

# STN<sup>®</sup>

ReaxysFile on STN<sup>®</sup>

Robert Austin – FIZ Karlsruhe

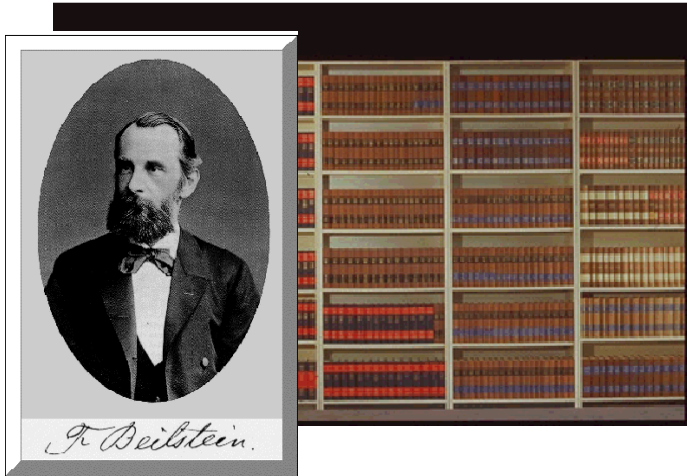
# Agenda

- What is ReaxysFile?
- Find substances
- Find reactions
- Searching bibliographic data
- Physical properties
- EcoPharm data
- Chemical data
- Basic tips for managing display costs

# What is ReaxysFile?

- The world's largest collection of organic reactions and chemical facts
- Substance based database of structures, substance identification and reaction data
- Citations to journal and patent references
- Numerically searchable physical properties
- Pharmacological and ecological data

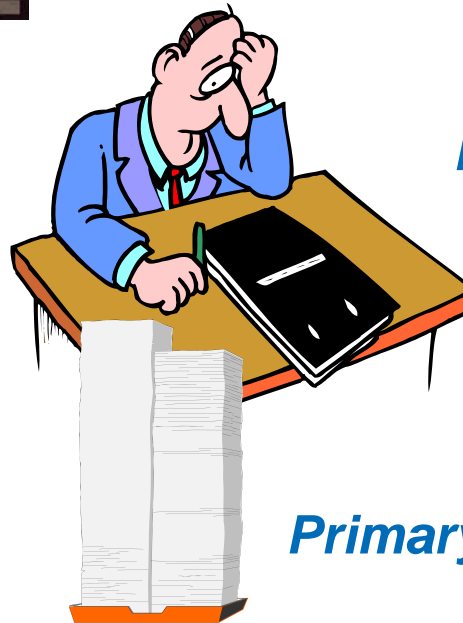
# ReaxysFile data sources



*Handbook 1771-1959*



*Primary literature >1979*



*Primary literature 1960 -1979*

# ReaxysFile on STN

- File REAXYSFILE
  - More than 10 million substances
  - More than 10 million reactions
  - More than 2 million citations 1771-date
- File BABS
  - Bibliographies and Abstracts of the ReaxysFile
  - Over 1 million abstracts and titles 1980-date

# New fields and new field names in ReaxysFile, December 2010

<u>Field qualifier</u>	<u>ReaxysFile field name</u>
<b>AN</b>	Accession Number
<b>BPR</b>	Basic Preferred Registry Number
<b>HSO</b>	Handbook Citation
<b>AAN</b>	ALL Accession Numbers
<b>COMPAN</b>	Composition: Compound Accession Number
<b>FAN</b>	Fragment Accession Number
<b>RX.AAN</b>	All Accession Numbers Reaction
<b>RX.RAN</b>	Reactant Accession Number
<b>RX.PAN</b>	Product Accession Number
<b>xxxx.PAAN</b>	[ <i>property</i> ] Partner Accession Number
<b>xxxx.AN</b>	[ <i>property</i> ] Accession Number

A full list of all new fields and new field names is available:  
[http://www.stn-international.com/stn\\_chemistry\\_reaxysfile.html](http://www.stn-international.com/stn_chemistry_reaxysfile.html)

# Typical questions for ReaxysFile

- Determine if a substance has been described in past chemical literature, e.g. a prior art search
- Find comprehensive chemical/physical data for a substance via a CAS Registry Number<sup>®</sup>
- Search for members of a substance family with boiling points in a certain temperature range measured at 760 Torr
- Find ways to synthesize a substance

# Ways to search ReaxysFile

- Structure/Substructure
- Chemical Name
- Chemical Name Segment
- CAS Registry Numbers
- Physical properties or keyword
- EcoPharm data
- Bibliographic data
- .....

# ReaxysFile sample record

=> FILE REAXYSFILE

=> S 9759486/AN

L1 1 9759486/AN

=> D IDE

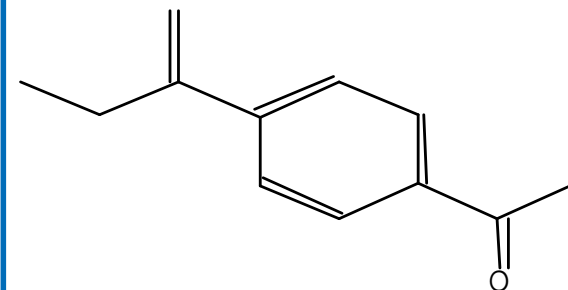
L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier

ReaxysFile substance records can be retrieved via their unique Accession Number (AN).

Substance Identification Information (IDE) display.

Accession Number (AN):	9759486
CAS Reg. No. (RN):	42427-52-1
Chemical Name (CN):	2-(4-acetylphenyl)but-1-ene
Autonom Name (AUN):	1-<4-(1-ethyl-vinyl)-phenyl>-ethanone
Molec. Formula (MF):	C12 H14 O
Molecular Weight (MW):	174.24
Lawson Number (LN):	7276
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	8220680
Entry Date (DED):	2005/01/21
Update Date (DUPD):	2005/01/21

Chemical Structure.



# ReaxysFile sample record (cont.)

## Field Availability:

Code	Name	
AN	Accession Number	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
DED	Entry Date	1
DUPD	Update Date	1
NMR	Nuclear Magnetic Resonance	2

Substance Identification Information (IDE) (cont.)

Field Availability (FA) Table.

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXPRO	Substance is Reaction Product	2

# ReaxysFile sample record (cont.)

=> D NMR

Property data, e.g. NMR.

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Nuclear Magnetic Resonance:

NMR

Coupling Nuclei (.NUI) 1H-1H

Solvents (.SOL): CDC13

Frequency (.F): 300 MHz

Reference(s):

1. Peyroux, Eugenie; Berthiol, Florian; Doucet, Henri; Santelli, Maurice, Eur. J. Org. Chem., CODEN: EJOCFK(5), <2004>, 1075 - 1082; BABS-6451267

NMR

Description (.KW): Chemical shifts

Nucleus (.NUC): 1H

Solvents (.SOL): CDC13

Frequency (.F): 300 MHz

Reference(s):

1. Peyroux, Eugenie; Berthiol, Florian; Doucet, Henri; Santelli, Maurice, Eur. J. Org. Chem., CODEN: EJOCFK(5), <2004>, 1075 - 1082; BABS-6451267

# ReaxysFile sample record (cont.)

=> D RX

Reaction data, RX.

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier E

Reaction:

RX  
Reaction ID (.ID): 9659517  
Reactant AN (.RAN): 386015, 9757604  
Reactant (.RCT): 1-(4-bromo-phenyl)-ethanone,  
but-1-en-2-ylboronic acid  
Product AN (.PAN): 9759486  
Product (.PRO): 1-<4-(1-ethyl-vinyl)-phenyl>-ethanone  
No. of React. Details (.NVAR): 1

Reaction Details:

RX  
Reaction RID (.RID): 9659517.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 93 percent (AN =9759486)  
Reagent (.RGT): K2CO3,  
cis,cis,cis-tetrakis<(diphenylphospha  
nyl)methyl>cyclopentane  
Catalyst (.CAT): <Pd(C3H5)Cl>2  
Solvent (.SOL): xylene  
Time (.TIM): 20 hour(s)  
Temperat ( ) Cel  
Reaction BABS Accession Number. Suzuki reaction  
References:  
1. Peyroux, Eugenie; Berthiol, Florian; Doucet, Henri; Santelli,  
Maurice, Eur. J. Org. Chem., CODEN: EJOCFK(5), <2004>, 1075 -  
1082, **BABS-6451267**

# BABS sample record

=> FILE BABS

=> S 6451267/AN

L2 1 6451267/AN

BABS Accession Number (AN).

=> D IALL

L2 ANSWER 1 OF 1 BABS COPYRIGHT 2010 Elsevier Properties SA. on STN

ACCESSION NUMBER:

6451267 BABS

TITLE:

Suzuki Cross-Coupling Reactions between Alkenylboronic Acids and Aryl Bromides Catalysed by a Tetrakisphosphane-Palladium Catalyst

AUTHOR(S):

Peyroux, Eugenie; Berthiol, Florian; Doucet, Henri; Santelli, Maurice

SOURCE:

Eur. J. Org. Chem. (2004), (5), 1075 - 1082  
CODEN: EJOCFK

DOCUMENT TYPE:

Journal

ABSTRACT:

A range of alkenylboronic acids undergo Suzuki cross-coupling with aryl bromides in good yields in the presence of [PdCl(C<sub>3</sub>H<sub>5</sub>)]<sub>2</sub>/cis/cis/cis-1,2,3,4-[(tetrakis(diphosphanyl)methyl)cyclopentane as a catalyst. A wide variety of 1-arylprop-1-enes, 2-arylprop-1-enes, 2-arylbut-1-enes and 1,1-diarylethylene or styrene derivatives have been prepared. Moreover, the reaction tolerates several functions, such as acetyl, formyl, nitrile or nitro. Furthermore, this catalyst can be used at low loading, even for reactions of sterically hindered substrates.

CONTROLLED TERM(S):

alkenes; aryl halides; catalysis; cross-coupling; palladium; phosphanes

# Agenda

- What is ReaxysFile?
- **Find substances**
- Find reactions
- Searching bibliographic data
- Physical properties
- EcoPharm data
- Chemical data
- Basic tips for managing display costs

# How to search for substances

- Chemical Name (/CN)
- Chemical Name Segment (/CNS)
- CAS Registry Numbers (/RN)
- Molecular Formula (/MF)
- Structure/Substructure
- .....

# ReaxysFile substances

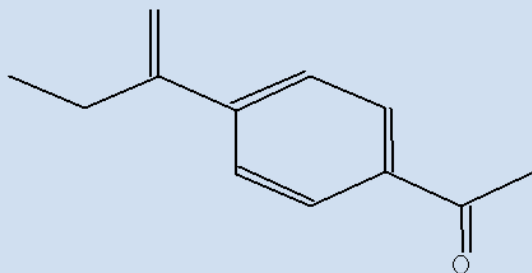
- Classical ReaxysFile Compounds
  - Organic compounds which contain only carbon and selected atoms from Group I, II, III, IV, V, VI, VII
  - Substances with one or more fragments
  - Peptides, Polysaccharides (small molecules)
- Other compound types
  - Biomolecules, Mixtures, Polymers

**Note:** “Other compound types” are included in ReaxysFile from 1995 onwards.

# How to search for substances

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):	9759486	/RN
CAS Reg. No. (RN):	42427-52-1	
Chemical Name (CN):	2-(4-acetylphenyl)but-1-ene	
Autonom Name (AUN):	1-<4-(1-ethyl-vinyl)-phenyl>-ethanone	/CN /CNS
Molec. Formula (MF):	C12 H14 O	/MF
Molecular Weight (MW):	174.24	
Lawson Number (LN):	7276	
Compound Type (CTYPE):	isocyclic	
Constitution ID (CONSID):	8220680	
Entry Date (DED):	2005/01/21	
Update Date (DUPD):	2005/01/21	



Structure search.

# Chemical Name Segments (/CNS)

- Name fragments from Chemical Name and Autonom Name fields
- Parsed at special characters and spaces
- Special characters are not indexed, e.g. “-”, “(“...

## Example:

**2- (2,4-dinitro-styryl) -1H-benzimidazole  
acetic acid**

# Search options related to MF

- Atom count /ATC
  - Total number of atoms in a molecule
- Element Count /ELC
  - Number of different elements in a molecule
- Element Count specific
  - Element index for each element in a molecule
  - E.g. 3 sulfur atoms: “S 3/S”

# Search options related to MF

- Element Ratio **/ELR**
  - Element count ratio for elements C, O, H and N
- Element Symbol **/ELS**
  - Element symbols of each element in molecules
- Periodic Group **/PG**
  - Periodic groups of each element in a molecule
- Number of Fragments **/NF**
  - Total number of fragments of a molecule

# Search example: MF related fields

## Search Question:

Find substances containing N, O, P and S elements with 5-10 carbon atoms, an H/C ratio greater than 2, excluding salts/adducts (multi-fragment compounds).

=> S N/ELS AND O/ELS AND P/ELS AND S/ELS

5392433 N/ELS

7286769 O/ELS

382810 P/ELS

1727736 S/ELS

L1 50964 N/ELS AND O/ELS AND P/ELS AND S/ELS

=> S L1 AND 5-10/C

1521245 5-10/C

L2 13544 L1 AND 5-10/C

Search for N, O, P, and S elements in /ELS.

Search the hit set for compounds with 5 - 10 carbon atoms.

# Search example: MF related fields (cont.)

```
=> S L2 AND ELR.HC>2
      352236 ELR.HC>2
L3      5716 L2 AND ELR.HC>2
```

Search the hit set for compounds with an element ratio H/C bigger than 2.

```
=> S L3 AND 1/NF
      7554162 1/NF
L4      3857 L3 AND 1/NF
```

Remove salts/adducts (limit to single fragment compounds).

```
=> D HIT
```

```
L4 ANSWER 1 OF 3857 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN
```

Molecular Formula (MF):

**C10 H23 N2 O6 P S3**

# Structure searching in ReaxysFile

- Standard STN structure search options
  - Exact (EXA), Family (FAM)
  - Substructure (SSS), Closed Substructure (CSS)
  - Full file (FULL), Sample (SAM)
- Subset structure searching is available

Learn more about the basics of structure searching:  
<http://www.cas.org/support/stngen/stndoc/structure.html>.

# CAS Registry Numbers (RN) in ReaxysFile

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):	2035920
Basic Pref. RN (BPR):	286-08-8
CAS Reg. No. (RN):	286-08-8, 54376-67-9
Chemical Name (CN):	
Autonom Name (AUN):	
Molec. Formula (MF):	
Molecular Weight (MW):	
Lawson Number (LN):	
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	1752035
Handbook Citation (HSO):	4-05-00-00257, 5-05, 6-05
Entry Date (DED):	1989/06/29
Update Date (DUPD):	2003/01/18
. . . .	

CAS Registry Numbers are:

- Extracted from the primary literature
- Derived from a match between ReaxysFile and CAS Registry

# ReaxysFile preferred CAS RN

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN) :	2035920
Basic Pref. RN (BPR) :	286-08-8
CAS Reg. No. (RN) :	286-08-8, 54376-67-9
Chemical Name (CN) :	
Autonom Name (AUN) :	
Molec. Formula (MF) :	
Molecular Weight (MW) :	
Lawson Number (LN) :	
File Segment (FS) :	
Compound Type (CTYPE) :	
Constitution ID (CONSID) :	1752035
Handbook Citation (HSO) :	4-05-00-00257, 5-05, 6-05
Entry Date (DED) :	1989/06/29
Update Date (DUPD) :	2003/01/18
. . . .	

## ReaxysFile Preferred CAS RN:

- Single CAS RN that has been selected as best choice from one or more RN's present in the database for a substance
- Not always present

# Stereoisomers and Constitution IDs

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN) :	2054549
CAS Reg. No. (RN) :	68-26-8, 2052-63-3, 6018-74-2, 17706-49-9, 22737-96-8, 22737-97-9, 29444-25-5, 34218-73-0, 39815-04-8, 69686-68-6, 69686-69-7, 74743-94-5, 84415-27-0, 84415-28-1, 85354-09-2, 85354-10-5, 93380-02-0, 98462-62-5, 137121-52-9
Chemical Name (CN) :	(7 $\xi$ ,11 $\xi$ )-retinol
Autonom Name (AUN) :	3,7-dimethyl-9-(2,6,6-trimethyl- cyclohex-1-enyl)-nona-2,4,6,8-tetraen-1
Molec. Formula (MF) :	C20 H30
Molecular Weight (MW) :	286.46
Lawson Number (LN) :	5494
File Segment (FS) :	Stereo compound
Compound Type (CTYPE) :	isocyclic
Constitution ID (CONSID) :	400280
. . . .	

Stereoisomers have different ANs, but have the same Constitution ID (CONSID).

# Stereoisomers and Constitution IDs (cont.)

```
=> S 400280/CONSID
L2      15 400280/CONSID
=> D
```

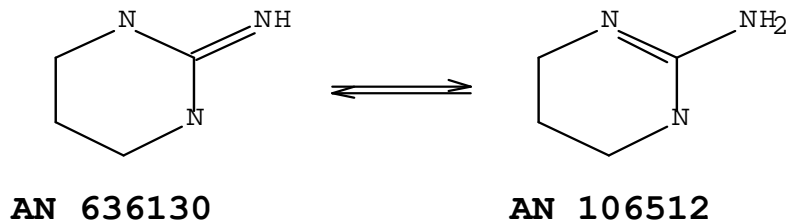
A search for the CONSID retrieves  
15 stereoisomer records.

```
L2 ANSWER 1 OF 15 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN
```

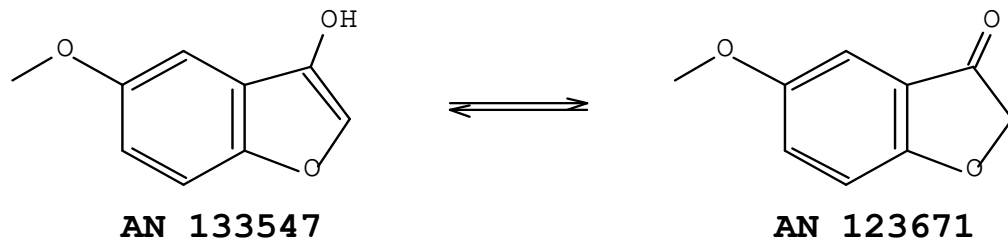
```
Accession Number (AN):      8920721
Chemical Name (CN):         3,7-dimethyl-9-(2,6,6-trimethyl-
                             cyclohex-1-enyl)-nona-2,4,6,8-te
                             traen-1-ol
Autonom Name (AUN):        3,7-dimethyl-9-(2,6,6-trimethyl-
                             cyclohex-1-enyl)-nona-2,4,6,8-te
                             traen-1-ol
Molec. Formula (MF):       C20 H30 O
Molecular Weight (MW):     286.46
Lawson Number (LN):       5494
File Segment (FS):        Stereo compound
Compound Type (CTYPE):    isocyclic
Constitution ID (CONSID):  400280
Entry Date (DED):         2002/01/24
Update Date (DUPD):       2002/01/24
. . . .
```

# A note on tautomers in ReaxysFile

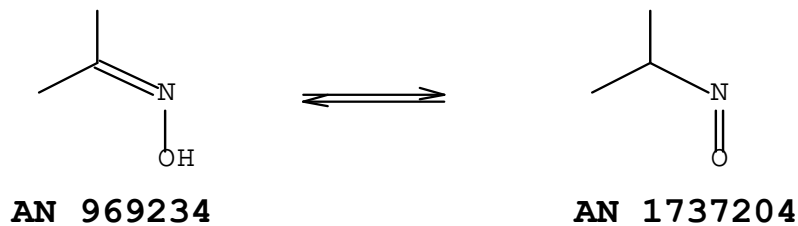
- Imino-amino tautomers



- Enol-keto tautomers



- Nitroso-oxime tautomers



Tautomers are assigned unique Accession Numbers (ANs).

# ReaxysFile substances

- Classical ReaxysFile Compounds
  - Organic compounds which contain only carbon and selected atoms from Group I, II, III, IV, V, VI, VII
  - Substances with one or more fragments
  - Peptides, Polysaccharides (small molecules)
- Other compound types
  - Biomolecules, Mixtures, Polymers

**Note:** “Other compound types” are included in ReaxysFile from 1995 onwards.

# ReaxysFile Compound Types (CTYPE)

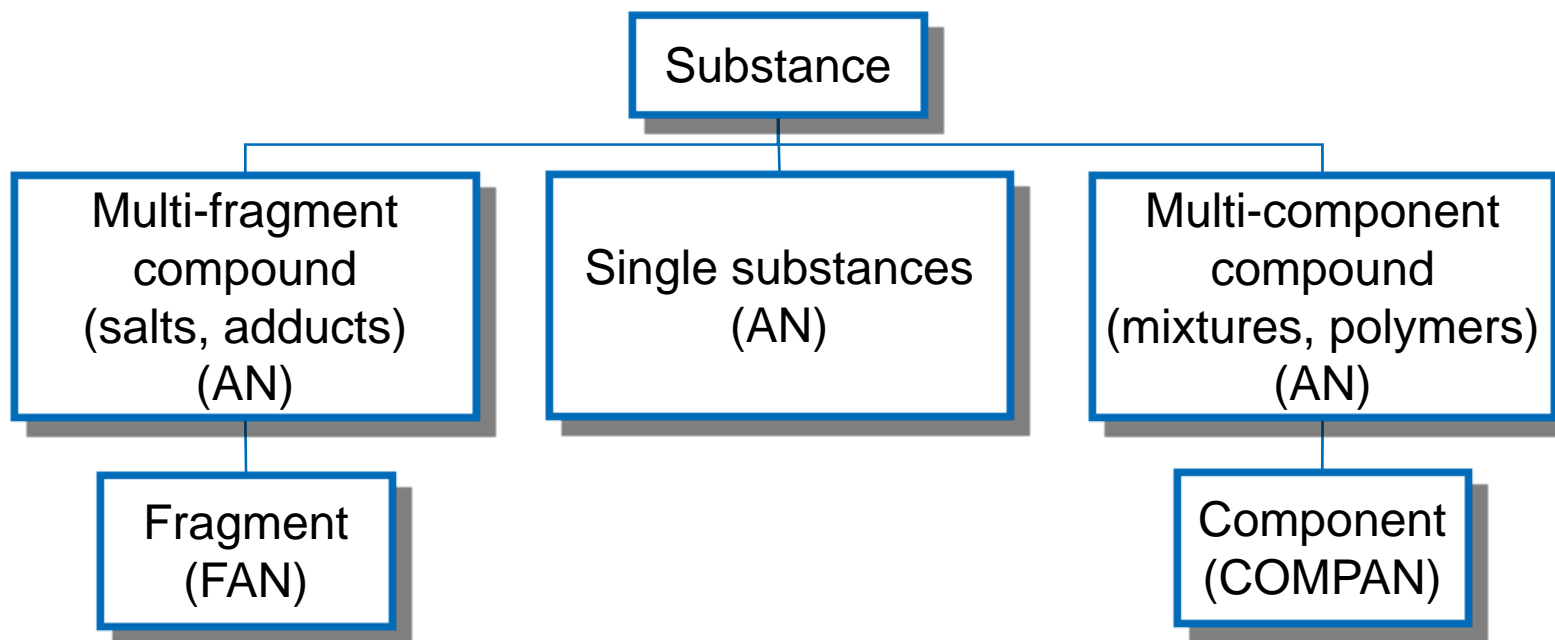
L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN): 8808326  
Chemical Name (CN): (R)-  
ydrc  
iniu  
Autonom Name (AUN): 4-te  
2-ph  
chlc  
Lin. Struct. Formula (LSF): C18H  
Fragm. Molec. Formula (FMF): C18  
Molecular Formula (MF): C18  
Molecular Weight (MW): 270.  
Fragment AN (FAN): 8778  
Lawson Number (LN): 2425  
File Segment (FS): Stereo compound  
Compound Type (CTYPE): heterocyclic  
Constitution ID (CONSID): 7455846  
Entry Date (DED): 2001/07/25  
Update Date (DUPD): 2001/07/25  
. . . .

CTYPE controlled terms:

- acyclic
- isocyclic
- heterocyclic
- polymer (monomers given)
- polymer (monomers not given)
- biomolecules
- mixtures (composition completely given) ...

# Multi-fragment and multi-component compounds in ReaxysFile



FAN = Fragment Accession Number. COMPAN = Component Accession Number.

# Multi-fragment Compounds: salts and adducts

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):	8808326
Chemical Name (CN):	(R)-4-(1,1-dimethylethyl)-1-(1-hydroxy-3-phenylpropan-2-yl)pyridinium chloride
Autonom Name (AUN):	4-tert-butyl-1-(1-hydroxymethyl-2-phenyl-ethyl)-pyridinium; chloride
Lin. Struct. Formula (LSF):	C18H24NO(1+)*Cl(1-)
Fragment Molec. Formula (FMF):	C18 H24 N O , Cl
Molecular Formula (MF):	C18 H24 N O . Cl
Molecular Weight (MW):	270.39, 35.45
Fragment AN (FAN):	8778869, 3587171
Lawson Number (LN):	24256, 14919
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7455846
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2001/07/25
. . . .	

FMF, MW and FAN are given for each fragment.

# Multi-component compounds: mixtures and polymers

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN): 8829001  
Chemical Name (CN): Polymer; Monomer(s):  
formaldehyde;  
N-methyl-p-methoxyphenethylamine;  
Compound Type (CTYPE): polymer (monomers given)  
Compos.: Comp. AN (COMPAN): 1209228, 2413387  
Compos.: Comp. Name (COMPN): formaldehyde,  
(4-methoxy-phenethyl)-methyl-  
amine  
Entry Date (DED): 2001/07/25  
Update Date (DUPD): 2001/07/25

No structure diagram available for this Document

. . . .

The name (COMPAN) and Accession Number (COMPAN) are provided for each component.

# Agenda

- What is ReaxysFile?
- Find substances
- **Find reactions**
- Searching bibliographic data
- Physical properties
- EcoPharm data
- Chemical data
- Basic tips for managing display costs

# Which reactions are indexed?

- Preparation
  - Chemical or biochemical methods suitable for large-scale preparations – new and useful preparative methods
  - General methods which are applicable for the preparation of several compounds
- Chemical Behavior
  - Publication provides quantitative results pertaining to the course of a reaction, rather than to its product(s)
  - Publication is focused on the investigation of how chemicals react/interact, rather than on synthesis

# ReaxysFile Reaction File Segment

- Each reaction is a separate database record
- All reaction data concentrated in field RX
- Reaction data for a substance can be displayed directly from a substance record
- Crossover from Substance to Reaction File segments is achieved by identifying ANs and searching them as reactants or products
- Detailed reaction searching is possible

# Reaction sample record

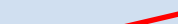
L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Reaction:

RX

Reaction ID:	8619548
Reactant AN (.RAN):	203413, 3588525
Reactant (.RCT):	2-phenothiazin-10-yl-ethanol, 2-cyanoethyl diisopropyl chlorophosphoramidite
Product AN (.PAN):	8645640
Product (.PRO):	diisopropyl-phosphoramidous acid 2-cyano-ethyl ester 2-phenothiazin-10-yl-ethyl ester
No. of React. Details (.NVAR):	3

RX.ID



## Reaction Identification Data:

- Reactions are defined by reactants and products (RX.ID)
- Reactant and Product names & ANs are given
- Number of Reaction Details is the number of different ways of preparing the same product from the same reactants

# Reaction sample record (cont.)

## Reaction Details:

RX

Reaction RID (.RID):	8619548.1	Reaction Detail 1.
Reaction Classification (.CL):	Preparation	
Yield (.YDT):	89 percent (AN =8645640)	
Reagent (.RGT):	DIPEA	
Solvent (.SOL):	acetonitrile	
Reaction Type (.TYP):	Substitution	
Reference(s):		
1. Tierney, Mark T.; Sykora, Milan; Khan, Shoeb I.; Grinstaff, Mark W., J. Phys. Chem. B, CODEN: JPCBFK, 104(32), <2000>, 7574 - 7576; BABS-6683760		

RX

Reaction RID (.RID):	8619548.2	Reaction Detail 2.
Reaction Classification (.CL):	Preparation	
Yield (.YDT):	95 percent (AN =8645640)	
Reagent (.RGT):	diisopropylethylamine	
Solvent (.SOL):	CH2Cl2	
Temperature (.T):	25 Cel	
Reaction Type (.TYP):	Substitution	
Reference(s):		
1. Tierney, Mark T.; Grinstaff, Mark W., J.Org.Chem., CODEN: JOCEAH, 65(17), <2000>, 5355 - 5359; BABS-6262693		
2. Tierney, Mark T.; Grinstaff, Mark W., J. Org. Chem., CODEN: JOCEAH, SIR65(17), <2000>, 5355 - 5359; BABS-6568080		

# How to access Reaction Data

- Substance File Segment
  - Identify substances with reaction information
  - Display reaction data for a substance
  - Most cost-effective display of reaction information
- Reaction File Segment
  - Crossover ANs from substance segment
  - Combine reactants and/or products
  - Combine reactants/products with reaction details

# Searching for substances with reaction references

- S RX**PRO**/FA for substances which are products in reaction records (or PRE/FA)
- S RX**REA**/FA for substances which are reactants in reaction records (or REA/FA)
- S RX/FA for substances which are reactants and/or products in reaction records

FA = Field Availability.

## Reaction display formats for substance records

- D RXPRO or FRXPRO (or PRE / FPRE)
  - Reactions in which the compound is the product
- D RXREA or FRXREA (or REA / FREA)
  - Reactions in which the compound is a reactant
- D RX or FRX
  - All reactions which the substance is either a reactant or a product

**Note:** include the Full “F” prefix to display more than 20 reaction references.

# Example: display product data (RXPRO) for a substance

```
=> S 42427-52-1/RN AND RXPRO/FA
L1      1 42427-52-1/RN AND RXPRO/FA
```

Search for Substances and limit to records with reaction product references (RXPRO/FA).

```
=> D IDE RXPRO
```

```
L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier
```

Display Substance data (IDE) and reaction references (RXPRO).

Accession Number (AN):	9759486
CAS Reg. No. (RN):	42427-52-1
Chemical Name (CN):	2-(4-acetylphenyl)but-1-ene
Autonom Name (AUN):	1-<4-(1-ethyl-vinyl)-phenyl>-ethanone
Molec. Formula (MF):	C12 H14 O
Molecular Weight (MW):	174.24
Lawson Number (LN):	7276
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	8220680
Entry Date (DED):	2005/01/21
Update Date (DUPD):	2005/01/21
. . . . .	

IDE Display.

# Example: display product data (RXPRO) for a substance (cont.)

Field Availability:

IDE Display (cont.)

Code	Name	Occurrence
AN	Accession Number	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
DED	Entry Date	1
DUPD	Update Date	1
NMR	Nuclear Magnetic Resonance	2

Field Availability  
(FA) Table.

This substance also occurs in Reaction Documents:

Indication of  
reactions.

Code	Name	Occurrence
RX	Reaction Documents	2
RXPRO	Substance is Reaction Product	2

# Example: display product data (RXPRO) for a substance (cont.)

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2

Reactions in which the compound is the product, => **D RXPRO**.

Reaction:

RX

Reaction ID (.ID): 9659517  
Reactant AN (.RAN): 386015, 9757604  
Reactant (.RCT): 1-(4-bromo-phenyl)-ethanone,  
but-1-en-2-ylboronic acid  
**Product AN (.PAN): 9759486**  
Product (.PRO): 1-<4-(1-ethyl-vinyl)-phenyl>-ethanone  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 9659517.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 93 percent (AN =9759486)  
Reagent (.RGT): K2CO3,  
cis,cis,cis-tetrakis<(diphenylphospha  
nyl)methyl>cyclopentane  
Catalyst (.CAT): <Pd(C3H5)Cl>2  
Solvent (.SOL): xylene  
Time (.TIM): 20 hour(s)  
Temperature (.T): 130 Cel  
Reaction Type (.TYP): Suzuki reaction  
Reference(s):  
1. Peyroux, Eugenie; Berthiol, Florian; Doucet, Henri; Santelli,  
Maurice, Eur. J. Org. Chem., CODEN: EJOCFK(5), <2004>, 1075 -  
1082; BABS-6451267

# How to access Reaction Data

- Substance File Segment
  - Identify substances with reaction information
  - Display reaction data for a substance
  - Most cost-effective display of reaction information
- Reaction File Segment
  - Crossover ANs from substance segment
  - Combine reactants and/or products
  - Combine reactants/products with reaction details

# AN link between File Segments

## Substance File Segment.

Accession Number (AN): 1724426


Basic Pref. RN (BPR): 616-91-1

CAS Reg. No. (RN): 616-91-1, 7218-04-4, 26117-28-2

Chemical Name (CN): N-acetyl-L-cysteine, A-8199, ACC, NAC, N $\alpha$ -acetyl-L-cysteine, N $\alpha$ -acetylcysteine, N $\alpha$ -acetyl-L-cysteine

Autonom Name (AUN): (R)-2-Acetylamino-3-mercapto-propionic acid

**AN**



## Reaction File Segment.

Reaction:  
RX

Reaction ID: 9891975

Reactant AN (.RAN): 1724426, 605349

Reactant (.RCT): N-acetyl-L-cysteine, acrylamide

Product AN (.PAN): 8985353

Product (.PRO): N-acetyl-S-(3-amino-3-oxopropyl) cysteine

No. of React. Details (.NVAR): 1

**RX.RAN**

# AN link between File Segments (cont.)

## Substance File Segment.

Accession Number (AN): **1724426**


Basic Pref. RN (BPR): 616-91-1

CAS Reg. No. (RN): 616-91-1, 7218-04-4, 26117-28-2

Chemical Name (CN): N-acetyl-L-cysteine, A-8199, ACC, NAC, N $\alpha$ -acetyl-L-cysteine, N $\alpha$ -acetylcysteine, N $\alpha$ -acetyl-L-cysteine

Autonom Name (AUN): (R)-2-Acetylamino-3-mercapto-propionic acid

**AN**



## Reaction File Segment.

Reaction:  
RX

Reaction ID: 9609016

Reactant AN (.RAN): 773648, 9726965

Reactant (.RCT): 2-mercapto-ethanol, N $\alpha$ -acetyl-S-(2,4-dinitro-5-(dimethylaminomethyl)phenyl)-L-cysteine

Product AN (.PAN): 9708798, **1724426**

Product (.PRO): 2-(5-dimethylaminomethyl-2,4-dinitrophenylsulfanyl)-ethanol, N-acetyl-L-cysteine

No. of React. Details (.NVAR): 1

**RX.PAN**

# Example: retrieving reaction records

=> S A-8199/CN

L1 1 A-8199/CN

Search for the substance.

=> D IDE

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):

1724426

Identify the AN.

Basic Pref. RN (BPR):

616-91-1

CAS Reg. No. (RN):

616-91-1, 7218-04-4, 26117-28-2

Chemical Name (CN):

N-acetyl-L-cysteine, A-8199, ACC,  
NAC, N $\alpha$ -acetyl-L-cysteine,  
N $\alpha$ -acetylcysteine,  
N $\alpha$ -acetyl-L-cysteine

Autonom Name (AUN):

(R)-2-Acetylamino-3-mercapto-propionic  
c acid

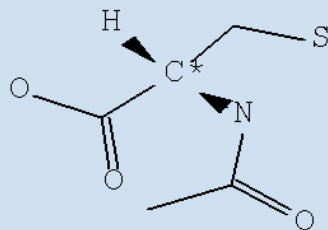
Lin. Struct. Formula (LSF):

C3H7SNO2C2H2O

Molec. Formula (MF):

C5 H9 N O3 S

. . . . .



# Example: retrieving reaction records (cont.)

```
=> S 1724426/RX.RAN
L2          392 1724426/RX.RAN
```

Search the substance AN in the Reactant AN field (/RX.RAN).

```
=> D RX
```

Display Reactions (RX) in which the substance is the reactant.

```
L2 ANSWER 1 OF 392 REAXYSFILE COPYRIGHT 2
```

```
Reaction:
```

```
RX
  Reaction ID:                23009186
  Reactant AN (.RAN):         11529574, 1724426
  Reactant (.RCT):            methyl
                               3-formyl-4-methoxy-2-(2-oxoethyl)
                               benzoate, N-acetyl-L-cysteine
  Product AN (.PAN):          11529585
  Product (.PRO):              C17H21NO8S
```

```
Reaction Details:
```

```
RX
  Reaction RID (.RID):         23009186.1
  Reaction Classification (.CL): Preparation
  Solvent (.SOL):              CH2Cl2
  Reference(s):
  1. Ling, Qing; Huang, Yue; Zhou, Yueyang; Cai, Zhengliang; Xiong,
     Bing; Zhang, Yahui; Ma, Lanping; Wang, Xin; Li, Xin; Li, Jia;
     Shen, Jingkang, Bioorganic & Medicinal Chemistry, CODEN:
     BMECEP, 16(15), <2008>, 7399 - 7409; BABS-7115813
```

Searchable  
Reaction Details.

# Example: retrieving reaction records (cont.)

```
=> S 1724426/RX.PAN
L3      8 1724426/RX.PAN
```

```
=> D RX
```

```
L3 ANSWER 1 OF 8 REAXYSFILE COPYRIGHT
```

```
Reaction:
```

```
RX
  Reaction ID: 9609016
  Reactant AN (.RAN): 773648, 9726965
  Reactant (.RCT): 2-mercapto-ethanol,
  N.alpha.-acetyl-S-(2,4-dinitro-5-(dimethylaminomethyl)phenyl)-L-cysteine
  Product AN (.PAN): 9708798, 1724426
  Product (.PRO): 2-(5-dimethylaminomethyl-2,4-dinitrophenylsulfanyl)-ethanol,
  N-acetyl-L-cysteine
  No. of React. Details (.NVAR): 1
```

```
Reaction Details:
```

```
RX
  Reaction RID (.RID): 9609016.1
  Reaction Classification (.CL): Preparation
  Reagent (.RGT): sodium phosphate buffer
  Time (.TIM): 1 hour(s)
  pH Value (.PH): 8.0
  . . . .
```

Search the substance AN in the Product AN field (/RX.PAN).

Display Reactions (RX) in which the substance is the product.

Searchable Reaction Details.

# Remember D RX from a substance record is often a more cost-effective display choice

=> D L1 RX ; D COST FULL

Display RX records for a substance from the substance record for one charge.

FILE & COST CENTER

QUANTITY @ RATE ESTIMATED COST  
DOLLARS

. . .

REAXYSFILE FILE COST=

SFE SESSION CONNECT HOURS

REACTION DATA

. . .

0.04	@	0.00	0.00
1	@	8.30	8.30

=> D L3 RX 1-8 ; D COST FULL

Displaying each RX individually is much more expensive!!

FILE & COST CENTER

QUANTITY @ RATE ESTIMATED COST  
DOLLARS

. . .

REAXYSFILE FILE COST=

SFE SESSION CONNECT HOURS

REACTION DATA

. . .

0.02	@	0.00	0.00
8	@	8.30	66.40

# Detailed reaction searching in the Reaction File Segment

- Search within Reaction Details
  - 18 fields available for precise Reaction Detail searching
  - Use (P)-operator to keep terms within a Reaction Detail
- Combine reactants and/or products
  - Multiple reactants and products can be linked
  - Use AND-operator to link reactants and/or products
- Combine reactants and/or products with Reaction Detail searches using AND

# Available data in Reaction Details

Reaction Detail ID	/RX.RID
Reaction Classification	/RX.CL
Yield	/RX.YD
Reagent	/RX.RGT
Catalyst	/RX.CAT
Solvent	/RX.SOL
Time	/RX.TIM
Temperature	/RX.T
Pressure	/RX.P

## Available data in Reaction Details (cont.)

pH Value	/RX.PH
Reaction Type	/RX.TYP
Subject Studied	/RX.SUBJ
Prototype Reaction	/RX.PRT
Other Conditions	/RX.COND
Note	/RX.COM
Stage Reactant AN	/RX.SRAN
Stage Reactant	/RX.SRCT
Number of Stages	/RX.SNR

# Individual reaction detail fields are also searchable in the /RX supersearch field

=> S CHCL3/RX

```
    71 CHCL3/RX.RCT
   9072 CHCL3/RX.RGT
    204 CHCL3/RX.PRO
     0 CHCL3/RX.SUBJ
 136602 CHCL3/RX.SOL
     3 CHCL3/RX.CAT
     0 CHCL3/RX.TYP
     0 CHCL3/RX.PRT
     5 CHCL3/RX.SRCT
```

Content of /RX.

```
L1    145732 CHCL3/RX
      (CHCL3/RX.RCT ,RX.RGT ,RX.PRO ,RX.SUBJ ,RX.SOL ,RX.CAT
      ,RX.TYP ,RX.PRT ,RX.SRCT)
```

=>

# Example: searching for preparations of Aspirin with a yield over 90%

=> S ACETYLSALICYLIC ACID/CN  
L1 2 ACETYLSALICYLIC ACID/CN

Search for a substance.

=> D IDE

L1 ANSWER 1 OF 2 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):	779271	Identify the AN.
Basic Pref. RN (BPR):	50-78-2	
CAS Reg. No. (RN):	50-78-2, 000050-78-2	
Chemical Name (CN):	2-(acetyloxy)benzoic acid, 2-(acetoxy)benzoic acid, O-acetyl salicylic acid, 2-acetoxybenzoic acid, acetyl salicylic acid, acetylsalicylic acid, Aspirin(R)	
Autonom Name (AUN):	2-Acetoxy-benzoic acid	
Lin. Struct. Formula (LSF):	C6H4(COOH)OCOCH3	
Molec. Formula (MF):	C9 H8 O4	
Molecular Weight (MW):	180.16	
Compound Type (CTYPE):	isocyclic	
Handbook Citation (HSO):	5-10, 0-10-00-00067, 1-10-00-00028, 2-10-00-00041, 3-10-00-00102, 4-10-00-00138, 6-10	
Entry Date (DED):	1989/06/29	
Update Date (DUPD):	2009/10/16 . . . .	

# Example: searching for preparations of Aspirin with a yield over 90% (cont.)

```
=> S 779271/RX.PAN AND (PREPARATION OR MULTISTAGE)/RX.CL (P)
    RX.YD>90
```

```
L2      1 779271/RX.PAN A
        RX.YD>90 %
```

Search aspirin AN in the product AN field (/RX.PAN), limited with (P) to >90% yield.

```
=> D RX
```

```
L2      ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN
```

```
Reaction:
```

```
RX
Reaction ID: 89050
Reactant AN (.RAN): 89001
Reactant (.RCT): 2-methylene-benzo<1,3>dioxin-4-one
Product AN (.PAN): 779271
Product (.PRO): 2-acetoxy-benzoic acid
No. of React. Details (.NVAR): 1
```

Display Reactions (RX) in which the aspirin is the product.

```
Reaction Details:
```

```
RX
Reaction RID (.RID): 89050
Reaction Classification (.CL): Preparation
Yield (.YDT): 100 percent (AN =779271)
Reagent (.RGT): H2O
Time (.TIM): 1 hour(s)
Temperature (.T): 25 Cel
pH Value (.PH): 7
. . . .
```

(P) keeps reaction detail search terms within a single reaction detail.

## A quick note on multi-stage reactions

- Multistage reactions are multi-step syntheses in which intermediate structures are not known
- They are classified “Multistage” rather than “Preparation” in the /RX.CL field
- All starting materials for all stages are grouped together in the reactant fields
- Each stage has separately searchable reaction details, e.g. temperature, reaction time, etc

# Typical multistage reaction record

=> D RX

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Reaction:

RX

Reaction ID:	8700547
Reactant AN (.RAN):	8685258, 605969
Reactant (.RCT):	3-trifluoromethyl-5,6-dihydro-<1,4>dioxine-2-carbonyl chloride, 3-chloro-aniline
Product AN (.PAN):	8704888
Product (.PRO):	3-trifluoromethyl-5,6-dihydro-<1,4>dioxine-2-carboxylic acid (3-chloro-phenyl)-amide
No. of React. Details (.NVAR):	1

Reactants for all stages listed in the Reactant field.

# Typical multistage reaction record (cont.)

## Reaction Details:

RX

Reaction RID (.RID): 8700547.1  
Reaction Classification (.CL): Multistage  
Yield (.YDT): 100 percent (AN =8704888)  
Nr. of Stages (.SNR): 2

Stage 1

Reagent (.RGT): polystyrene-bound  
4-hydroxy-3-nitrobenzophenone,  
pyridine  
Solvent (.SOL): CH2Cl2  
Time (.TIM): 24 hour(s)  
Temperature (.T): 20 Cel  
Reaction Type (.TYP): Condensation

Stage 2

Reagent (.RGT): Et3N  
Stage reactant (.SRCT): 3-chloro-aniline  
Stage Reactant AN (.SRAN): 605969  
Solvent (.SOL): acetonitrile  
Time (.TIM): 14 hour(s)  
Other Conditions (.COND): Heating  
Reaction Type (.TYP): Condensation  
Reference(s): . . . .

Multistage Reaction Detail.

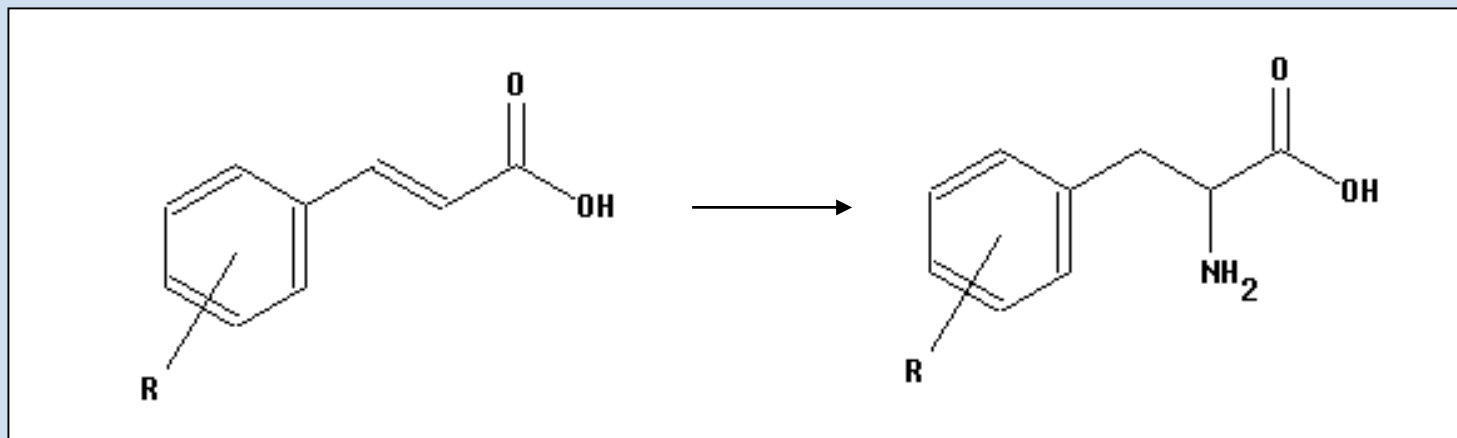
Stage 1

Stage 2

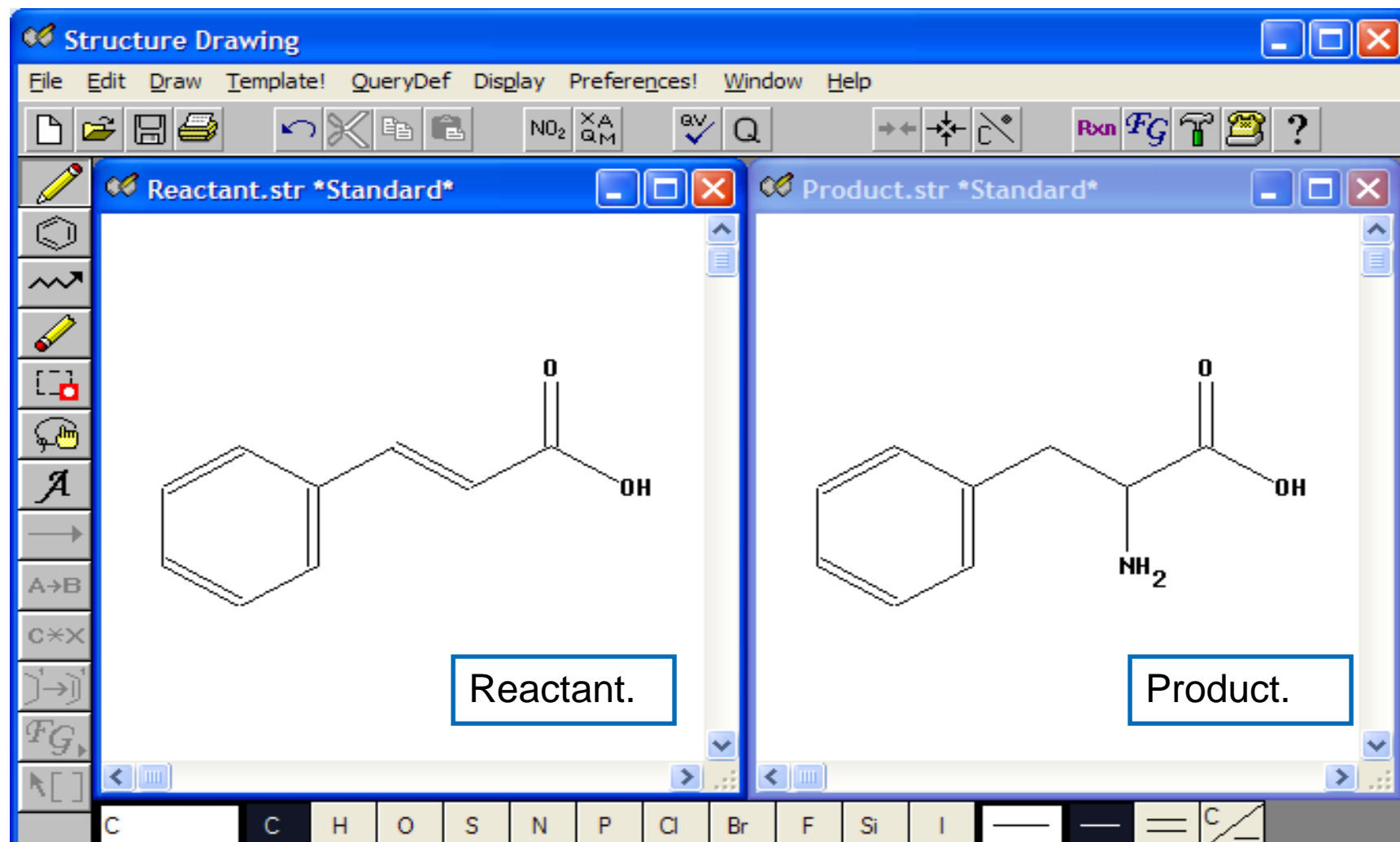
# Example: searching for reactions with specific reactant and product

## Search Question:

Searching for references to the amination of unsaturated carboxylic acids – with a date restriction prior to 1987.



# Using STN Express<sup>®</sup> structure drawing to prepare queries for reactant and product



# Example: searching for reactions with specific reactant and product (cont.)

=> FILE REAXYSFILE

=>

Uploading C:\. . .\My Documents\STN Express 8.4\Queries\Reactant.str

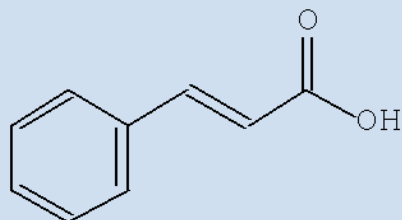
L1 STRUCTURE UPLOADED

Upload the **Reactant** query structure (L1).

=> D

L1 HAS NO ANSWERS

L1 STR



Structure search for the unsaturated carboxylic acid **Reactants** (L2).

=> S L1 SSS FULL

L2 12122 SEA SSS FUL L1

=> S L2 AND RXREA/FA

L3 5321 L2 AND RXREA/FA

Use **RXREA/FA** to find substances with **Reactant** references (L3).

=> TRANSFER L3 AN 1- /RX.RAN

L4 TRANSFER L3 1- AN : 5321

L5 16588 L4/RX.RAN

**TRANSFER** to **RX.RAN** field (L5).

# Example: searching for reactions with specific reactant and product (cont.)

Uploading C:\. . .\My Documents\STN Express 8.4\Queries\Product.str

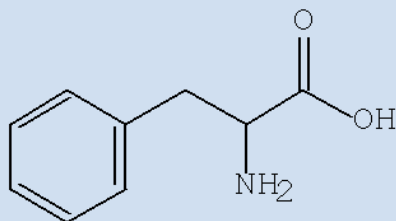
L6 STRUCTURE UPLOADED

Upload the **Product** query structure (L6).

=> D

L6 HAS NO ANSWERS

L6 STR



Structure search for the alpha amino acid **Products** (L7).

=> S L6 SSS FULL

L7 4344 SEA SSS FUL L6

=> S L7 AND RXPRO/FA

L8 3249 L7 AND RXPRO/FA

Use **RXPRO/FA** to find substances with Product (preparation) references (L8).

=> TRANSFER L8 AN 1- /RX.PAN

L9 TRANSFER L8 1- AN :

L10 5336 L9/RX.PAN

3249

TRANSFER to **RX.PAN** field (L10).

# Example: searching for reactions with specific reactant and product (cont.)

```
=> S L5 AND L10 AND PY<1987
L11          31 L5 AND L10 AND PY<1987
```

```
=> D RX 3
```

```
L11 ANSWER 3 OF 31 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN
```

```
Reaction:
```

```
RX
Reaction ID: 2659374
Reactant AN (.RAN): 4684533
Reactant (.RCT): (Z)-2-acetamido-3-(p-hydroxyphenyl)-2-propenic acid
Product AN (.PAN): 4675160
Product (.PRO): L-tyrosine
No. of React. Details (.NVAR): 2
. . . .
```

```
Reference(s):
```

1. Riley, Dennis P.; Shumate, Robert E., J.Org.Chem., CODEN: JOCEAH, 45(25), <1980>, 5187-5193; BABS-5556935

Search for the Reactants (L5) and Products (L10) in reaction records with pre-1987 references.

Product, reactant and year hit terms.

Note: BABS Accession Number.

# Example: searching for reactions with specific reactant and product (cont.)

=> FILE BABS; S 5556935/AN; D ALL

L12 1 5556935/AN

L12 ANSWER 1 OF 1 BABS COPYRIGHT 2010 Elsevier  
AN 5556935 BABS

TI 1,2-Bis(diphenylphosphino)-1-cyclohexylethane. A New Chiral Phosphine Ligand for Catalytic Chiral Hydrogenations

AU Riley, Dennis P.; Shumate, Robert E.

SO J.Org.Chem. (1980), 45(25), 5187-5193

CODEN: JOCEAH

DT Journal

LA English

SL English

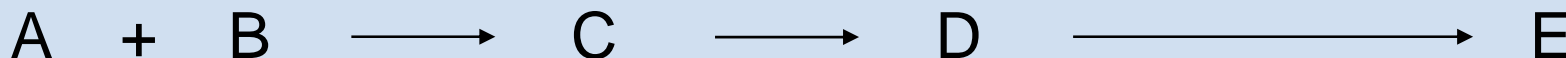
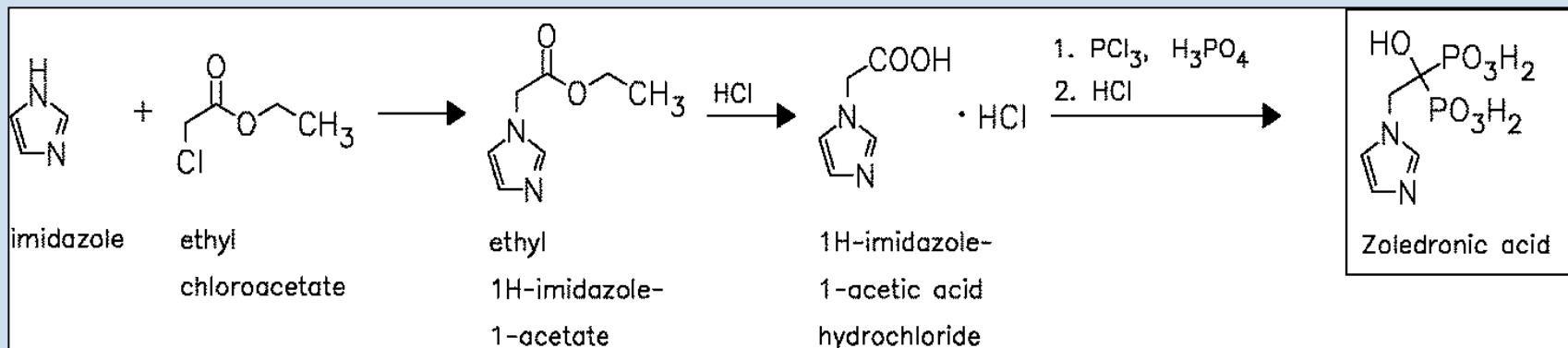
AB The new chiral bidentate phosphine ligand (R)-1,2-bis(diphenylphosphino)-1-cyclohexylethane ((R)-Cycphos) has been prepared. The rhodium(I) cationic complex of this phosphine serves as an effective homogeneous asymmetric hydrogenation catalyst for the reduction of (Z)- $\alpha$ -amidoacrylic acids at ambient temperature and pressure. Optical yields for the corresponding (S)- $\alpha$ -amino acid derivatives that are produced are generally above 90percent. The success of this ligand in giving higher optical yields than those obtained from other structurally analogous phosphines is rationalized in terms of the bulky cyclohexyl substituent affording a more stereochemically rigid chelating phosphine.

English abstracts are available for all ReaxysFile references from 1980 to date in BABS.

# How to approach multi-step synthesis searches in ReaxysFile

## Multi-step Reaction example:

The preparation of zoledronic acid.



**Note:** ReaxysFile reaction records are all single-step reactions.

# How to approach multi-step synthesis searches in ReaxysFile (cont.)

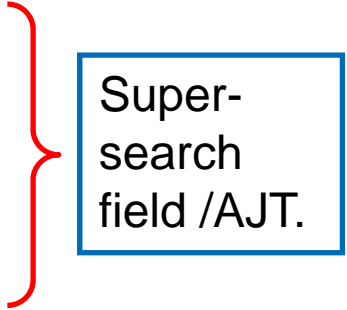
- Preparation of zoledronic acid search
  - Search for  $D \longrightarrow E$
  - Search for  $C \longrightarrow E$
  - Search for  $A \longrightarrow E$
- To be comprehensive also consider
  - Search for  $A \longrightarrow C$  in addition
  - Search for  $A \longrightarrow D$  in addition
  - Search for  $C \longrightarrow D$  in addition

# Agenda

- What is ReaxysFile?
- Find substances
- Find reactions
- **Searching bibliographic data**
- Physical properties
- EcoPharm data
- Chemical data
- Basic tips for managing display costs

# Journal reference searching

- Author (/AU)
- Coden (/ISN)
- Document Type (/DT)
- Language (/LA)
- Journal Title (/JT)
- Journal/Review without Coden (/JTW)
- Unresolved Citation (/URES)
- Publication Year (PY)



Super-search field /AJT.

# Search bibliography with (S)-operator

```
=> S OLAH?/AU (S) J.ORG.CHEM./JT
L2          3973 OLAH?/AU (S) J.ORG.CHEM./JT
```

```
=> D HIT
```

Use the (S) operator to restrict search for different bibliographic data to one reference.

```
L2 ANSWER 1 OF 3973 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA on STN
```

## Reaction Details:

```
RX
Reaction RID (.RID):          9421572.1
Reaction Classification (.CL): Preparation
Yield (.YDT):                51 percent (AN =9481667)
Reagent (.RGT):              m-chloroperbenzoic acid
Solvent (.SOL):              CH2Cl2
Temperature (.T):            0 - 20 Cel
Reference(s):
1. Prakash, G. K. Surya; Hu, Jinbo, Olah, George A.,
   J.Org.Chem., CODEN: JOCEAH, 68(11), <2003>, 4457 - 4463;
   BABS-6411170
```

# Searching bibliography in file segments

## Substance file segment

- AU.SUB
- ISN.SUB
- JT.SUB
- PY.SUB

## Reaction file segment

- AU.RX
- ISN.RX
- JT.RX
- PY.RX

# File segment specific searching

=> S SHARPLESS?/AU

L1 5771 SHARPLESS?/AU

Search for author in both file segments.

=> S SHARPLESS?/AU.SUB

5771 SHARPLESS?/AU

10864115 ALL/FA

L2 2126 SHARPLESS?/AU.SUB

(SHARPLESS?/AU AND ALL/FA)

Search for author in substance file segment.

=> D HIT

L2 ANSWER 1 OF 2126 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA on STN

Mass Spectrum:

MS

Hit: Reference in substance data.

Description (.KW):

HRMS (High resolution mass spectrometry), ESI (Electrospray ionisation)

Note(s) (.COM):

mol peak

Reference(s):

1. Kalisiak, Jarostaw; Fokin, Valery V., **Sharpless, K. Barry;** Trauger, Sunia A.; Kalisiak, Ewa; Morita, Hirotoishi; Siuzdak, Gary; Adams, Mike W. W., Journal of the American Chemical Society, CODEN: JACSAT, 131(1), <2009>, 378 - 386; BABS-7142045

# File segment specific searching (cont.)

=> S SHARPLESS?/AU.RX

5771 SHARPLESS?/AU

10864115 ALL/FA

L3 3645 SHARPLESS?/AU.RX

(SHARPLESS?/AU NOT ALL/FA)

Search for author in reaction file segment.

=> D HIT

L3 ANSWER 1 OF 3645 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA on STN

Reaction Details:

RX

Reaction RID (.RID): 23258099.1  
Reaction Classification (.CL): Preparation  
Reagent (.RGT): hydrazine monohydrate  
Solvent (.SOL): ethyl alcohol  
Time (.TIM): 4  
Other Conditions (.COND): Reflux

Reference(s):

1. Kalisiak, Jarostaw; Fokin, Valery V., **Sharpless, K. Barry;** Trauger, Sunia A.; Kalisiak, Ewa; Morita, Hirotoishi; Siuzdak, Gary; Adams, Mike W. W., Journal of the American Chemical Society, CODEN: JACSAT, 131(1), <2009>, 378 - 386; BABS-7142045

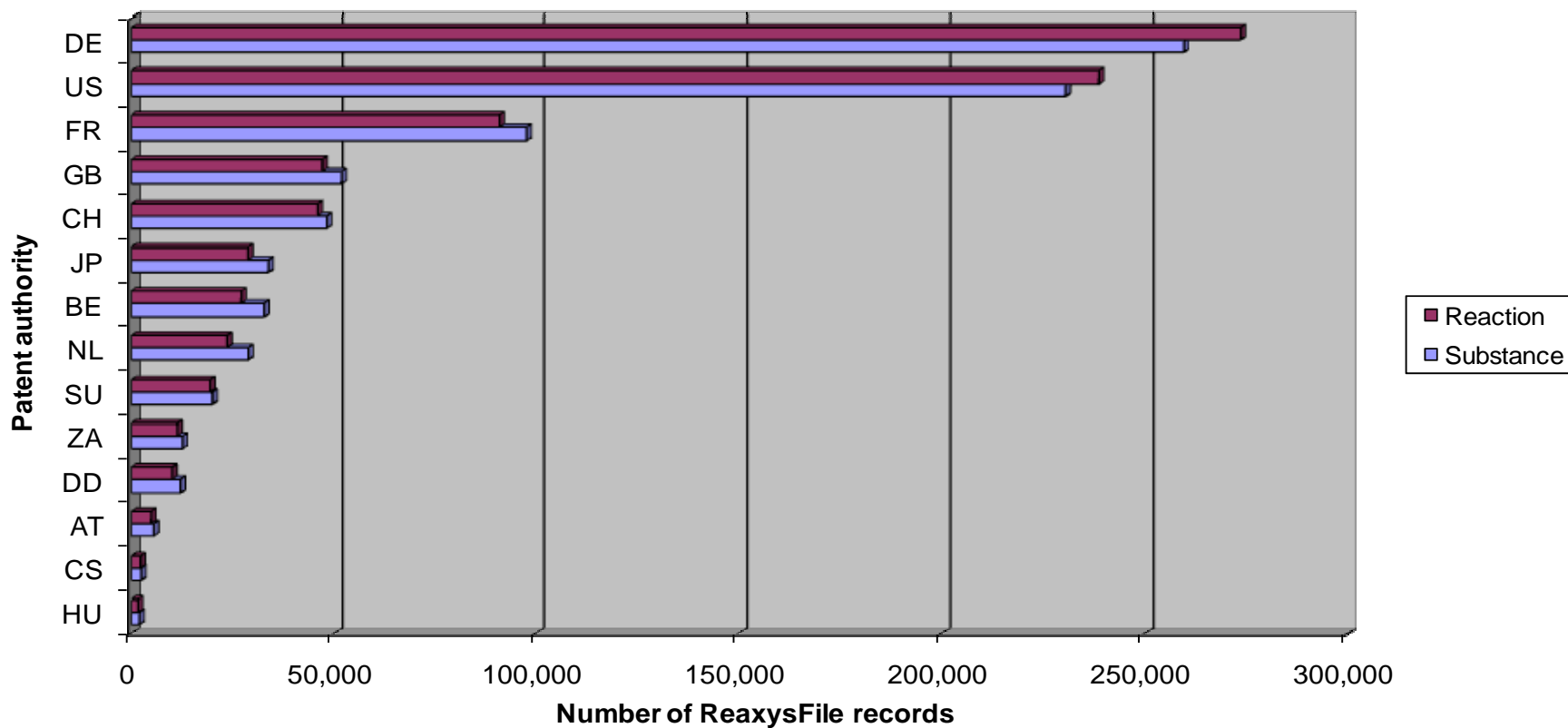
Hit: Reference in reaction data.

# Patents in ReaxysFile

- Earliest patent 1869 and most recent 1981
- Primarily from literature period 1925-1980
- Some unique patent data ~ 1930-1960
- Mainly US and DE patents
- Unique material from early AT, AU, JP, SU
- Other countries: FR, GB, CH, JP, BE, NL

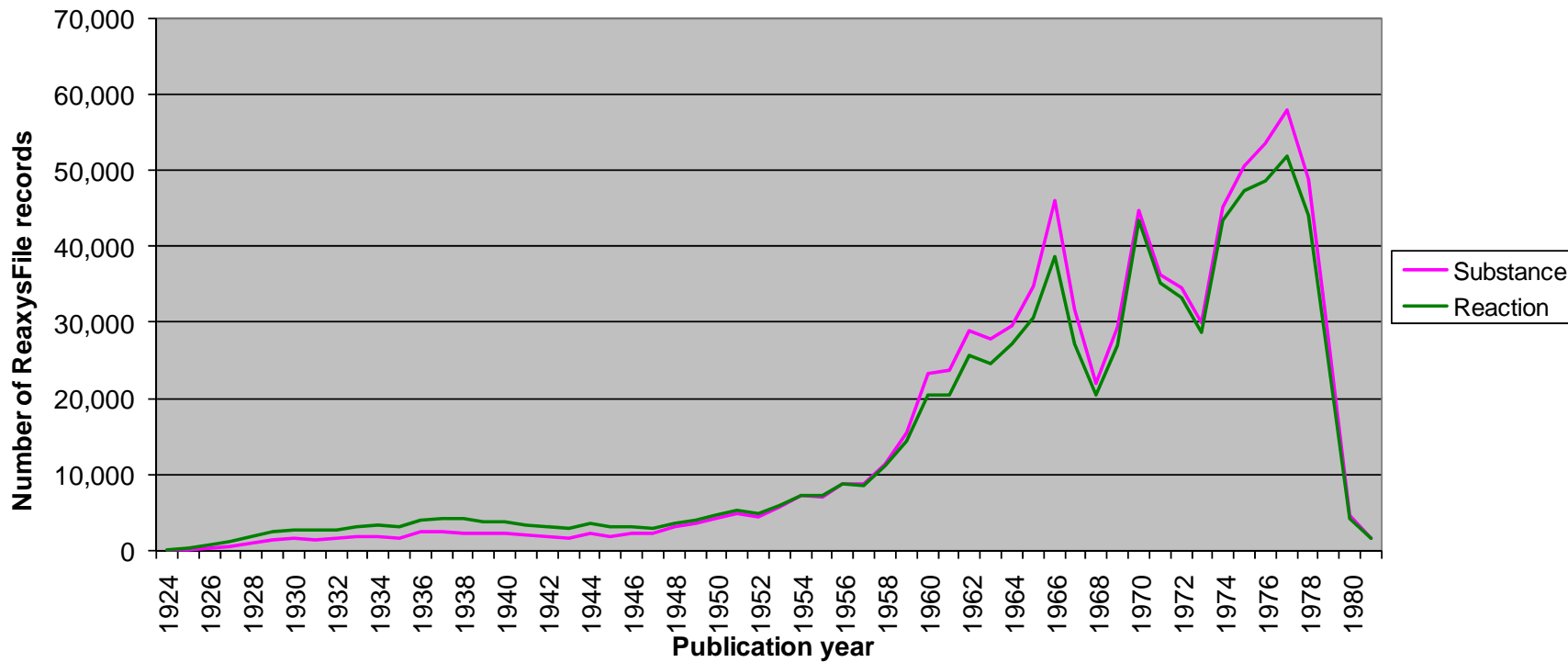
# Patents in ReaxysFile

Number of ReaxysFile records with patent references by patent authority



# Patents in ReaxysFile (cont.)

Number of ReaxysFile records with patent references



# Patent reference searching

- Document Type (/DT)
- Patent Number (/PN)
- Patent Assignee (/PA)
- Publication Year (PY)
- Publication Country (/PC)
- Substance (/xx.SUB) and Reaction (/xx.RX)
- Sentence (S) proximity

# Example: patent and property search

```
=> S (DUPONT OR DU(S)PONT)/PA (L) BP/FA AND CYCLOPROP?/CNS
L1          36 (DUPONT OR DU(S)PONT)/PA (L) BP/FA AND CYCLOPROP?/CNS
```

```
=> D
```

```
L1 ANSWER 1 OF 36 REAXYSFILE COPYRIGHT 2010 Elsevier
```

```
Accession Number (AN):          2874357
Basic Pref. RN (BPR):          59864-49-2
CAS Reg. No. (RN):            59864-49-2
Chemical Name (CN):            3-Chloro-N-cyclopropylmethyl-10
                                ,11-dihydro-5H-dibenzocyclohepte
                                n-5-imine
Autonom Name (AUN):            (3-chloro-10,11-dihydro-dibenzo
                                <a,d>cyclohepten-5-ylidene)-cycl
                                opropylmethyl-amine
Molec. Formula (MF):           C19 H18 Cl N
Molecular Weight (MW):         295.81
Lawson Number (LN):            14006, 7475
File Segment (FS):             Stereo compound
Compound Type (CTYPE):         isocyclic
Constitution ID (CONSID):       2613369
Handbook Citation (HSO):        5-12
Entry Date (DED):              1989/07/11
Update Date (DUPD):            1989/07/26
```

DuPont patents with Boiling Point references for cyclopropyl containing compounds.

# Example: patent and property search (cont.)

## Field Availability:

Code	Name	Occurrence
BP	Boiling Point	1
NMR	Nuclear Magnetic Resonance	1

## Boiling Point:

Value	Press.	Ref.
(BP)	(.P)	
(Cel)	(Torr)	
140 - 150	0.2	1

Hit: Patent reference  
with boiling point data.

## Reference (s) :

1. Patent: E.I. Du Pont de Nemours a. Comp. US 3954865 1976,  
Chem. Abstr., 85(46269)

CAplus reference: => S 85:46269/DN

# Example: DuPont reaction patent search

```
=> S (DUPONT? OR DU(S)PONT?)/PA (S) US/PC (S) 1930-1934/PY  
L1 1630 (DUPONT? OR DU(S)PONT?)/PA (S) US/PC (S) 1930-1934/PY
```

```
=> S L1 NOT ALL/FA  
L2 1217 L1 NOT ALL/FA
```

Limit to Reaction Records with NOT ALL/FA.

```
=> D RX
```

```
L2 ANSWER 1 OF 1217 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA on STN
```

Reaction:

```
RX  
Reaction ID: 8288020  
Reactant AN (.RAN): 3144247  
Reactant (.RCT): air,  
2.6-dichloro-1.4-dihydro-anthrac  
enediol-(9.10)  
Product (.PRO): substance of mp: 273-274 degree  
No. of React. Details (.NVAR): 1
```

Hit: Patent reference  
with reaction data.

Reaction Details:

```
RX  
Reaction RID (.RID): 8288020.1  
Reaction Classification (.CL): Chemical behaviour (half  
reaction)  
Note(s) (.COM): Handbook  
Reference(s):  
1. Patent: du Pont de Nemours & Co. US 1967862 1931
```

# ReaxysFile bibliographic display formats and related SELECT fields for cross-file searching

D ALLREF	all unique references
D ALLP	all unique patent numbers
D BABSAN	all unique BABS ANs
SEL PN	patent publication numbers
SEL BABSAN	BABS Accession Numbers

# ReaxysFile property and reaction data for a substance comes from one or more references

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN): 3084620

. . . .

Melting Point:

. . . .

This means that, e.g. when more than one property is indexed from a single reference, the citation is repeated.

Reference(s):

1. Hamdouchi, C.; Topolski, M.; Goedken, V.; Walborsky, H. M., J.Org.Chem., CODEN: JOCEAH, 58(11), <1993>, 3148-3155; BABS-5755167
2. Patent: Bristol Labor.Inc. US 2787637 1953
3. Zvejnieks, Sven.Kem.Tidskr., CODEN: SKTIAF, 66, <1954>, 316,321

Boiling Point:

. . . .

Reference(s):

1. Aleksandrova,E.K. et al., J.Org.Chem.USSR (Engl.Transl.), CODEN: JOCYA9, 9, <1973>, 778-780, Zh.Org.Khim., CODEN: ZORKAE, 9, <1973>, 756-758
2. Patent: Bristol Labor.Inc. US 2787637 1953
3. Zvejnieks, Sven.Kem.Tidskr., CODEN: SKTIAF, 66, <1954>, 316,321
4. Wenkert,E. et al., Can.J.Chem., CODEN: CJCHAG, 41, <1963>, 1924-1936

# ALLREF provides a simple de-duplicated list of all the unique property and reaction data references

=> D L1 ALLREF

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

All References:  
ALLREF

Compare this de-duplicated ALLREF display, to the property displays given on the previous slide.

1. Jiang, Xianxing; Zhang, Yifu; Wang, Rui; Chan, Albert S. C., Organic Letters, CODEN: ORLEF7, 11(1), <2009>, 153 - 156; BABS-7137874  
. . . .
30. Patent: Bristol Labor.Inc. US 2787637 1953
31. Zvejnieks, Sven.Kem.Tidskr., CODEN: SKTIAF, 66, <1954>, 316,321
32. Campbell et al., J.Amer.Chem.Soc., CODEN: JACSAT, 79, <1957>, 1127
33. Patent: Cheney US 2812325 1953
34. Aleksandrova,E.K. et al., J.Org.Chem.USSR (Engl.Transl.), CODEN: JOCYA9, 9, <1973>, 778-780, Zh.Org.Khim., CODEN: ZORKAE, 9, <1973>, 756-758  
. . . .

# SELECT PN provides cross-file searching options with other patent files, e.g. CAplus

```
=> S PENTANOIC ACID PHENYL ESTER/CN
L1          1 PENTANOIC ACID PHENYL ESTER/CN

=> SEL PN
E1 THROUGH E2 ASSIGNED

=> FILE HCAPLUS

=> S E1-E2
L2          2 ("DE 1288094"/PN OR "US 2139550"/PN)

=> D BIB 2
```

```
L2 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2010 ACS on STN
AN  1939:15371 HCAPLUS
TI  Alkylchlorophenols
IN  Klarmann, Emil
PA  Lehn & Fink Products Corp.
FAN.CNT 1
```

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	US 2139550		19381206	US 1934-752835	19341113
OSC.G	2	THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD			(2 CITINGS)

Search for ReaxysFile substance(s) of interest.

SELECT the PNs.

Enter HCAplus and search the E-numbers.

Display HCAplus bibliographic (BIB) details.

# SELECT and SEARCH for BABSANs provides cross-file searching options with BABS

=> FILE REAXYSFILE

=> SEL L1 BABSAN

E3 THROUGH E12 ASSIGNED

=> FILE BABS

=> S E3-E12

L3 10 (5510115/BABSAN OR 5697493/BABSAN OR 5745405/BABSAN OR . . .

=> D IALL

L3 ANSWER 1 OF 10 BABS COPYRIGHT 2010 Elsevier Pr

ACCESSION NUMBER: 6471013 BABS

TITLE: O-Acylation Mechanism of p

with Various Alkanoyl Chlorides Under Phase  
Transfer Catalysis Conditions

AUTHOR(S) : Hashimoto, Iwao; Kawaji, Takatoshi; Mitoma,  
Yoshiharu; Simion, Alina M.; Simion, Cristian;  
Ishimoto, Keiko; Prakash, G. K. Surya; Olah,  
George A.; Tashiro, Masashi

SOURCE: Rev. Roum. Chim. (2004), 49(2), 149 - 156

CODEN: RRCHAX

DOCUMENT TYPE: Journal

ABSTRACT: The phenolic ester synthesis between . . . .

L1 is the search on the previous slide.

SELECT the BABSANs.

Enter BABS and search  
the E-numbers (L3).

Display ALL in BABS  
for full bibliographic  
details and an abstract.

# Agenda

- What is ReaxysFile?
- Find substances
- Find reactions
- Searching bibliographic data
- **Physical properties**
- EcoPharm data
- Chemical data
- Basic tips for managing display costs

# Typical physical property questions

- Do my measurements for compounds I synthesized in the lab match characterization data in the chemical literature?
- Where in the literature can I find a MS spectrum for my compound?
- Will my compound dissolve in water?

# Physical property data

## Available for

- Single component systems
  - Information on physical properties of the pure title substance
- Multi-component systems
  - Information on physical properties of the title substance in a multi-component system (e.g liquid/liquid or liquid/solid systems)

# ReaxysFile physical property categories

- Electrical and Magnetic Properties (ELEP)
- Electrochemical Behavior (ECB)
- Physical and Mechanical Properties (MECP)
- Optical Properties (OPTP)
- Safety Data (SF)
- Spectroscopic Data (SPE)
- Structure and Energy Parameter (SEP)
- State of Aggregation (SAG)
- Thermodynamic Properties (THE)
- Transport Phenomena (TRA)
- Multi-Component Systems (MCS)

# Example: spectroscopic data

- ESR (ESR)
- Fluorescence (FLU)
- Infrared Spectrum (IR)
- Luminescence (LUM)
- Nuclear Magnetic Resonance (NMR)
- Nuclear Quadrupole Resonance (NQR)
- Phosphorescence (PHO)
- Raman Spectrum (RAS)
- Rotational Spectrum (ROT)
- UV and Visible Spectrum (UVS)

# Property Field Availability (/FA)

- All property display field names and codes are searchable in the /FA field

```
=> FILE REAXYSFILE
```

```
=> E NMR/FA 5
```

Over 3 million ReaxysFile substances have NMR property information (E3).

```
E1          3079      MUT/FA
E2          3079      MUTAROTATION/FA
E3         3104245  --> NMR/FA
E4          5866      NQR/FA
E5         3104245      NUCLEAR MAGNETIC RESONANCE/FA
```

```
=>
```

# Property keywords (.KW) are also available for many physical properties

- Example: mechanical property (/MEC) keywords

=> E A/MEC.KW 25

```
**** START OF FIELD ****
E3          0 --> A/MEC.KW
E4          310    COMPRESSIBILITY/MEC.KW
E5          210    ELASTICITY CONSTANTS/MEC.KW
E6          115    INTERNAL PRESSURE/MEC.KW
E7          2229   MOLAR VOLUME/MEC.KW
E8          348    PVT RELATIONSHIP/MEC.KW
E9          29     SECOND VIRIAL COEFFICIENT OF THE EQUATION OF STATE
                /MEC.KW
E10         579    SPECIFIC VOLUME/MEC.KW
E11         2     THIRD VIRIAL COEFFICIENT OF TE EQUATION OF STATE/MEC.KW
E12         400    VIRIAL COEFFICIENTS OF THE EQUATION OF STATE/MEC.KW
E13        3099   VISCOSITY/MEC.KW
E14         198    VOLUME CHANGE ON MELTING/MEC.KW
**** END OF FIELD ****
```

# The all Keywords (/AKW) field combines keywords from all the individual xxx.KW fields

=> E MOLAR VOLUME/AKW

E1	128	MOLAR EXCESS GIBBS FREE ENERGY/AKW
E2	1029	MOLAR POLARIZATION/AKW
E3	2229	--> MOLAR VOLUME/AKW
E4	18	MULTIPHOTON IONIZATION (MPI)/AKW
E5	3	MULTIPLE RESONANCE STUDIES/AKW
E6	2	MUTAROTATION COEFFICIENT/AKW
E7	856	MUTUAL SOLUBILITY/AKW
E8	303	NATURAL BIREFRINGENCE/AKW
E9	179	NEAR IR BANDS/AKW
E10	168	NEAR IR SPECTRUM/AKW
E11	246	NEGATIVE CHEMICAL IONIZATION/AKW
E12	4725	NEGATIVE ION SPECTROSCOPY/AKW

# The Property Hierarchy (/PH) combines all /FA and /AKW terms into one index

- All property field names and field codes from /FA indexed as bound phrase
- All physical property keywords for all properties indexed as bound phrase
- Browse /PH when you are unsure whether a topic is property field or a keyword term

# The Property Hierarchy (/PH) combines all /FA and /AKW terms into one index (cont.)

=> E CRYSTAL/PH 25

E1	1168	CRYOSCOPIC CONSTANT/PH
E2	85777	CRYPH/PH
E3	0	--> CRYSTAL/PH
E4	570	CRYSTAL GROWTH/PH
E5	2077	CRYSTAL HABIT/PH
E6	855	CRYSTAL MORPHOLOGY/PH
E7	85777	CRYSTAL PHASE/PH
E8	382655	CRYSTAL PROPERTY DESCRIPTION/PH
E9	718	CRYSTAL REFRACTIVE INDICES/PH
E10	59656	CRYSTAL SPACE GROUP/PH
E11	73856	CRYSTAL STRUCTURE DETERMINATION/PH
E12	61031	CRYSTAL SYSTEM/PH
E13	3386	CRYSTAL TRANSITION POINT/PH
E14	59656	CSG/PH
E15	61031	CSYS/PH
...		

*Entries from  
keywords*

*Entries from  
field codes*

# Search example: physical data

- What is the absorption maximum in the UV/VIS spectrum of nitrofen?

```
=> FILE REAXYSFILE
```

```
=> S NITROFEN/CN
```

```
L1          1 NITROFEN/CN
```

```
=> S L1 AND UVS/FA
```

```
839879 UVS/FA
```

```
L2          1 L1 AND UVS/FA
```

Search for the chemical name and availability of the physical property of interest (UVS/FA).

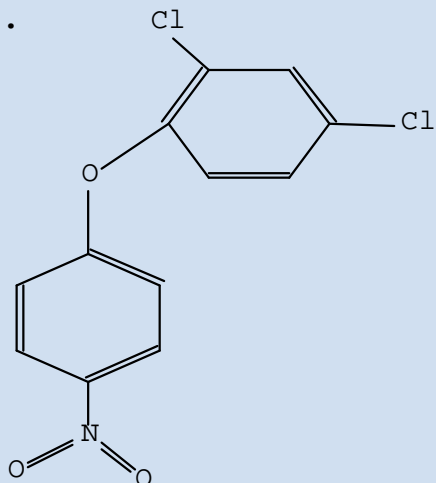
# Search example: physical data (cont.)

=> D IDE

L2 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):	1887356
Basic Pref. RN (BPR):	1836-75-5
CAS Reg. No. (RN):	1836-75-5
Chemical Name (CN):	Chlomethoxyfen, Nitrofen, NIP, 2,4-Dichlorophenyl 3-methoxy-4-nitrophenyl ether, . . .
Autonom Name (AUN):	2,4-Dichloro-1-(4-nitro-phenoxy)-benzene
Lin. Struct. Formula (LSF):	C12H7Cl2NO3
Molec. Formula (MF):	C12 H7 Cl2 N O3

. . . . .



Display substance  
identification data (IDE).

# Search example: physical data (cont.)

Field Availability:

The IDE format includes the field availability (FA) table.

Code	Name	Occurrence
AN	Accession Number	1
BRP	Basic Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	7
.		
.		
UVS	UV and Visible Spectrum	2
.		
.		

# Search example: physical data (cont.)

=> **D UVS**

Display UV and Visible Spectrum information (**UVS**).

L2 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

## UV and Visible Spectrum:

Description	Solvent	Absorption	Ref.
(.KW)	(.SOL)	Maxima	
		(nm)	
====+====+====+====			
Absorption maxima	ethanol	292	1
UV/VIS			2

## Reference(s):

1. Dahlgard; Brewster, J.Amer.Chem.Soc., CODEN: JACSAT, 80, <1958>, 5861
2. Fujikawa et al., Agric.Biol.Chem., CODEN: ABCHA6, 34, <1970>, 68,76

# Searching numeric properties

## Melting Point:

Value	Solvent	Ref.	Note
(MP)	(.SOL)		
(Cel)			
=====			
176		1	1
176 - 177	methanol	2	1
175 - 176		3	1
174 - 175		4	2, 1
170 - 172		5	

## Numeric Values

## Reference(s):

1. Wolodkowitsch et al., Zh.Obshch.Khim., CODEN: ZOKHA4, 29, <1959>, 2837; engl. Ausg. S. 2797
2. Patent: N.V. de Bataafsche Petr. Mij. DE 945448 1950
3. Lidov et al., Adv. Chemistry Ser., 1, <1950>, 175, 178
4. Wasicky; Unti, Anais Fac. Farm. Odont. Univ. Sao Paulo, 11, <1953>, 169, 173
5. Ebing, Chimia, CODEN: CHIMAD, 21, <1967>, 132

## Notes(s):

1. Handbook
2. Sublimation.

# Numeric operators

- within a range
- > greater than
- < less than
- >= greater or equal to
- <= less or equal to

# Examples: numeric searching

- Value

=> S 100/BP

- Range

=> S BP>100

=> S 100-110/BP

Boiling Point:

Value	Press.	Ref.
(BP)	(.P)	
(Cel)	(Torr)	

100	1	1
-----	---	---

Boiling Point:

Value	Press.	Ref.
(BP)	(.P)	
(Cel)	(Torr)	

126	0.2	1
-----	-----	---

Boiling Point:

Value	Press.	Ref.
(BP)	(.P)	
(Cel)	(Torr)	

105	7.5e-05	1
-----	---------	---

# STN Units System: unit conversion

- Values in default units may be entered without unit

```
=> S 0/MP
```

```
L1      856 0 CEL/MP
```

- Values in other accepted units are converted automatically into the default unit

```
=> S 273.15 K/MP
```

```
L2      856 273.15 K/MP
```

```
=> D HIT
```

```
L1 ANSWER 1 OF 856 REAXYSFILE...
```

```
Melting Point:
```

```
Value |Ref.
```

```
(MP) |
```

```
(Cel) |
```

```
=====+=====
```

```
0 | 1
```

```
=> D HIT
```

```
L2 ANSWER 1 OF 856 REAXYSFILE...
```

```
Melting Point:
```

```
Value |Ref.
```

```
(MP) |
```

```
(Cel) |
```

```
=====+=====
```

```
0 | 1
```

# STN Units System

- General Information on the STN Units system  
<http://www.cas.org/support/stngen/doc/stnunits/>
- **HELP UNIT** for units in ReaxysFile
  - Points to specific HELPs on property groups, e.g. mechanical properties – HELP SMEC
- **D UNIT <field>** to see the file default and current units for an individual ReaxysFile property
  - D UNIT ALL to see the complete list
- **SET UNIT** to change units in ReaxysFile
  - HELP SET UNIT for instructions

# Valid units systems for searching

- CGS - The centimeter-gram-second system
- ENG - Customary U. S. Engineering units
- FPS - The foot-pound-second system
- MKS - The meter-kilogram-second system
- SI - Systeme Internationale (International System), based on the MKS system
- STN - Customary units based on the SI system (note: Celsius instead of Kelvin for temperature)

# Search example: changing default units

```
=> SET UNIT BP=K
SET COMMAND COMPLETED

=> S 473.15/BP
L1      10109 473.15 K /BP

=> D HIT
```

```
L1 ANSWER 1 OF 10109 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA on STN
```

Boiling Point:

Value	Press.	Ref.
(BP)	(.P)	
(K)	(Torr)	
=====+=====+=====		
473.15 - 475.15	1	1

Reference(s) :

1. Lazareva, N. F.; Brodskaya, E. I., Russ.J.Gen.Chem., CODEN: RJGCEK, 71(2), <2001>, 201 - 205, Zh.Obshch.Khim., CODEN: ZOKHA4, 71(2), <2001>, 226 - 231; BABS-6307426

Here the default unit for Boiling Point (BP) is changed to Kelvin (K).

SET UNIT changes both the search default unit, and the unit seen in displays.

# The importance of proximity searching

- The **(P)**-operator must be used to restrict numeric terms to the same experiment
- The **(P)**-operator must be used to combine property values with property conditions

## Examples

- Find substances with a refractive index of 1.3590, measured at 20° C and a wavelength of 589 nm
- Find substances with a sublimation point of 100° C measured at 0.1 Torr pressure

# Physical property subfields (numeric)

- Temperature /xxx.T
- Pressure /xxx.P
- Wavelength /xxx.W
- Concentration /xxx.C
- Partner AN /xxx.PAAN
- . . .

**Note:** the (P)-operator must be used to combine property values with property conditions (subfields).

# Physical property subfields (text)

- Comment /xxx.COM
- Description /xxx.KW
- Partner /xxx.PA
- Solvent /xxx.SOL
- Test System, Species /xxx.SP
- ...

**Note:** the (P)-operator must be used to combine property values with property conditions (subfields).

# Search example: physical property subfields

=> S 1.3590/RI (P) 589/RI.W (P) 20/RI.T

L1 43 1.3590/RI (P) 589 NM /RI.W (P) 20 CEL /RI.T

=> D RI 10

L1 ANSWER 10 OF 43 REAXYSFILE COPYRIGHT

Find substances with a refractive index of 1.3590, measured at 20° C and a wavelength of 589 nm.

## Refractive Index:

Value (RI) (--)	Temperature (.T) (Cel)	Wavelen. (.W) (nm)	Reference
1.369	20	589	1
1.359	20	589	2

## Reference(s):

1. Filatov, A.S. et al., J.Gen.Chem.USSR (Engl.Transl.), CODEN: JGCHA4, 37, <1967>, 787-791, Zh.Obshch.Khim., CODEN: ZOKHA4, 37(4), <1967>, 837-841
2. Ginsburg, V.A. et al., Dokl.Chemical(Engl.Transl.), CODEN: DKCHAY, 142, <1962>, 4-7, Dokl.Akad.Nauk SSSR, CODEN: DANKAS, 142, <1962>, 88-91

# Search example: importance of (P)-proximity

=> S 100/SP (P) 0.1/SP.P

745 100 CEL /SP

786 0.1 TORR /SP.P

L1 71 100 CEL /SP (P) 0.1 TORR /SP.P

=> S 100/SP AND 0.1/SP.P

745 100 CEL /SP

786 0.1 TORR /SP.P

L2 73 100 CEL /SP AND 0.1 TORR /SP.P

=> S L2 NOT L1

L3 2 L2 NOT L1

=> D HIT

L3 ANSWER 1 OF 2 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Sublimation Point:

Value	Press.	Ref.
(SP)	(.P)	
(Cel)	(Torr)	
100	2.000001	1
60	0.1	2

Find substances with a sublimation point of 100° C measured at 0.1 Torr.

Two additional answers (L3) are retrieved if AND is used instead of (P).

The two additional answers (L3) are false hits – the property and condition do not come from the same reference.

# Subset structure searching within answer sets retrieved by physical property searches

- Find pyrrole derivatives with a boiling point lower than or equal to 30° C?

=> S BP<=30

L1 5481 BP<=30 CEL

=>

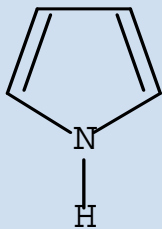
Uploading C:\STNEXP\QUERIES\Pyrrole.str

L2 STRUCTURE UPLOADED

=> D

L2 HAS NO ANSWERS

L2 STR



Search for the boiling point range less than or equal to 30° C.

Build and upload the structure of pyrrole (L2) to conduct a subset substructure search within L1 (next slide).

Structure attributes must be viewed using STN Express query preparation.

# Subset structure searching within answer sets retrieved by physical property searches

```
=> S L2 SSS SUBSET
```

Conduct a substructure search within subset L1 using structure query L2.

```
ENTER SUBSET L# OR (END): L1
```

```
ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END): FULL
```

```
FULL SUBSET SEARCH INITIATED 17:53:18 FILE 'REAXYSFILE'
```

```
FULL SUBSET SCREEN SEARCH COMPLETED - 17 TO ITERATE
```

```
100.0% PROCESSED 17 ITERATIONS
```

```
3 ANSWERS
```

```
SEARCH TIME: 00.00.01
```

```
L3 3 SEA SUB=L1 SSS FUL L2
```

3 substances (L3) have a pyrrole ring system, and a boiling point less than or equal to 30° C.

# Subset structure searching within answer sets retrieved by physical property searches

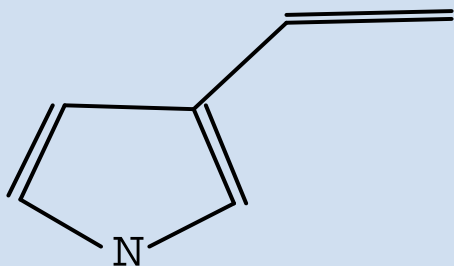
=> D IDE BP

Display IDE and Boiling Point (BP) data.

L3 ANSWER 1 OF 3 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):	6642346
Chemical Name (CN):	3-Vinylpyrrole
Autonom Name (AUN):	3-vinyl-1H-pyrrole
Molec. Formula (MF):	C6 H7 N
Molecular Weight (MW):	93.13
Lawson Number (LN):	24232
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	5716778
Handbook Citation (HSO):	6-20
Entry Date (DED):	1994/07/18
Update Date (DUPD):	2000/02/29

# Subset structure searching within answer sets retrieved by physical property searches



Display IDE and Boiling Point (BP) data (cont.).

. . . .

## Boiling Point:

Value	Press.	Ref.
(BP)	(.P)	
(Cel)	(Torr)	
30	0.006	1

## Reference(s) :

1. Settambolo, Roberta; Lazzaroni, Raffaello; Messeri, Tommaso; Mazzetti, Michele; Salvadori, Piero, *J.Org.Chem.*, CODEN: JOCEAH, 58(27), <1993>, 7899-7902; BABS-5856964

# Option: Boiling Point (BP) data can be tabulated (BPTAB) from multiple records

=> D L3 1-3 BPTAB

L3 3 ANSWERS REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Boiling Point:

ANS	AN	Value	Press.	Ref.	Note
		(BP)	(.P)		
		(Cel)	(Torr)		
=====+	=====+	=====+	=====+	=====+	=====+
1	6642346	30	0.006	1	
2	4402618	30	0.5	2	
3	1159	130 - 130.05	771	3	
.	.	.	.	.	.

Reference(s) :

1. Settambolo, Roberta; Lazzaroni, Raffaello; Messeri, Tommaso; Mazzetti, Michele; Salvadori, Piero, J.Org.Chem., CODEN: JOCEAH, 58(27), <1993>, 7899-7902; BABS-5856964
  2. Ceacereanu, Dimitru M.; Gerstenberger, Michael R. C.; Haas, Alois, J.Heterocycl.Chem., CODEN: JHTCAD, 22, <1985>, 281-285; BABS-5559606
  3. Bak et al., J.Chem.Phys., CODEN: JCPSA6, 24, <1956>, 720, 721
- . . . . .

# Physical property data

Available for

- Single component systems
  - Information on physical properties of the pure title substance
- Multi-component systems
  - Information on physical properties of the title substance in a multi-component system (e.g liquid/liquid or liquid/solid systems)

# Multi-component Systems (MCS)

- Solution Behavior (SOL) (Solubility (SLB), Solubility Product (SLBP), Henry Constant (HNC)...)
- Mixtures (Liquid/Vapour (LVS), Liquid/Liquid (LLSM), Liquid/Solid (LSSM))
- Mechanical and Physical Properties (MECM)
- Optical Data (ODM) (KW: Kerr Constant...)
- Transport Phenomena (TRAM) (KW: Diffusion...)
- Adsorption (ADSM)
- ...

# Multicomponent Systems

## *Equilibrium Systems*

Property is cross-indexed  
in all partners

If a physical property can be  
ascribed to one AN,  
*it is only indexed with  
this compound*

Examples:  
Azeotropes, Eutectics,  
Liquid/Vapour Equilibria

Examples:  
Solubility, Adsorption,  
Critical Micelle  
Concentration

AN = ReaxysFile Accession Number.

# Example: equilibrium system (eutectic)

=> S 472792/AN AND 774890/LSSM.PAAN

L1 1 472792/AN AND 774890/LSSM.PAAN

=> D LSSM

L1 1 ANSWERS REAXYSFILE COPYRIGHT 2010 Elsevier

LSSM

Description (.KW):

Partner AN (.PAAN):

Partner (.PA):

Note(s):

Reference(s):

1. Opfer-Schaum; Piristi, Z.Lebensm.Unters., 87, <1944>, 65,66

Eutectic

774890

2-hydroxy-benzoic acid

Handbook

=> S 774890/AN AND 472792/LSSM.PAAN

L2 1 774890/AN AND 472792/LSSM.PAAN

=> D LSSM

L2 1 ANSWERS REAXYSFILE COPYRIGHT 2010 Elsevier

LSSM

Description (.KW):

Partner AN (.PAAN):

Partner (.PA):

Note(s):

Reference(s):

1. Opfer-Schaum; Piristi, Z. Lebensm.-Unters., 87, <1944>, 65, 66

Eutectic

472792

4-hydroxy-3-methoxy-benzaldehyde

Handbook

Eutectic system:

472792 = vanillin

774890 = salicylic acid

The Eutectic property and the other partner compound, are indexed in each partner record.

# Example: Critical Micelle Concentration

=> S CMC<10 (P) H2O/CMC.SOL (P) CMC.T<20

L2 16 CMC<10 G/L (P) H2O/CMC.SO

Search for substances with a CMC of less than 10 g/L in water, when measured at less than 20 °C.

=> D HIT

L2 ANSWER 1 OF 16 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Critical Micelle Concentration:

Value	Temp.	Solvent	Ref.
(CMC)	(.T)	(.SOL)	
(g/L)	(Cel)		
6.2	11.9	H2O	1
6.458	12.9	H2O	1

Reference(s) :

1. Paula, Stefan; Sues, Willy; Tuchtenhagen, Juergen; Blume, Alfred, J.Phys.Chem., CODEN: JPCHAX, 99(30), <1995>, 11742-11751; BABS-5965508

# Agenda

- What is ReaxysFile?
- Find substances
- Find reactions
- Searching bibliographic data
- Physical properties
- **EcoPharm data**
- Chemical data
- Basic tips for managing display costs

# EcoPharm data

- Pharmacological and Ecological data
- Influence and chemical behavior of substances in the environment, including man, animals and plant and complex ecosystems air, soil and water

# Typical EcoPharm queries

- Which structures, showing anaesthetic activity, have been described recently in the literature?
- What are the ecotoxic effects of *nitrofen*?
- Was the antibacterial effect of *cefpirome* in combination with *rifampin* investigated before?

# EcoPharm topics

- Pharmacological data (PHARM)
  - Human and mammalian pharmacology and toxicology
- Ecological data (ECO)
  - Effect and interaction of substances with nature
- Laboratory Use and Handling (USC)
  - Application or handling, use of substance in preparative chemistry

# New Journals for EcoPharm

- Toxicology
- Toxicology Letters
- Aquatic Toxicology
- Archives of Toxicology
- Environmental Science and Technology
- Environmental Pollution
- Biodegradation
- Journal of Applied Toxicology
- Life Sciences
- Reproductive Toxicology
- Water Research



# EcoPharm: related physical data

- Henry Constant
- Vapor Pressure
- Partition Constant POW
- Solubility
- Viscosity
- Dissociation Exponent
- Boundary Surface Phenomena
- Adsorption
- Melting Point
- Boiling Point
- Molecular Weight

# Pharmacological Data (PHARM)

- Human/mammalian pharmacology
  - Therapeutic effects, pharmacokinetics, pharmacodynamics
- Human/mammalian toxicology
  - Empirical data (e.g. LD50), evaluated and classified data, regulations for handling, storage, transport etc., risk assessment

**Tip:** Use the **PHARM** format to display all available pharmacological data.

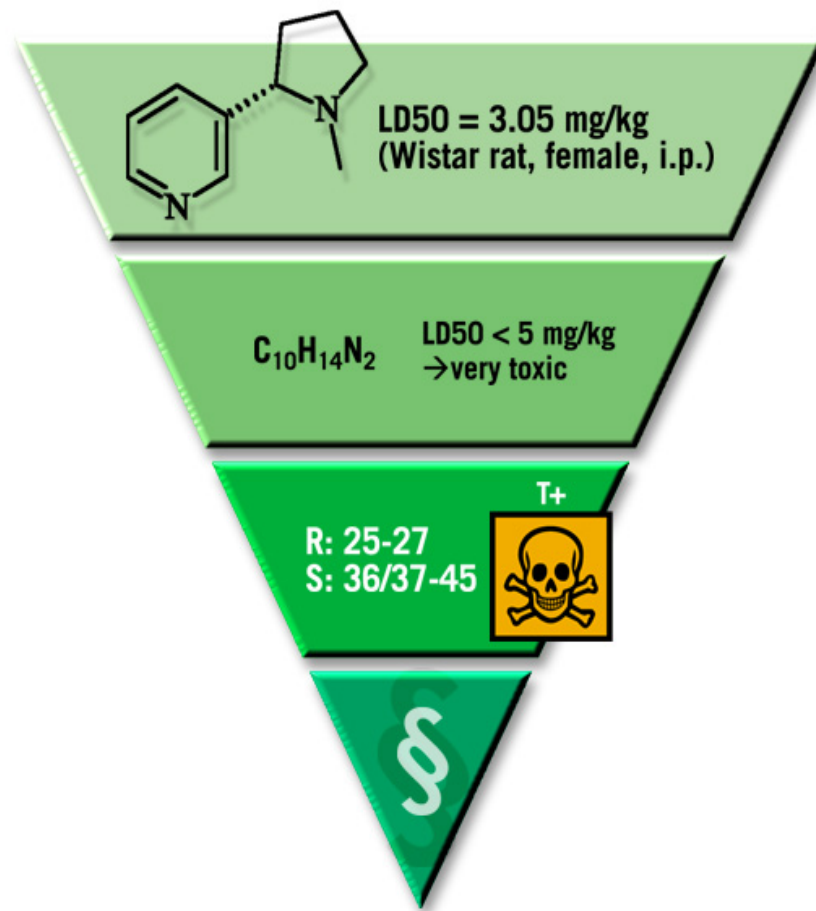
# Toxicological Data

**1** Level 1  
Basic Scientific Data

**2** Level 2  
Evaluation and Classification

**3** Level 3  
Regulation

**4** Level 4  
Risk Assessment



# Detailed data structure for PHARM

## Effect

- Acute toxicity
- Chronic toxicity. . .

## Test System

- Escheria coli
- Lumbricus terrestris

## Test Method

- in vitro
- Amersham kit

## Endpoint of Effect

- Mortality
- Luminescence

## Metabolite

- Chemical name
- AN

## Type of Data/Values

- MTD
- LD50

# PHARM search fields

- Effect /PHARM.E
- Species or Test system /PHARM.SP
- Route of Application /PHARM.RA
- Type /PHARM.TYP
- Value /PHARM.V
- Result /PHARM.RE
- Metabolite /PHARM.META
- Method /PHARM.MR
- ...

# Example: Pharmacological data

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN): 754371  
Basic Pref. RN (BPR): 439-14-5  
CAS Reg. No. (RN): 439-14-5, 65854-76-4, 0000439-14-5  
Chemical Name (CN): Valium(R), diazemuls, diazepam, . . .  
. . . .

## PHARM

Effect (.E): biotransformation  
Species or Test-System (.SP): human liver microsomes  
Concentration (.C): 200 .my.mol/l  
Method, Remarks (.MR): in vitro; title comp. as substrate;  
potassium phosphate buffer, pH 7.4; 37  
deg C; NADPH; incub. for 20 min;  
formation of TMZ and NDZ measured by HPLC  
Further Details (.FD): TMZ: temazepam; NDZ: N-desmethyldiazepam  
Results (.RE): title comp. was metabolized to TMZ and  
NDZ with the rate of 9.2 and 2  
nmol/min/nmol of P450, respectively  
Metabolite AN (.AN): 759300, 751823  
Metabolite (.META): Normison, desmethyldiazepam

Reference(s):  
1. Gelboin, Harry V.; Krausz, Kristopher W.; Goldfarb, Inna; Buters,  
Jeroen T. M.; Yang, Shen K.; Gonzalez, Frank J.; Korzekwa, Kenneth R;  
Shou, Magang, Biochem.Pharmacol., CODEN: BCPCA6, 50(11), <1995>,  
1841 - 1850; BABS-6282690  
. . . .

EcoPharm data provides concise, practical details.

# Ecological data (ECO)

- Effects and interactions of compounds with living and non-living nature
  - Influence on ecosystems (air, soil, water)
  - Behavior in the environment (distribution, accumulation potential, transformation)

**Tip:** Use the **ECO** format to display all available Ecological Data.

# Ecological data

## Ecotoxicology

Toxic effects on  
indicator organisms

## Mobility

- Ability to move through  
the environment
- Bioaccumulation/  
Biomagnification

## Exposure

- Exposure assessment
- Concentration in  
environment

## Transformation and Degradation

- Decomposition by chemical  
or biological reactions

# Ecological data: subjects

- Ecotoxicology (ECTOX)
- Biological Behavior (BIO)
- Ecological Mobility: Transport and Distribution (ECTD)
- Exposure Assessment (EXCA)
- Concentration in Environment (COEV)

## Ecological data: subjects (cont.)

- Biodegradation (BIOD)
- Abiotic Degradation, Hydrolysis (ECDH)
- Abiotic Degradation, Photolysis (ECDP)
- Stability in Soil (ECS)
- Oxygen Demand (EOD)

D  
E  
G  
R  
A  
D  
A  
T  
I  
O  
N

**Tip:** Use the **PED** format to display all available Pharmacological (**PHARM**) and Ecological (**ECO**) Data.

# Example: Ecotoxicology (ECTOX)

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN): 754371  
Basic Pref. RN (BPR): 439-14-5  
CAS Reg. No. (RN): 439-14-5, 65854-76-4, 0000439-14-5  
Chemical Name (CN): Valium(R), diazemuls, diazepam, . . .  
. . . .

EcoPharm data provides  
concise, practical details.

## ECTOX

Effect (.E): toxicity to aquatic invertebrates (acute)  
Endpoint of Effect (.EP): acute toxicity  
Species or Test-System (.SP): Brachionus calyciflorus  
Exposure Period (.EX): 24 h  
Method, Remarks (.MR): Brachionus calyciflorus (Rotokit F) test  
Further Details (.FD): human acute toxicity prediction by a  
battery of ecotoxicological tests and  
physicochemical properties; best partial  
least squares (PLS) model; Multicentre  
Evaluation of In Vitro Cytotoxicity  
programme  
Results (.RE): no L(E)C50 obtained within the  
concentration range tested  
Reference(s):  
1. Calleja, M. C.; Personne, G.; Geladi, P., Food Chem.Toxicol., CODEN:  
FCTOD7, 32(2), <1994>, 173 - 188; BABS-6195315  
. . . .

# Laboratory Use and Handling (USC)

- This topic is focused on:
  - Application or handling of a substance
  - Use of a substance in preparative chemistry, and/or in a laboratory

# Examples: laboratory use and handling

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN  
. . . .

Use of Compound:

USC

Use Pattern (.PT): flame retardant

Reference(s):

1. Ruffin, Catherine; Fischbach, Urs; Gruetzmacher, Hansjoerg; Levalois-Gruetzmacher, Joelle, Heteroatom Chemistry, CODEN: HETCE8, 18(7), <2007>, 721 - 731; BABS-7072061

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN  
. . . .

Use of Compound:

USC

Use Pattern (.PT): phase transfer catalyst

Reference(s):

1. Shinde, Sandip S.; Lee, Byoung Se; Chi, Dae Yoon, Tetrahedron Letters, CODEN: TELEAY, 49(27), <2008>, 4245 - 4248; BABS-7105185

# Old versus modern EcoPharm structure

## Old

Toxicity (TOX)

Biological Function (BF)

Ecological Data (ECOL)

Use (USC)

## Modern

⇒ Pharmacological Data (PHARM)

⇒ Pharmacological Data (PHARM)

⇒ Ecological Data (ECO)

⇒ Laboratory Use & Handling (USC)

**Note:** Modern EcoPharm data was introduced in 1995.

# EcoPharm Basic Index (/BIPED)

=> S ENDOCRINE/BIPED

L1 249 ENDOCRINE/BIPED

=> D HIT 20

The EcoPharm Basic Index (/BIPED) includes all fields from the from EcoPharm data.

L1 ANSWER 20 OF 249 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA on STN

Ecotoxicology:

ECTOX

Effect (.E): **endocrine** system effects  
Species or Test-System (.SP): Carassius auratus gibelio, Crucian Carp  
Sex (.S): male and female  
Exposure Period (.EX): 2 week(s)  
Method, Remarks (.MR): 200/sex one-year old fish with ca. 12-15 cm length and 150 g body weight; temperature of water 20 deg C; 12:12 light-dark rhythm; fed daily with commercial fish pellets; . . . .  
Further Details (.FD): control group: 5 ml acetone in 500 L water; concentration levels of 17.beta.-estrodinol (estrogen) . . . .  
Results (.RE): estrogen (E) and androgen (T) alterations in serum (figures); synergistic effect  
Reference(s):  
1. Zhan, W.; Xu, Y.; Li, A. H.; Zhang, J.; Schramm, K.-W.; Kettrup, A., Bull.Environ.Contam.Toxicol., CODEN: BECTA6, 65(5), <2000>, 560 - 566; BABS-6272429

# EcoPharm: search examples

- Find toxicological data for nitrofen

=> S NITROFEN/CN AND PHARM/FA

L1 1 NITROFEN/CN AND PHARM/FA

Use Field Availability (/FA).

=> D IDE

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):	1887356
Basic Pref. RN (BPR):	1836-75-5
CAS Reg. No. (RN):	1836-75-5
Chemical Name (CN):	Chlomethoxyfen, Nitrofen, NIP, 2,4-Dichlorophenyl 3-methoxy-4-nitrophenyl ether, . . . .
Autonom Name (AUN):	2,4-Dichloro-1-(4-nitro-phenoxy)-benzene
Lin. Struct. Formula (LSF):	C12H7Cl2NO3
Molec. Formula (MF):	C12 H7 Cl2 N O3
Molecular Weight (MW):	284.098
Compound Type (CTYPE):	isocyclic
Handbook Citation (HSO):	5-06, 3-06-00-00821, 4-06-00-01288, 6-06
Entry Date (DED):	1989/06/29
Update Date (DUPD):	2009/06/20
. . . .	

# EcoPharm: search examples (cont.)

=> D PHARM

Display the pharmacological (PHARM) data.

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN  
. . . .

## PHARM

Effect (.E): cytotoxicity  
Endpoint of Effect (.EP): cell growth  
Species or Test-System (.SP): SIRC cells, rabbit eye derived cell  
line  
Concentration (.C): <= 1 mmol/l  
Exposure Period (.EX): 72 h  
Further Details (.FD): cells were cultured in Eagle's MEM  
medium supplemented with 10 percent  
calf serum  
Type (.TYP): IC50  
Value of Type (.V): > 1 mmol/l

## Reference(s):

1. Ohno, Y.; Miyajima, A.; Su  
TOLED5, 102, <1998>, 569 -

Remember to use the "F" prefix to display more than 20 entries, i.e. FPHARM.

. . . .

Only first 20 entries are displayed. Total number of entries = 44.  
Use "DIS F<prop>" for full format, e.g. FCPD instead of CPD.

# EcoPharm: search examples (cont.)

- Find antihistamines which are not ethylene diamine derivatives

```
=> S ANTIHISTAMINIC/PHARM.E  
L1          655 ANTIHISTAMINIC/PHARM.E
```

Search for the pharmacological effect (/PHARM.E).

```
=>  
Uploading C:\...\My Documents\STN Express 8.4\Queries\ethylene diamine.str
```

```
L2          STRUCTURE UPLOADED
```

Draw, save and upload the ethylene diamine structure.

```
=> D  
L2 HAS NO ANSWERS  
L2          STR
```



Structure attributes must be viewed using STN Express query preparation.

# EcoPharm: search examples (cont.)

=> S L2 SUBSET

Conduct structure search in subset.

ENTER SUBSET L# OR (END) :L1

ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END) :FULL

FULL SUBSET SEARCH INITIATED 19:20:18 FILE 'REAXYSFILE'

FULL SUBSET SCREEN SEARCH COMPLETED - 190 TO ITERATE

100.0% PROCESSED 190 ITERATIONS 190 ANSWERS

SEARCH TIME: 00.00.01

L3 190 SEA SUB=L1 SSS FUL L2

=> S L1 NOT L3

Exclude all records retrieved by substructure search.

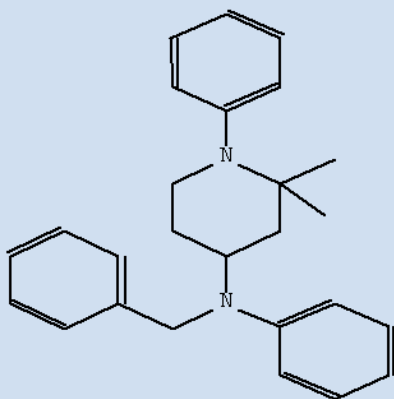
L4 465 L1 NOT L3

# EcoPharm: search examples (cont.)

=> D

L4 ANSWER 1 OF 465 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):	11681414
Chemical Name (CN):	(RS)-4-(N-benzylanilino)-2,2-dimethyl-1-phenylpiperidine
Lin. Struct. Formula (LSF):	C26H30N2
Molec. Formula (MF):	C26 H30 N2
Molecular Weight (MW):	370.538
Entry Date (DED):	2009/05/09
Update Date (DUPD):	2009/05/14



The ReaxysFile default display format is Query Related Data (QRD), i.e. IDE + HIT.

# EcoPharm: search examples (cont.)

Pharmacological Data:

PHARM

Query Related Data  
(QRD) (cont.)

Effect (.E): **antihistaminic**

Species or Test-System (.SP): ileum segments of guinea pig

Concentration (.C): 3E-08 - 3E-05 mol/l

Kind of Dosing (.KD): title comp. used as dihydrochloride

Results (.RE): molecular target: H1 histaminic  
receptor

Reference(s):

1. Weis, Robert; Schweiger, Klaus; Faist, Johanna; Rajkovic, Erich; Kunzl, Andreas J.; Seebacher, Werner; Fabian, Walter M. F.; Schunack, Walter, Bioorganic & Medicinal Chemistry, CODEN: BMECEP, 16(24), <2008>, 10326 - 10331; BABS-7131693

# Agenda

- What is ReaxysFile?
- Find substances
- Find reactions
- Searching bibliographic data
- Physical properties
- EcoPharm data
- **Chemical data**
- Basic tips for managing display costs

# Chemical data

- Chemical Derivative
  - Derivative name, AN and comment may be given
  - Derivatives for characterization are recorded as individual compounds
- Isolation from Natural Product
  - Names of natural sources from which compound has been isolated in scientific nomenclature
- Purification
  - Description of purification method
- Related Structure
  - Indicates differences in structure (constitution, configuration) given in former literature references
  - Contains new AN assigned to compound

# Search example: chemical data (CDER)

- Find a derivative of 7-chloro-3-methyl-1-phenyl-isoquinoline to help characterize the compound

```
L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Pr  
Accession Number (AN): 1345900  
Basic Pref. RN (BPR): 21158-93-0  
CAS Reg. No. (RN): 21158-93-0  
Chemical Name (CN): 7-chloro-3-methyl-1-phenyl-isoquinoline  
Autonom Name (AUN): 7-chloro-3-methyl-1-phenyl-isoquinoline  
Molec. Formula (MF): C16 H12 Cl N  
Molecular Weight (MW): 253.73  
Lawson Number (LN): 24514  
Compound Type (CTYPE): heterocyclic  
Constitution ID (CONSID): 1251297  
Handbook Citation (HSO): 5-20-08-00385, 6-20  
Entry Date (DED): 1988/11/29  
Update Date (DUPD): 1996/01/03  
. . . .
```

IDE display for 7-chloro-3-methyl-1-phenyl-isoquinoline.

# Search example: chemical data (cont.)

IDE display for 7-chloro-3-methyl-1-phenyl-isoquinoline (cont.)

Field Availability:

Code	Name	Occurrence
AN	Accession Number	1
BRP	Basic Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
HSO	Handbook Citation	2
DED	Entry Date	1
DUPD	Update Date	1
CDER	Chemical Derivative	2
DE	Dissociation Exponent	1
MP	Melting Point	2
NMR	Nuclear Magnetic Resonance	1
UVS	UV and Visible Spectrum	3
. . . . .		

# Search example: chemical data (cont.)

=> D CDER

Display chemical derivative (CDER).

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Chemical Derivative:

CDER

(CDER) :

C16H12C1N\*C6H3N3O7

Derivative AN (.AN) :

6468957

Reference(s) :

1. Zielinski, Wojciech, Pol.J.Chem., CODEN: PJCHDQ, 54(11/12), <1980>, 2209-2215; BABS-5804357

CDER

Note(s) (.COM) :

Pikrat C16H12C1N\*C6H3N3O7: F: 193-194grad (aus A.)

Reference(s) :

1. Bhattacharya, Indian J.Chem., CODEN: IJOCAP, 6, <1968>, 341,343

# Search example: chemical data (cont.)

=> S 6468957/AN

L2 1 6468957/AN

Search for the AN of  
the derivative (picrate).

=> D IDE

L2 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Accession Number (AN):	6468957
Fragm. Molec. Formula (FMF):	C16 H12 Cl N , C6 H3 N3 O7
Molecular Formula (MF):	C16 H12 Cl N . C6 H3 N3 O7
Molecular Weight (MW):	253.73, 229.11
Fragment AN (FAN):	1345900, 423400
Lawson Number (LN):	24514, 5222
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	5627885
Handbook Citation (HSO):	6-20
Entry Date (DED):	1994/01/24
Update Date (DUPD):	1994/01/24
. . . .	

# Search example: chemical data (cont.)

Field Availability:

Field availability for the derivative (picrate).

Code	Name	Occurrence
AN	Accession Number	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FAN	Fragment AN	2
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
HSO	Handbook Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1

# Search example: chemical data (cont.)

=> D MP

L2 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

Melting Point:

Value	Ref.
(MP)	
(Cel)	
=====+=====	
190 - 191	1

Characterization  
of derivative.

Reference(s) :

1. Zielinski, Wojciech, Pol.J.Chem., CODEN: PJCHDQ, 54(11/12),  
<1980>, 2209-2215; BABS-5804357

# Agenda

- What is ReaxysFile?
- Find substances
- Find reactions
- Searching bibliographic data
- Physical properties
- EcoPharm data
- Chemical data
- **Basic tips for managing display costs**

# Basic tips for managing display costs

- The ReaxysFile pricing model
  - Connection time charge (\$51.00 / hour)
  - Structure search charge (\$96.60 / SSS FULL)
  - SELECT charge for PN and RN (\$0.49 / record)
  - Per display field charge (\$8.30 / record)
  - No search term charges
  - No free-of-charge display formats

**Note:** For more detail on ReaxysFile prices enter **HELP COST** at the command prompt (=>), or visit: <http://www.stn-international.com/prices.html>

## Basic tips for managing display costs (cont.)

- Always think twice about the ALL format
- IDE format already includes the FA table
- Display RX from the substance segment
- HIT format is often not a full field display
- QRD format (default) is IDE + HIT
- Full “F” prefix for >20 references
- ALLREF format provides a simple list of all unique references for one display charge
- Super display formats for a single fee (next...)

# Basic tips for managing display costs (cont.)

Use ReaxysFile **Super Display Fields** for displaying multiple related fields for a single display charge.

IDE	Identification of substance
CRY	Crystals
ECB	Electrochemical behavior
ECO	Ecological
PED	ECO + PHARM
ELEP	Electrical
GAS	Gases
LIQ	Liquids
MAGP	Magnetic
MECP	Physical and mechanical

OPTP	Optical
SEP	Structure and energy
SF	Safety
SOL	Solution behavior
THE	Thermodynamic
TRA	Transport phenomena
CHE	Chemical
LVS	Liquid/Vapor system
RX	Reactions

## Example: the super display field Crystal Properties (CRY) includes

- Density of the Crystal (CDEN)
- Crystal Property (CPD)
- Crystal Space Group (CSG)
- Crystal System (CSYS)
- Crystal Phase Transition Point (CTP)
- Decomposition Point (DP)
- Melting Point (MP)
- Sublimation Point (SP)

# Summary

- What is ReaxysFile?
- Find substances
- Find reactions
- Searching bibliographic data
- Physical properties
- EcoPharm data
- Chemical data
- Basic tips for managing display costs

# Resources for searching ReaxysFile

- ReaxysFile user documentation:

[http://www.stn-international.com/stn\\_chemistry\\_reaxysfile.html](http://www.stn-international.com/stn_chemistry_reaxysfile.html)

- ReaxysFile database summary sheet:

<http://www.stn-international.com/reaxysfile.html>

- BABS database summary sheet:

<http://www.stn-international.com/babs.html>

# STN<sup>®</sup>

For more information ...

CAS

E-mail: [help@cas.org](mailto:help@cas.org)

Support and Training:

[www.cas.org](http://www.cas.org)

FIZ Karlsruhe

[helpdesk@fiz-karlsruhe.de](mailto:helpdesk@fiz-karlsruhe.de)

Support and Training:

[www.stn-international.de](http://www.stn-international.de)