

STN[®]

ReaxysFile on STN[®]

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Agenda

- What is ReaxysFile?
- Find substances
- Find properties
- 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>
AN	Accession Number
BPR	Basic Preferred Registry Number
HSO	Handbook Citation
AAN	ALL Accession Numbers
COMPAN	Composition: Compound Accession Number
FAN	Fragment Accession Number
RX.AAN	All Accession Numbers Reaction
RX.RAN	Reactant Accession Number
RX.PAN	Product Accession Number
xxxx.PAAN	[<i>property</i>] Partner Accession Number
xxxx.AN	[<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

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[®]
- 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

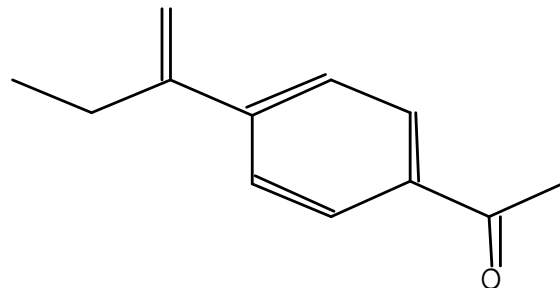
L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier

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.

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)
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(C₃H₅)]₂/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 properties
- Find reactions
- Basic tips for managing display costs

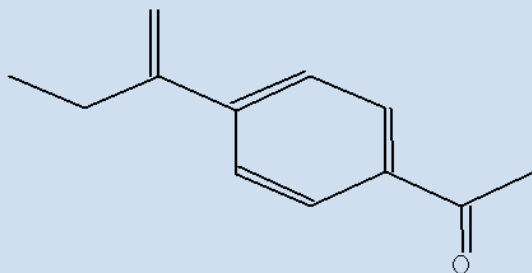
How to search for substances

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

How to search for substances

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.

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

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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).

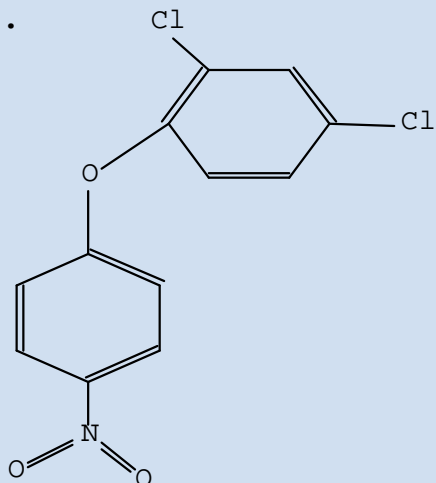
Search example: physical data (cont.)

=> 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	
		(.AM)	
		(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: °C instead of K for temperature)

Tip: Use e.g. `SET UNITS ALL=CGS` to convert all units to the centimeter-gram-second system.

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
```

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

```
=> 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
```

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

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

=>

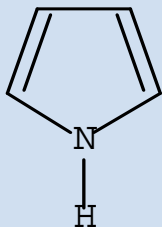
Uploading C:\STNEXP\QUERIES\Pyrrole.str

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

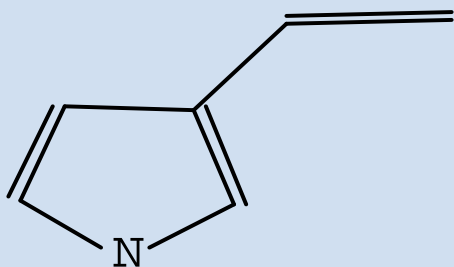
=> D IDE BP

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.

Agenda

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

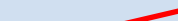
L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier Properties SA. on STN

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 / 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 α -acetyl-L-cysteine, N α -acetylcysteine, N α -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 α -acetyl-L-cysteine, N α -acetylcysteine, N α -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 α -acetyl-S-(2,4-dinitro-5-(dimethylaminomethyl)phenyl)-L-cysteine 9708798, **1724426**

Product AN (.PAN):

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 α -acetyl-L-cysteine,
N α -acetylcysteine,
N α -acetyl-L-cysteine

Autonom Name (AUN):

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

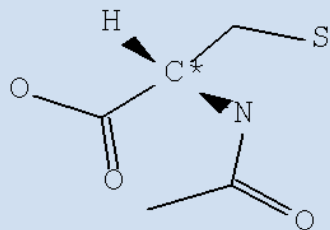
Lin. Struct. Formula (LSF):

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
```

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

```
=> D RX
```

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

```
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
  . . . .
```

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

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.

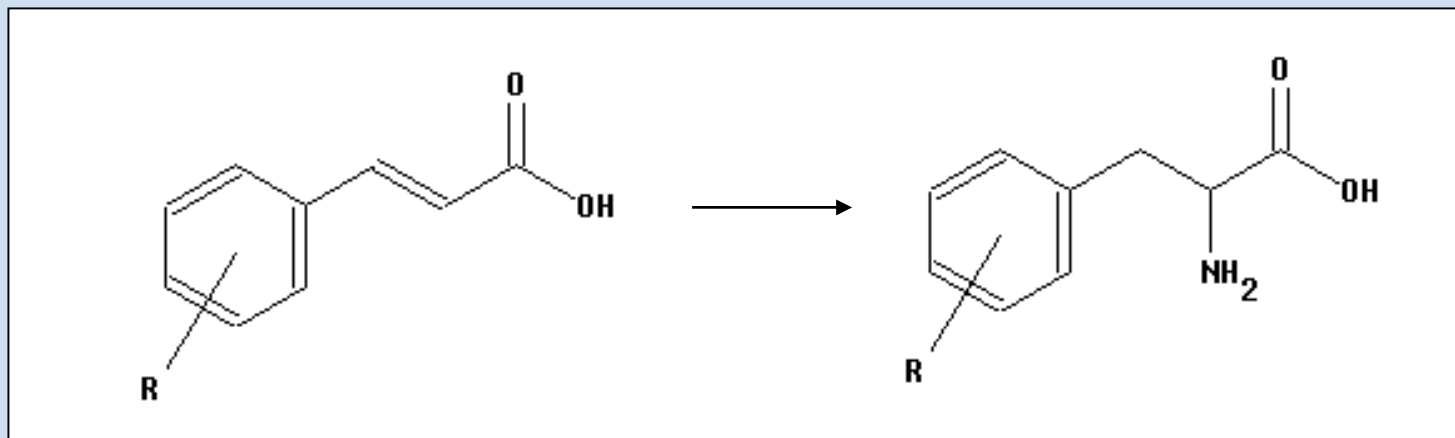
Stage 1

Stage 2

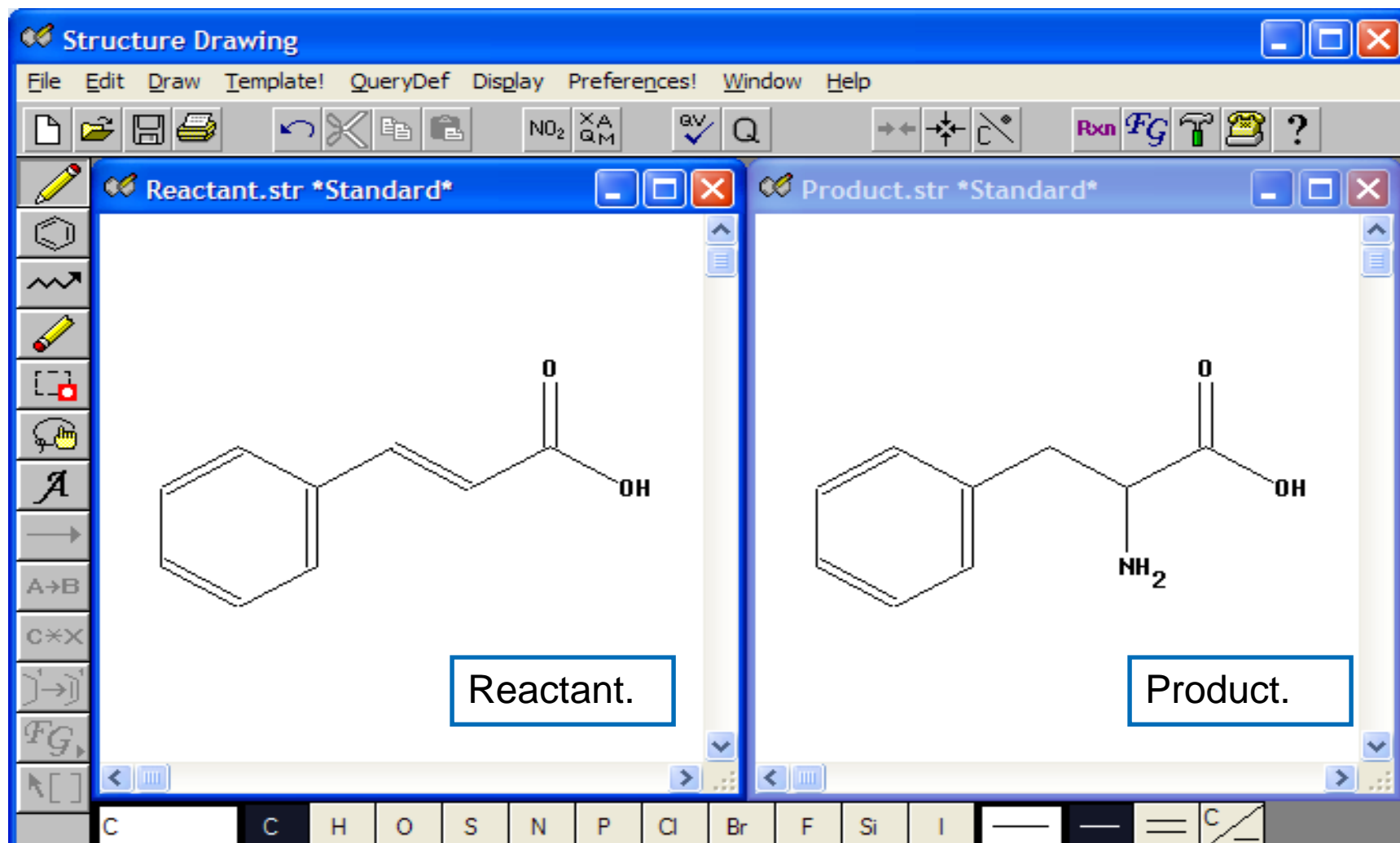
Example: searching for reactions with specific reactant and product

Search Question:

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



Using STN Express[®] 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

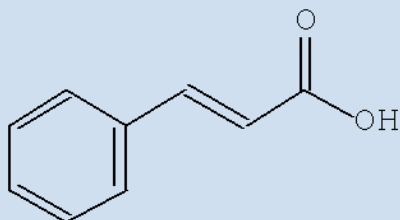
L1 STRUCTURE UPLOADED

=> 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

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

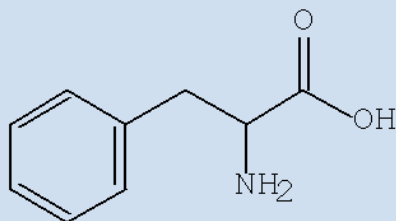
L6 STRUCTURE UPLOADED

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

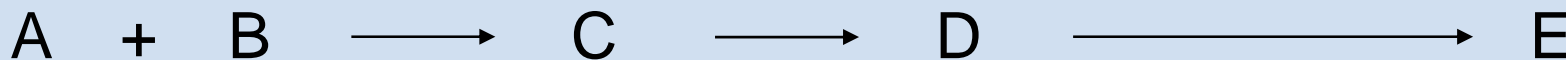
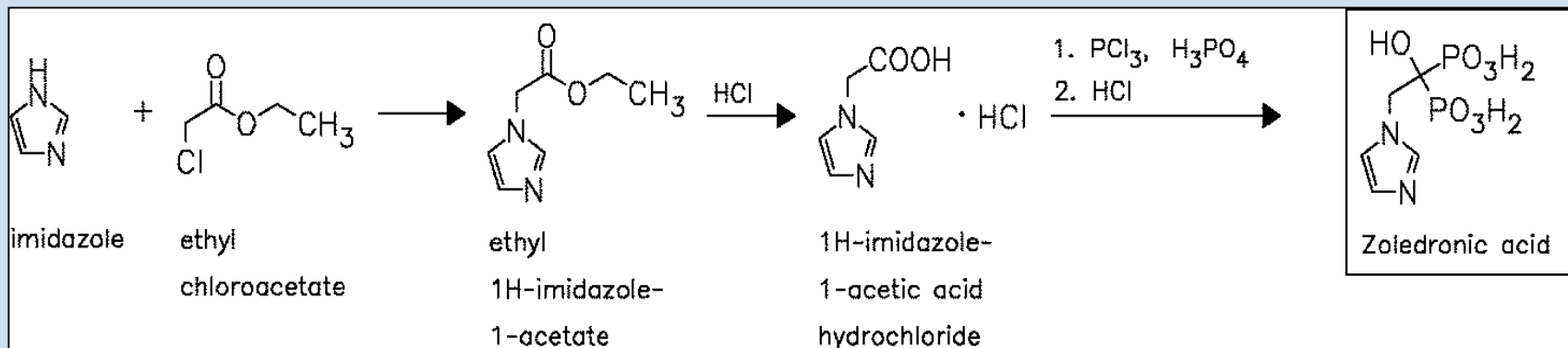
AB The new chiral bidentate phosphine ligand (R)-1,2-bis(diphenylphosphino)-1-cyclohexylethane ((R)-Cycphos) has been prepared. The rhodium(I) cationic complex of this phosphine serves as an effective homogeneous asymmetric hydrogenation catalyst for the reduction of (Z)- α -amidoacrylic acids at ambient temperature and pressure. Optical yields for the corresponding (S)- α -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 properties
- 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

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 physical properties
- Find reactions
- Basic tips for managing display costs

Resources for searching ReaxysFile

- ReaxysFile user documentation:

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>

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