILEBI

AB Shows that the compound of Formula: is converted into levocetirizine ...

# Searching for substances starting in ReaxysfileBib

- Searches may not be precise; however, this is an easier way to find substances that may be challenging to find through other searches
- Search in TI > AB > BI
- Useful for e.g. polymers and pharmaceuticals (formulations)
- Useful for “novel exotic” substances lacking well-defined structures, e.g. CH<sub>5</sub><sup>+</sup> (methanium ion, formation in space, only conceptual)
- Use S L<sub>x</sub> to evaluate indexed substances within bibliographic documents

# Search a class of substances in REAXYSFILEBIB

```
=> S ((?SUPER? OR ?ULTRA?) (T) (?HYDROPHOB?)) (5A) (?POLYMER? OR ?MACROMOLECUL?)
```

```
447964 ?SUPER?
```

```
303112 ?ULTRA?
```

```
107636 ?HYDROPHOB?
```

```
581255 ?POLYMER?
```

```
26221 ?MACROMOLECUL?
```

```
L8 377 ((?SUPER? OR ?ULTRA?) (T) (?HYDROPHOB?)) (5A) (?POLYMER? OR ?MACROMOLECUL?)
```

```
=> S L8 AND (?ANTIREFLECT? OR ANTI REFLECT? OR ?REFLECT?)
```

```
1887 ?ANTIREFLECT?
```

```
399620 ANTI
```

```
5 ANTIS
```

```
399623 ANTI
```

```
(ANTI OR ANTIS)
```

```
204883 REFLECT?
```

```
1144 ANTI REFLECT?
```

```
(ANTI(W)REFLECT?)
```

```
207281 ?REFLECT?
```

```
L9 9 L8 AND (?ANTIREFLECT? OR ANTI REFLECT? OR ?REFLECT?)
```

# Enter REAXYSFILESUB and retrieve indexed substances

```
=> FILE REAXYSFILESUB
```

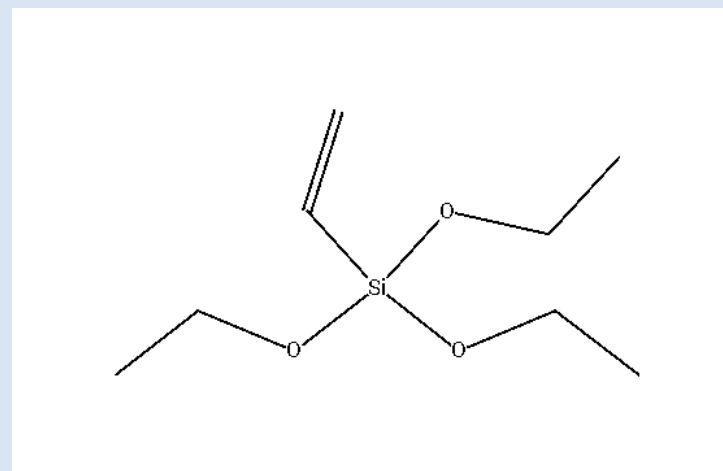
```
=> S L9
```

```
L10          14 L9
```

```
=> D L10 1-
```

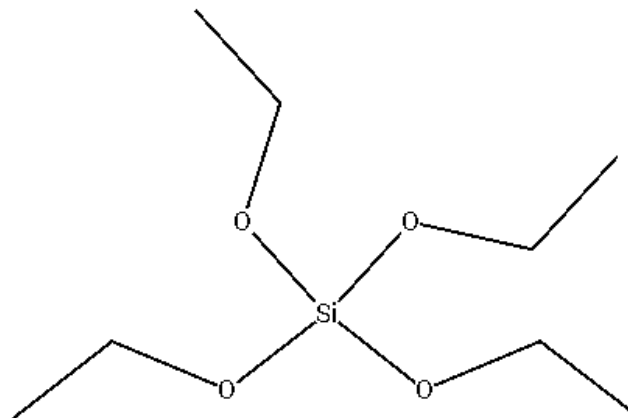
```
AN      1767229  REAXYSFILESU
RN      78-08-0
CN      Triethoxyvinylsilane; Vinyltriethoxysilan; triethoxyvinylsilane
SD      acyclic
MF      C8 H18 O3 Si
LSF     H2CCHSi(OC2H5)3
INCHI   FWDBOZPQNFPOLF-UHFFFAOYSA-N
AINCHI  FWDBOZPQNFPOLF-UHFFFAOYAZ
MW      190.315
MARKREF.CNT 13
REC     1781
ED      Entered STN: 14 Jul 2020
        Last updated on STN: 2 Mar 2021
```

The 9 documents that our keyword search retrieved contain 14 indexed substances.



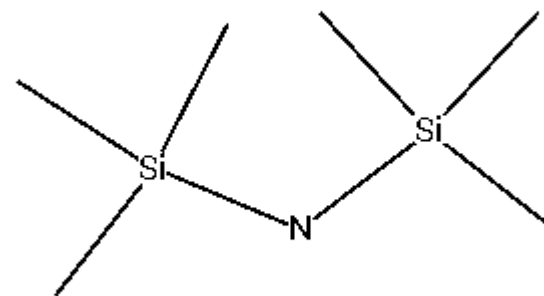
# View all indexed substances in bibliographic document set

AN 1422225 REAXYSFILESU  
RN 78-10-4  
CN tetraethoxy orthosilicate; tetr aethyl ortosilicate;  
tetraethoxyorthosilicate; teraethyl orthosilicate;  
teraethylorthosilicate; silicon tetraethoxide; tetraethoxysilicate  
SD acyclic  
MF C8 H20 04 Si  
LSF Si(OCH3CH2)4  
INCHI BOTDANWDWHJENH-UHFFFAOYSA-N  
AINCHI BOTDANWDWHJENH-UHFFFAOYAS  
MW 208.33  
MARKREF.CNT 26  
REC 21577  
ED Entered STN: 13 Jul 2020  
Last updated on STN: 2 Mar 2021



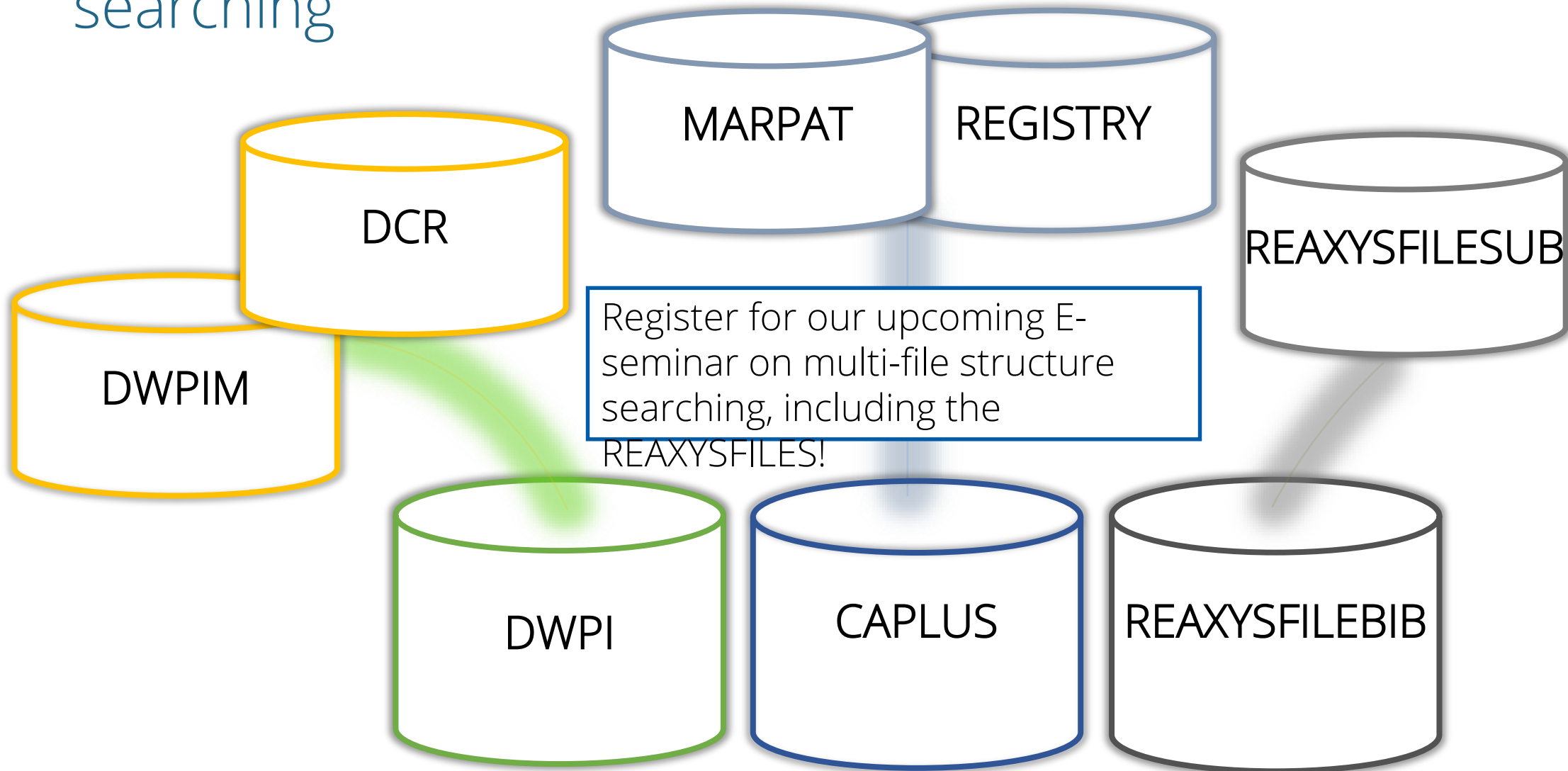
# View all indexed substances in bibliographic document set

AN 635752 REAXYSFILESU  
RN 999-97-3  
CN 1,1,1,3,3,3-hexamethyl-disilazane; 1,1,1,3,3,3-hexamethyldisilazane; ;  
1,1,3,3,3-hexamethyldisilazane; Hexamethyldisilazane;  
bis(trimethylsilyl)amine  
SD acyclic  
MF C6 H19 N Si2  
LSF Si2NH(CH3)6  
INCHI FFUAGWLWBBFQJT-UHFFFAOYSA-N  
AINCHI AVKNGPAMCBSNSO-UHFFFAOYAS  
MW 161.395  
MARKREF.CNT 14  
REC 8756  
ED Entered STN: 13 Jul 2020  
Last updated on STN: 2 Mar 2021





# Multiple Structure/Bib file pairs for more comprehensive searching



# Useful Tips

Especially before crossfile searching consider the following:

- In ReaxysfileSub after a structure or text search
  - S L# NOT 0/REC to eliminate substances without corresponding references in ReaxysfileBib
  - S L# NOT markush substance/SD or L# AND markush substance/SD to eliminate or split off the Markush Substances; Markush Substances are not structure-searchable
- In ReaxysfileBib
  - Many references have no substances assigned; indexing rules allow so-called “concepts” without specific or generic structures



# Summary

- Up-to-date Reaxysfile is available as REAXYSFILESUB and REAXYSFILEBIB on STNext
- Reaxysfile patent indexing contains additional relevant substance information, thus being an important source for e.g. FTO searches
- REAXYSFILESUB/BIB structure search options and cross-database searching is consistent with other substance/bibliographic database pairs on STNext



# Get the monthly STN Trainings & Events Newsletter

**STN**  
THE CHOICE OF PATENT EXPERTS™

ABOUT STN PRODUCTS & SERVICES CUSTOMER SUPPORT **RESOURCES** TRAINING CENTER

## Resources

We provide STN-related topics in our newsletters, and product introductions and overviews in our brochures.

- Announcements from Patent Offices (COVID-19)
- STNewline / STN News
- INPADOC on STN News and Newsletter
- STN Trainings & Events Newsletter**
- Brochures

39

# Questions? Feedback?



**Email:**  
[sarah.stokes@fiz-k.com](mailto:sarah.stokes@fiz-k.com)

**CAS** [help@cas.org](mailto:help@cas.org)  
[www.cas.org](http://www.cas.org)

**FIZ Karlsruhe** [helpdesk@fiz-](mailto:helpdesk@fiz-karlsruhe.de)  
[www.stn-](http://www.stn-international.de)  
[international.de](http://www.stn-international.de)

