

# STN<sup>®</sup>

## Reaction Searching in ReaxysFile on STN<sup>®</sup>

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# Agenda

- What is ReaxysFile?
- Find substances
- Find reactions
- 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 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

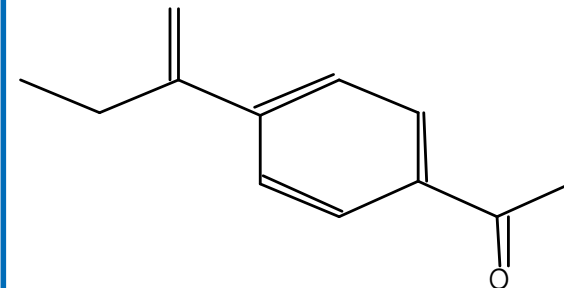
L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier

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.

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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.

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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 (.TEM): Cel  
Reaction Type (.RT): 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**

# 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(diphenylphosphanyl)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
- Basic tips for managing display costs

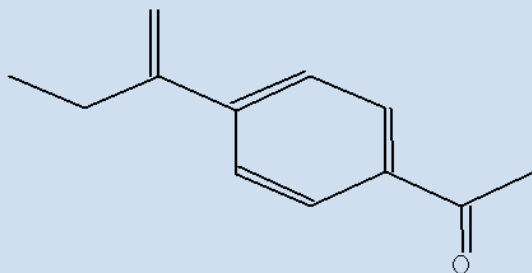
# How to search for substances

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

# How to search for substances

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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.

# 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>.

# Agenda

- What is ReaxysFile?
- Find substances
- **Find reactions**
- 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

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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



## 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 / FREAA)
  - 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

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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

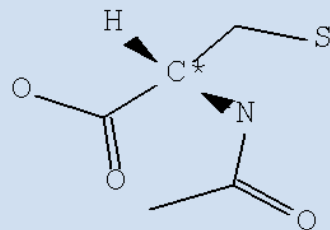
Lin. Struct. Formula (LSF):

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-dinitro-phenylsulfanyl)-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

# 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
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 . . . .

Identify the AN.

# 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

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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.

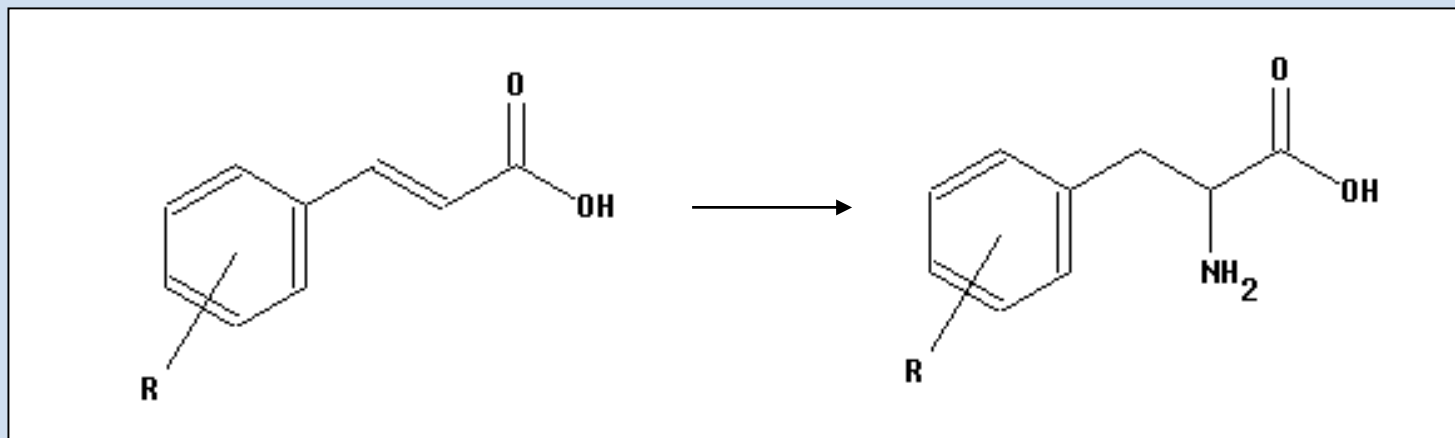
Stage 1

Stage 2

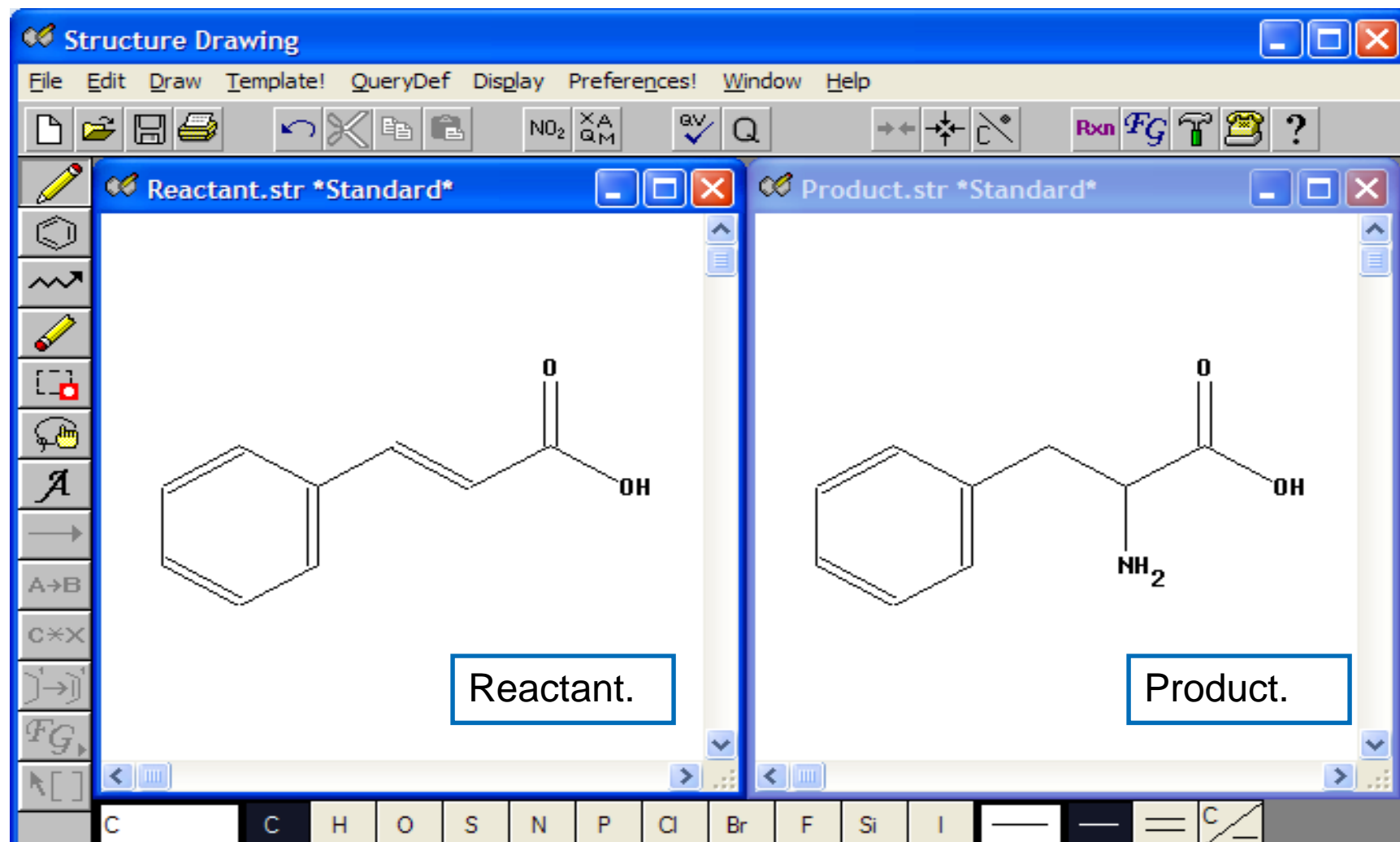
# Example: searching for reactions with specific reactant and product

## 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

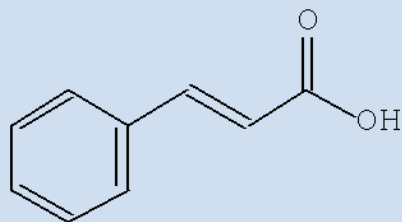
L1 STRUCTURE UPLOADED

=> D

L1 HAS NO ANSWERS

L1 STR

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



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

=> TRANSFER L3 AN 1- /RX.RAN

L4 TRANSFER L3 1- AN : 5321

L5 16588 L4/RX.RAN

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

**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

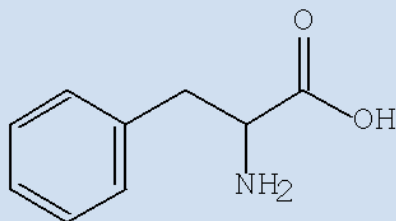
L6 STRUCTURE UPLOADED

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

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

=> S L7 AND RXPRO/FA

L8 3249 L7 AND RXPRO/FA

=> TRANSFER L8 AN 1- /RX.PAN

L9 TRANSFER L8 1- AN :

3249

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

L10 5336 L9/RX.PAN

# 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

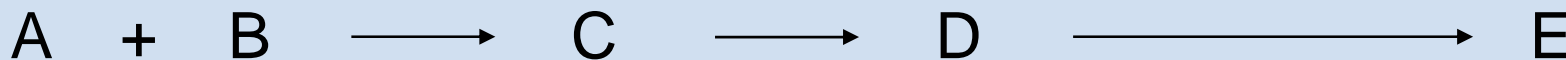
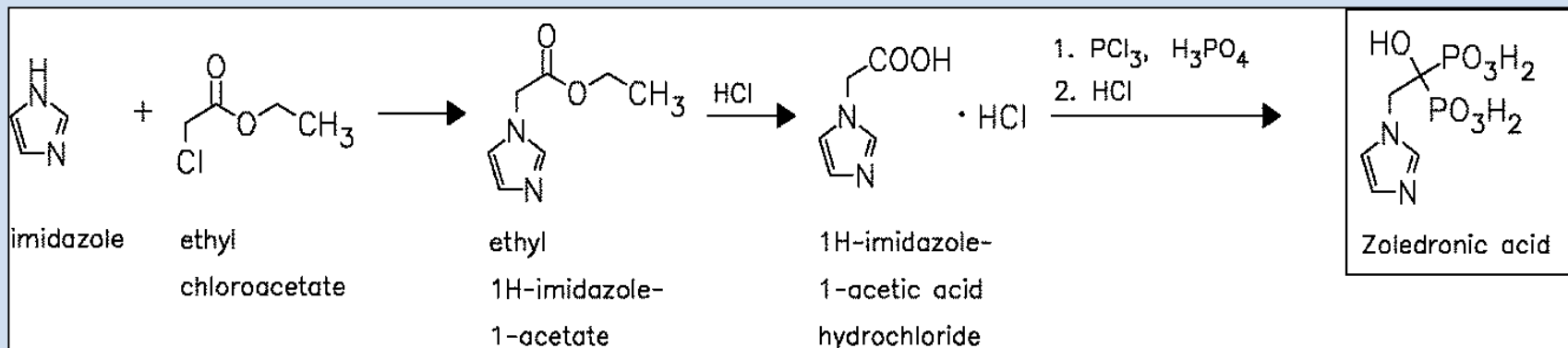
AB The new chiral bidentate phosphine ligand (R)-1,2-bis(diphenylphosphino)-1-cyclohexylethane ((R)-Cycphos) has been prepared. The rhodium(I) cationic complex of this phosphine serves as an effective homogeneous asymmetric hydrogenation catalyst for the reduction of (Z)- $\alpha$ -amidoacrylic acids 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
- **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

# Summary

- What is ReaxysFile?
- Find substances
- Find reactions
- 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>

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