

# STN<sup>®</sup>

## Physical Property Searching in ReaxysFile on STN<sup>®</sup>

Martine MICHEL

CAPADOC

[martine.michel@capadoc.fr](mailto:martine.michel@capadoc.fr)

# Agenda

- What is ReaxysFile?
- Find substances
- Find physical properties
- 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](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

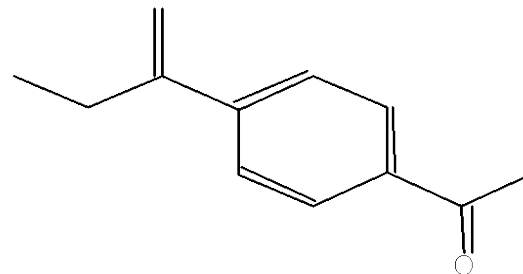
L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier

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): CDCl3

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): CDCl3

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

L1 ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2010 Elsevier F

Reaction data, RX.

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):

BABS Accession Number.

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 physical properties
- Basic tips for managing display costs

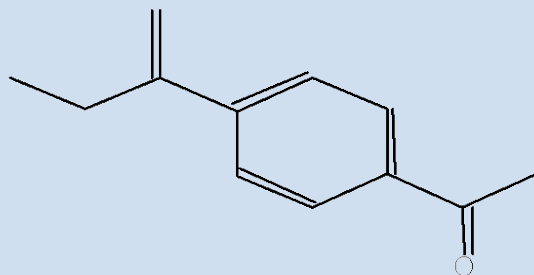
# How to search for substances

- 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

- What is ReaxysFile?
- Find substances
- **Find physical properties**
- 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).

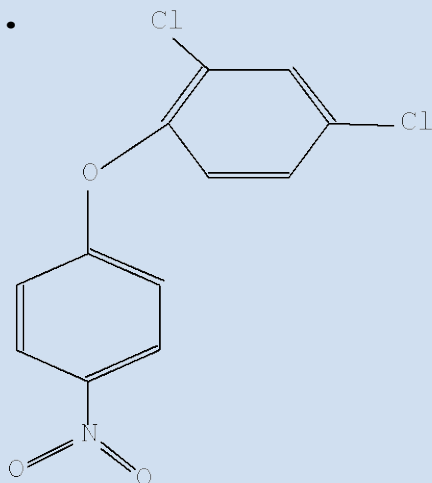
# Search example: physical data (cont.)

=> 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 Maxima	Ref.
(.KW)	(.SOL)	(.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 (MP) (Cel)	Solvent (.SOL)	Ref.	Note
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
```

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

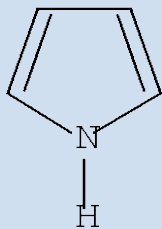
- Find pyrrole derivatives with a boiling point lower than or equal to 30° C?

```
=> 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

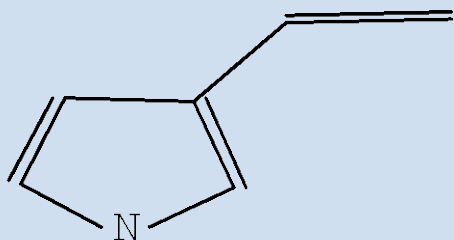
=> D IDE BP

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 (BP) (Cel)	Press. (.P) (Torr)	Ref.	Note
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 physical properties
- **Basic tips for managing display costs**

# Basic tips for managing display costs

- The ReaxysFile pricing model
  - Connection time charge (38 €/ hour)
  - Per display field charge (5,80 €/ record)
  - Structure search charge (72,10 €/ SSS FULL)
  - 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
- 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>

Thank you for your attention

**STN**<sup>®</sup>

For more information

[www.capadoc.com](http://www.capadoc.com)

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

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

**STN**

STN is available through FIZ Karlsruhe, Germany  
and Chemical Abstracts Service, U.S.A.