BEILSTEIN on STN

WORKSHOP MANUAL

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Contents

BEILSTEIN on STN

Robert Austin
FIZ Karlsruhe

Agenda

- What is Beilstein?
- Changes in 2002: file re-design and new content
- Find substances
- Find reactions
- Searching bibliographic data
- *New* EcoPharm data
- Physical properties
- Chemical data

What is BEILSTEIN?

What is BEILSTEIN?

- 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

BEILSTEIN on STN®

- File BEILSTEIN
  - More than 8 million substances
  - More than 9 million reactions
  - More than 2 million citations 1771-date
- File BABS
  - Over 800,000 abstracts and titles 1980-date

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Typical questions for BEILSTEIN

- Determine if a substance been described in past chemical literature, e.g. a novelty 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

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Ways to search BEILSTEIN

- Structure/Substructure
- Chemical Name
- Chemical Name Segment
- Molecular Formula
- CAS Registry Numbers
- Physical properties or keyword
- . . . .

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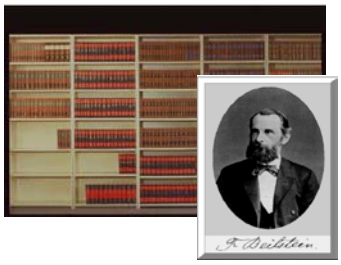
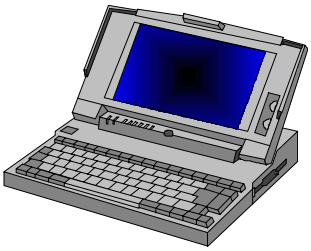
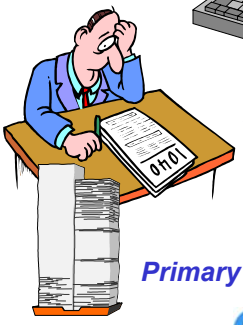
BEILSTEIN data sources



BEILSTEIN Handbook 1771-1959



Primary literature >1979



Primary literature 1960 -1979

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BEILSTEIN data sources

- New to STN in 2002
  - Three new molecule types: **biomolecules**, **polymers** and **mixtures**
  - A series of new property topics
  - Ecological and pharmacological data
  - Expanded journal coverage
  - Changes date back to 1995

BEILSTEIN journal list

- A list of source journals for the BEILSTEIN database is available

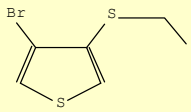
  www.stn-international.com/training_center/chemistry/beilstein/bjl.html

Sample record

```
L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

 Beilstein Records (BRN):      6188941
 Chemical Name (CN):           4-bromo-3-ethylmercaptothiophene
 Autonom Name (AUN):           3-bromo-4-ethylsulfanyl-thiophene
 Molec. Formula (MF):          C6 H7 Br S2
 Molecular Weight (MW):        223.15
 Lawson Number (LN):           17181, 301
 Compound Type (CTYPE):        heterocyclic
 Constitution ID (CONSID):     5319663
 Tautomer ID (TAUTID):         5797498
 Beilstein Citation (BSO):     6-17
 Entry Date (DED):             1993/10/20
 Update Date (DUPD):           1993/10/20
```

Substance Identifying Information



Structure

Sample record

```
 Field Availability:

 Code      Name                                      Occurrence
 ========================================================
 BRN       Beilstein Records                                1
 CN        Chemical Name                                    1
 AUN       Autonomname                                      1
 MF        Molecular Formula                                1
 FW        Formular Weight                                  1
 LN        Lawson Number                                    2
 CTYPE     Compound Type                                    1
 CONSID    Constitution ID                                  1
 TAUTID    Tautomer ID                                      1
 BSO       Beilstein Citation                               1
 ED        Entry Date                                       1
 UPD       Update Date                                      1
 BP        Boiling Point                                    1

This substance also occurs in Reaction Documents:

 Code      Name                                      Occurrence
 ========================================================
 RX        Reaction Documents                               2
 RXREA     Substance is Reaction Reactant                   1
 RXPRO     Substance is Reaction Product                    1
```

Field Availability Table

Sample record

```
L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Boiling Point:
 Value       | Press.      |Ref.
 (BP)        | (.P)        |
 (Cel)       | (Torr)      |
=============+=============+====
 117 - 120   | 14          | 1

Reference(s):
 1. Litvinov, V. P.; Dzhumaev, I. A.; Zolotarev, B. M., Bull.Acad.Sci.USSR
    Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 32(9), <1983>, 1901-1906,
    Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(9), <1983>, 2105-2110;
    BABS-5771950
```

Property data

Sample record

```
L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Reaction:
RX
     Reaction ID (.ID):              1558123
     Reactant BRN (.RBRN):           107642, 1098273
     Reactant (.RCT):                3,4-dibromo-thiophene, diethyldisulfane
     Product BRN (.PBRN):            6188941
     Product (.PRO):                 4-bromo-3-ethylmercaptothiophene
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):            1558123.1
     Reaction Classification (.CL):  Preparation
     Reagent (.RGT):                 1.) BuLi
     Other Conditions (.COND):       1) ether
     Note(s) (.COM):                 Yield given. Multistep reaction
     Reference(s):
     1. Litvinov, V. P.; Dzhumaev, I. A.; Zolotarev, B. M., Bull.Acad.Sci.USSR
        Div.Chem.Sci.(Engl.Transl.), CODEN: BACCAT, 32(9), <1983>, 1901-1906,
        Izv.Akad.Nauk SSSR Ser.Khim., CODEN: IASKA6(9), <1983>, 2105-2110;
        BABS-5771950
```

Reaction data

Changes to BEILSTEIN in 2002

Changes to BEILSTEIN

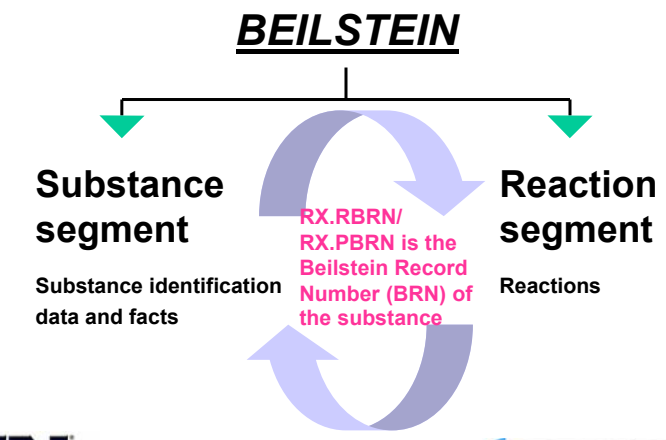
- New file structure
- New layout for reaction data
- New subject: EcoPharm Data
- New compound types
- New property topics
- Re-organization of existing topics
- Controlled terms in new Keyword fields
- All Keywords and Property Hierarchy fields
- Easier access to BEILSTEIN Abstracts

New file structure

Two file segments

- Substance segment (SUB)
  - Substance identification data and facts
- Reaction segment (RX)
  - Reaction data

BEILSTEIN file segments



BRN link between file segments

Substance File Segment

```
Beilstein Records (BRN):      1209327
Beilstein Pref. RN (BPR):     108-05-4
CAS Reg. No. (RN):            108-05-4
Chemical Name (CN):           acetoxyethene, acetic acid vinyl ester,
                              Essigsaeure-vinylester, acetic acid ethenyl
                              ester, vinyl acetate
Autonom Name (AUN):           acetic acid vinyl ester
Molec. Formula (MF):          C4 H6 O2 ...
```

BRN

Reaction File Segment

```
Reaction:
RX
     Reaction ID:             8743437
     Reactant BRN:            1209327
     Reactant:                acetoxyethene
     Product BRN:             506007
     Product:                 acetic acid
     No. of Reaction Details: 4 ...
```

RX.RBRN

New subject: EcoPharm data

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

New compound types added

- Biomolecules
  - e.g. carbohydrates, nucleic acids, proteins, enzymes, hormones
- Mixtures
  - composition completely, partially or not given
- Polymers
  - monomers given, monomers not given

New property topics

- Conformation (CNF) in ***Structure and Energy Parameter***
- Luminescence (LUM) in ***Spectral Data***
- Electrical Data (ELE) and Magnetic Data (MAG) in ***Electrical and Magnetic Properties***
- Henry Constant (HNC), Partition Constant Octan-1-ol/Water (POW), Complex Phase Equilibria (CPEM), Electrical Data (EDM), Optical Data (ODM) in ***Multi-Component Systems***

Removal of Topics

- Gibbs Energy of Formation
- Coefficient of Expansion
- Zero Point Energy
- Purity
- Moment of Inertia
- Some old topics are now keywords
  - e.g. Molar Volume ➢ Mechanical Properties

Reorganization of existing topics

- Additional fields for existing topics
  - e.g. ESR: Coupling Nuclei, Solvents, Temperature, Comment
- Systematic grouping of spectroscopic properties
  - NMR (NMR), IR (IR), RAMAN (RAS), UV/VIS (UVS)
  - Fluorescence (FLU), Phosphorescence (PHO)
  - Subfields gathered together logically, e.g. **/NMR.xxx**
- Redox Potential ➢ Electrochemical Characteristics

Controlled Terms / Keywords

- Controlled Terms moved to new keyword fields (.KW) of corresponding topics
- Data located in the old keyword field moved corresponding comments fields (.COM)
- Various keyword lists have been extended
- Use Expand to see keywords in a given topic

Example: mechanical property 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 ****
```

Controlled Terms / Keywords

- All Keywords (AKW)
  - Keywords from all .KW topic fields in one index
- Property Hierarchy (/PH)
  - Keywords plus topic field codes in one index
- Browse AKW and PH terms using Expand
  - BEILSTEIN is a zero connection hour file!

Basic Index (/BI)

- Basic Index (/BI) (default)
  - Substance Identification Data and property fields
  - All chemical name fields
  - All Beilstein Record Numbers (BRN) fields
  - Molecular formulae, and all keywords (AKW)
- Basic Index for Reactions (/BIRX)
- Basic Index for EcoPharm data (/BIPED)
- Use SET SFIELDS to change default Basic Index

Link to Beilstein Abstracts (BABS)

- BEILSTEIN Abstracts database (BABS): Titles & abstracts 1980 to date
- At the end of a BEILSTEIN reference a BABS Accession Number is given
- New link for STN on the Web: from a BEILSTEIN reference to the BABS record
- From BABS to full-text via Chemport

STN

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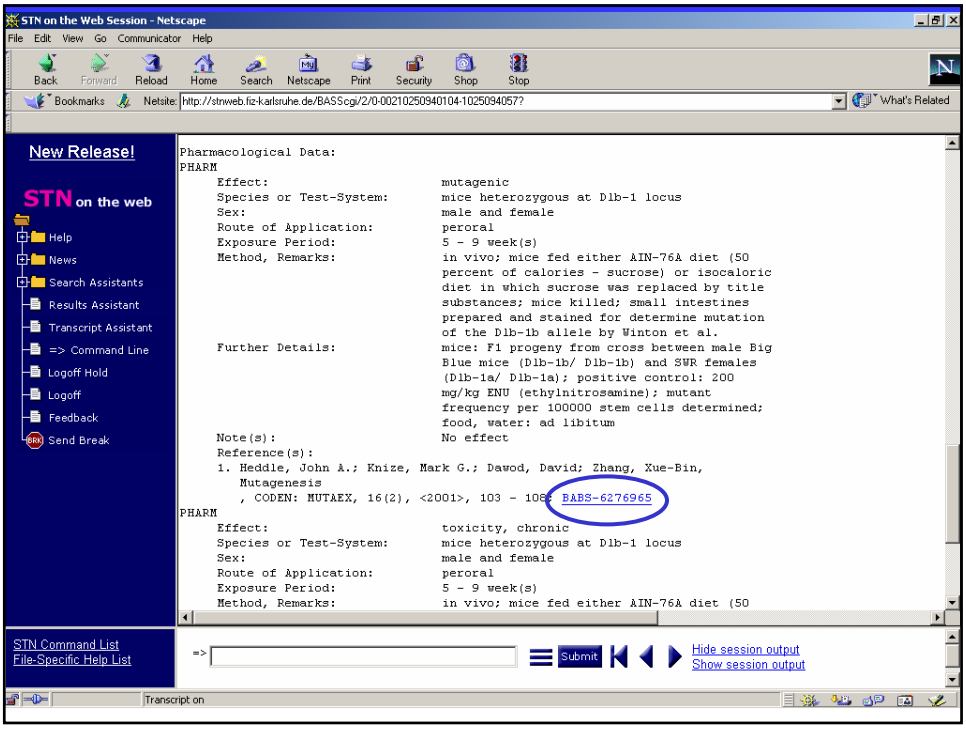
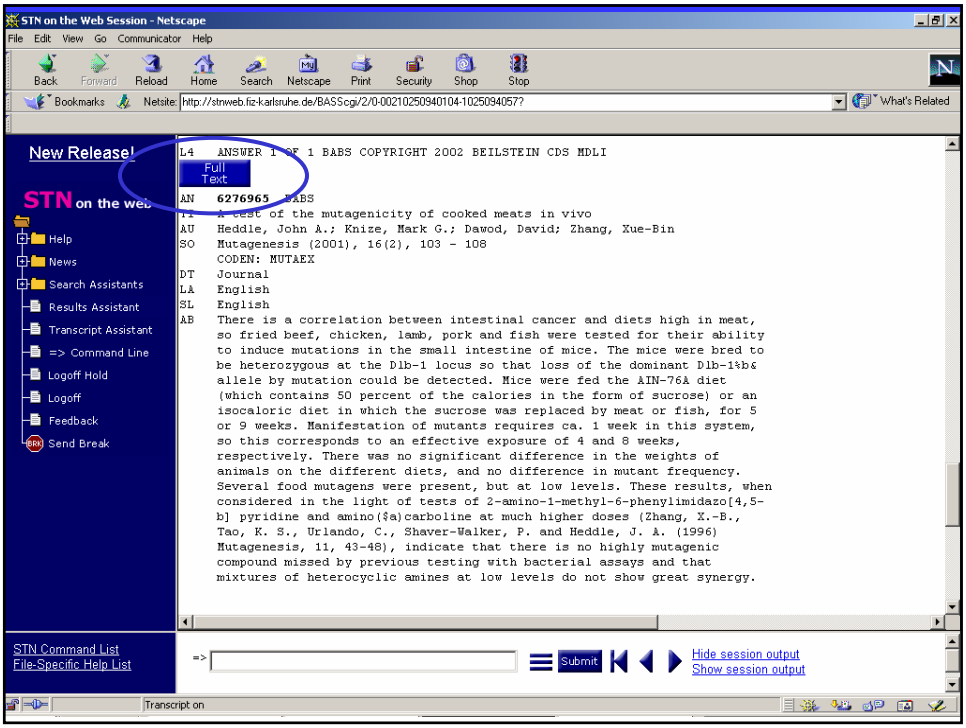
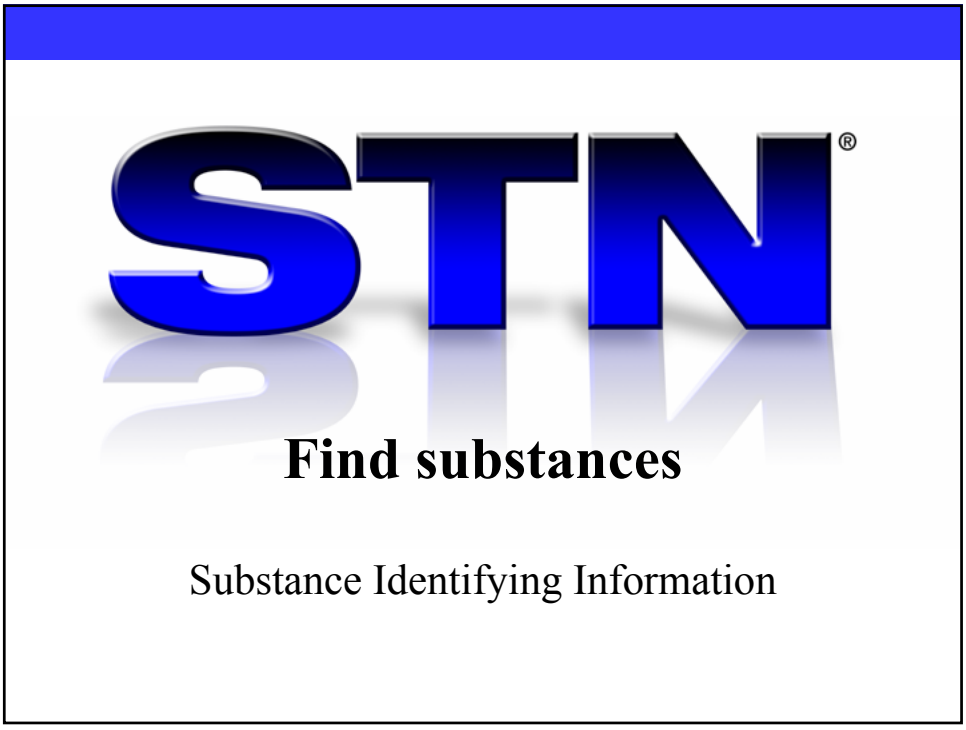


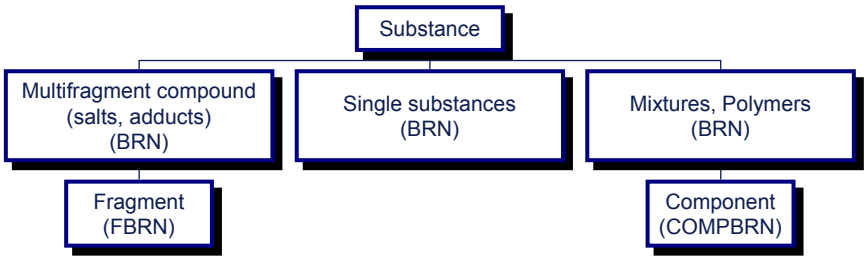

STN on the Web Session - Netscape
File Edit View Go Communicator Help
Back Forward Reload Home Search Netscape Print Security Shop Stop
Bookmarks Netsite: http://stnweb.fiz-karlsruhe.de/BASScgi/2/0-00210250940104-10250940577
What's Related
New Release!
STN on the Web
Help
News
Search Assistants
Results Assistant
Transcript Assistant
=> Command Line
Logoff Hold
Logoff
Feedback
Send Break
L4 ANSWER 1 OF 1 BABS COPYRIGHT 2002 BEILSTEIN CDS MDLI
Full Text
AN 6276965 BABS
TI A test of the mutagenicity of cooked meats in vivo
AU Heddle, John A.; Knize, Mark G.; Dawod, David; Zhang, Xue-Bin
SO Mutagenesis (2001), 16(2), 103 - 108
CODEN: MUTAEX
DT Journal
LA English
SL English
AB There is a correlation between intestinal cancer and diets high in meat, so fried beef, chicken, lamb, pork and fish were tested for their ability to induce mutations in the small intestine of mice. The mice were bred to be heterozygous at the Dlb-1 locus so that loss of the dominant Dlb-1%b& allele by mutation could be detected. Mice were fed the AIN-76A diet (which contains 50 percent of the calories in the form of sucrose) or an isocaloric diet in which the sucrose was replaced by meat or fish, for 5 or 9 weeks. Manifestation of mutants requires ca. 1 week in this system, so this corresponds to an effective exposure of 4 and 8 weeks, respectively. There was no significant difference in the weights of animals on the different diets, and no difference in mutant frequency. Several food mutagens were present, but at low levels. These results, when considered in the light of tests of 2-amino-1-methyl-6-phenylimidazo[4,5-b] pyridine and amino($a)carboline at much higher doses (Zhang, X.-B., Tao, K. S., Urlando, C., Shaver-Walker, P. and Heddle, J. A. (1996) Mutagenesis, 11, 43-48), indicate that there is no highly mutagenic compound missed by previous testing with bacterial assays and that mixtures of heterocyclic amines at low levels do not show great synergy.
STN Command List
File-Specific Help List
=>
Submit
Hide session output
Show session output
Transcript on


STN®
Find substances
Substance Identifying Information

BEILSTEIN substances

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

Indexing of substances



Substance Identifying Information

Beilstein Records (BRN):	6188941
Chemical Name (CN):	4-bromo-3-ethylmercaptothiophene
Autonom Name (AUN):	3-bromo-4-ethylsulfanyl-thiophene
Molec. Formula (MF):	C6 H7 Br S2
Molecular Weight (MW):	223.15
Lawson Number (LN):	17181, 301
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	5319663
Tautomer ID (TAUTID):	5797498
Beilstein Citation (BSO):	6-17
Entry Date (DED):	1993/10/20
Update Date (DUPD):	1993/10/20

Beilstein Record Number (BRN)

Accession Number of substance

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Substance Identifying Information

Beilstein Records (BRN):	6188941
Chemical Name (CN):	4-bromo-3-ethylmercaptothiophene
Autonom Name (AUN):	3-bromo-4-ethylsulfanyl-thiophene
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Entry Date (DED):	1993/10/20
Update Date (DUPD):	1993/10/20

Chemical Name and AutoNom Name

Chemical Name:
- preferred names
- names from publications
- trivial names

Autonom Name:
- Names generated by the program AutoNom

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Chemical Name Segments (/CNS)

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

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

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Substance Identifying Information

```
Beilstein Records (BRN):      2035920
Beilstein Pref. RN (BPR):     286-08-8
CAS Reg. No. (RN):            286-08-8, 54376-67-9
Chemical Name (CN):           norcarane, bicyclo<4.1.0>heptane
Autonom Name (AUN):           bicyclo<4.1.0>heptane
Molec. Formula (MF):          C7 H12
Molecular Weight (MW):        96.17
Lawson Number (LN):           3941
File Segment (FS):            Stereo compound
Compound Type (CTYPE):        isocyclic
Constitution ID (CONSID):     1752035
Tautomer ID (TAUTID):         1929282
Beilstein Citation (BSO):     4-05-00-00257, 5-
Entry Date (DED):             1989/06/29
Update Date (DUPD):           2001/07/25
```

CAS Registry Number

- Extracted from abstracted primary literature
- Derived from a match between database structures and CAS Registry file

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Substance Identifying Information

Beilstein Records (BRN):	2035920
Beilstein Pref. RN (BPR):	286-08-8
CAS Reg. No. (RN):	286-08-8, 54376-67-9
Chemical Name (CN):	norcarane, bicyclo<4.1.0>heptane
Autonom Name (AUN):	bicyclo<4.1.0>he
Molec. Formula (MF):	C7 H12
Molecular Weight (MW):	96.17
Lawson Number (LN):	3941
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	1752035
Tautomer ID (TAUTID):	1929282
Beilstein Citation (BSO):	4-05-00-00257, 5
Entry Date (DED):	1989/06/29
Update Date (DUPD):	2001/07/25

BEILSTEIN Preferred Registry Number

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

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Substance Identifying Information

Beilstein Records (BRN):	6188941
Chemical Name (CN):	4-bromo-3-ethylmercaptothiophene
Autonom Name (AUN):	3-bromo-4-ethylsulfanyl-thiophene
Molec. Formula (MF):	C6 H7 Br S2
Molecular Weight (MW):	223.15
Lawson Number (LN):	17181, 301
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	5319663
Tautomer ID (TAUTID):	5797498
Beilstein Citation (BSO):	6-17
Entry Date (DED):	1993/10/20
Update Date (DUPD):	1993/10/20

Molecular Formula

- Complete molecular formula given for single and multifragment compounds
- Given in Hill-order
- Accepted with or without blanks

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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 sulphur 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

- Find compounds containing N, O, P and S elements with 5-10 carbon atoms, an H/C ratio greater than 2, and excluding 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

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

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

=> D HIT

L4   ANSWER 1 OF 3857 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

     Molecular Formula (MF):         C10 H23 N2 O6 P S3
```

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

Restrict to compounds with only one fragment

Substance Identifying Information

Beilstein Records (BRN):	8808326
Chemical Name (CN):	(R)-4-(1,1-dimethylethyl)-1-(1-hydroxy-3-phenylpropan-2-yl)pyridinium chloride
Autonom Name (AUN):	4-tert-butyl-1-(1-hydroxymethyl-2-phenyl-ethyl)-pyridinium; chloride
Lin. Struct. Formula (LSF):	C18H24NO(1+)*Cl(1-)
Fragm. Molec. Formula (FMF):	C18 H24 N O , Cl
Molecular Formula (MF):	C18 H24 N O . Cl
Molecular Weight (MW):	270.39, 35.45
Fragment BRN (FBRN):	8778869, 3587171
Lawson Number (LN):	24256, 14919
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7455846
Tautomer ID (TAUTID):	8269668
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2001/07/25

Molecular Weight
- Given for single substances and multifragment compounds
- For multifragment compounds MW is given for **each fragment**

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Substance Identifying Information

Beilstein Records (BRN):	8808326
Chemical Name (CN):	(R)-4-(1,1-dimethylethyl)-1-(1-hydroxy-3-phenylpropan-2-yl)pyridinium chloride
Autonom Name (AUN):	4-tert-butyl-1-(1-hydroxymethyl-2-phenyl-ethyl)-pyridinium; chloride
Lin. Struct. Formula (LSF):	C18H24NO(1+)*Cl(1-)
Fragm. Molec. Formula (FMF):	C18 H24 N O , Cl
Molecular Formula (MF):	C18 H24 N O . Cl
Molecular Weight (MW):	270.39, 35.45
Fragment BRN (FBRN):	8778869, 3587171
Lawson Number (LN):	24256, 14919
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7455846
Tautomer ID (TAUTID):	8269668
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2001/07/25

File Segment
- Structure keywords
- Further information about identity of compounds
- Controlled vocabulary

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Substance Identifying Information

Beilstein Records (BRN):	8808326
Chemical Name (CN):	(R)-4-(1,1-dimethylethyl)-1-(1-hydroxy-3-phenylpropan-2
Autonom Name (AUN):	4-tert-butyl-1 ethyl)-pyridir
Lin. Struct. Formula (LSF):	C18H24NO(1+)*C
Fragm. Molec. Formula (FMF):	C18 H24 N O ,
Molecular Formula (MF):	C18 H24 N O .
Molecular Weight (MW):	270.39, 35.45
Fragment BRN (FBRN):	8778869, 35871
Lawson Number (LN):	24256, 14919
File Segment (FS):	Stereo compour
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7455846
Tautomer ID (TAUTID):	8269668
Entry Date (DED):	2001/07/25
Update Date (DUPD):	2001/07/25

Compound Type
Keywords from list of controlled terms:
- acyclic
- isocyclic
- heterocyclic
- polymer (monomers given)
- polymer (monomers not given)
- biomolecules
- mixtures (composition completely given) ...

STN

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Substance Identifying Information

Beilstein Records (BRN):	403040
Beilstein Pref. RN (BPR):	68-26-8
CAS Reg. No. (RN):	68-26-8, 2052-63-3, 6018-74-2, 17706-49-9, ...
Chemical Name (CN):	retinol, <7t,9t,11t,13t>- Retinol, vitamin-A alcohol, vitamin A, axerophthol, vitamin-A, vitamin-A1, vitamin-A1 alcohol
Autonom Name (AUN):	3,7-dimethyl-9-(2,6,6-trimethyl-cyclohex-1-enyl)-nona-2,4,6,8-tetraen-1-ol
Molec. Formula (MF):	C20 H30 O
Molecular Weight (MW):	286.46
Lawson Number (LN):	5494
File Segment (FS):	Stereo compoun
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	400280
Tautomer ID (TAUTID):	395507
Beilstein Citation (BSO):	3-06-00-02787, 4-06-00-04133, 5-06, 6-06
Entry Date (DED):	1989/06/29
Update Date (DUPD):	2002/01/24

Stereoisomers
*Each stereoisomer has a different BRN, but all possess the same **CONSID***

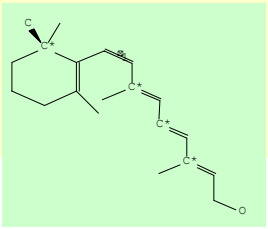
Search example: Constitution ID

```
=> S 400280/CONSID
L2          19 400280/CONSID
=> D

L2   ANSWER 1 OF 19 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

     Beilstein Records (BRN):        8920721
     Chemical Name (CN):             3,7-dimethyl-9-(2,6,6-trimethyl-cyclohex-1-
                                     enyl)-nona-2,4,6,8-tetraen-1-ol
     Autonom Name (AUN):             3,7-dimethyl-9-(2,6,6-trimethyl-cyclohex-1-
                                     enyl)-nona-2,4,6,8-tetraen-1-ol
     Molec. Formula (MF):            C20 H30 O
     Molecular Weight (MW):          286.46
     Lawson Number (LN):             5494
     File Segment (FS):              Stereo compound
     Compound Type (CTYPE):          isocyclic
     Constitution ID (CONSID):       400280
     ...
```

Search for the CONSID retrieves 19 records



Substance Identifying Information

```
     Beilstein Records (BRN):        8808326
     Chemical Name (CN):             (R)-4-(1,1-dimethylethyl)-1-(1-hydroxy-3-
                                     phenylpropan-2-yl)pyridinium chloride
     Autonom Name (AUN):             4-tert-butyl-1-(1-hydroxymethyl-2-phenyl-
                                     ethyl)-pyridinium; chloride
     Lin. Struct. Formula (LSF):     C18H24NO(1+)*Cl(1-)
     Fragm. Molec. Formula (FMF):    C18 H24 N O , Cl
     Molecular Formula (MF):         C18 H24 N O . Cl
     Molecular Weight (MW):          270.39, 35.45
     Fragment BRN (FBRN):            8778869, 3587
     Lawson Number (LN):             24256, 14919
     File Segment (FS):              Stereo compou
     Compound Type (CTYPE):          heterocyclic
     Constitution ID (CONSID):       7455846
     Tautomer ID (TAUTID):           8269668
     Entry Date (DED):               2001/07/25
     Update Date (DUPD):             2001/07/25
```

Tautomer ID

- Each tautomer of a compound has a different BRN
- All tautomers of a compound poses the same Tautomer ID

STN

FIZ KARLSRUHE

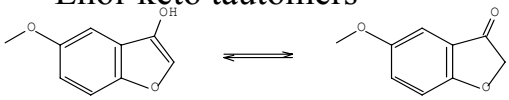
Tautomers

- Imino-amino tautomers

BRN 636130 BRN 106512

TAUTID 121350

- Enol-keto tautomers



BRN 133547 BRN 123671

TAUTID 130745

- Nitroso-oxime tautomers

BRN 969234 BRN 1737204

TAUTID 888467

STN FIZ KARLSRUHE

Substance Identifying Information

Beilstein Records (BRN):	8808326
Chemical Name (CN):	(R)-4-(1,1-dimethylethyl)-1-(1-hydroxy-3-phenylpropan-2-
Autonom Name (AUN):	4-tert-butyl-1- ethyl)-pyridin
Lin. Struct. Formula (LSF):	C18H24NO(1+)*C
Fragm. Molec. Formula (FMF):	C18 H24 N O ,
Molecular Formula (MF):	C18 H24 N O .
Molecular Weight (MW):	270.39, 35.45
Fragment BRN (FBRN):	8778869, 35871
Lawson Number (LN):	24256, 14919
File Segment (FS):	Stereo compoun
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7455846
Tautomer ID (TAUTID):	8269668
Data Entry Date (DED):	2001/07/25
Update Date (DUPD):	2001/07/25

Data Entry Date
•Date when the compound was first entered into the database

Data Update Date
•Date when the last update of the compound was entered into the database by the database producer

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Multi-fragment Compounds

```
Beilstein Records (BRN):        8808326
Chemical Name (CN):             (R)-4-(1,1-dimethylethyl)-1-(1-hydroxy-3-
                                phenylpropan-2-yl)pyridinium chloride
Autonom Name (AUN):             4-tert-butyl-1-(1-hydroxymethyl-2-phenyl-
                                ethyl)-pyridinium; chloride
Lin. Struct. Formula (LSF):     C18H24NO(1+)*Cl(1-)
Fragm. Molec. Formula (FMF):    C18 H24 N O , Cl
Molecular Formula (MF):         C18 H24 N O . Cl
Molecular Weight (MW):          270.39, 35.45
Fragment BRN (FBRN):            8778869, 3587171
Lawson Number (LN):             24256, 14919
File Segment (FS):              Stereo compound
Compound Type (CTYPE):          heterocyclic
Constitution ID (CONSID):       7455846
Tautomer ID (TAUTID):           8269668
Entry Date (DED):               2001/07/25
Update Date (DUPD):             2001/07/25
```

FMF, MW and FBRN given for each fragment

New types: mixtures and polymers

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

No structure diagram available for this BRN
```

COMPN and COMPBRN given for each component

Structure searching in BEILSTEIN

- Structure searching is *free-of-charge*
- Standard STN structure search options
  - Exact (EXA), Family (FAM)
  - Substructure (SSS), Closed Substructure (CSS)
  - Full file (FULL), Sample (SAM)
- STN Express / STN on the Web
- Subset searching available

STN

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STN®

Find reactions

Reaction Identification data and
Reaction Details

Which reactions are indexed?

- Preparation
  - Chemical or biochemical methods suitable for large-scale preparations, new and preparative useful methods
  - General methods which are applicable for the preparation of several compounds
- Chemical Behavior
  - Quantitative results pertaining to the course of the reaction available
  - Publication is focused on the investigation of the chemical behavior

Reaction file segment

- Each reaction is a separate record
- All reaction data concentrated in the field RX
- Reaction data possess a new, more user-friendly structure and are enhanced by additional data
- No concatenation of substance data and reaction data in a search query possible
- Convenient method available to show reaction data for a compound from the substance file segment

Reaction sample record

```
Reaction:
RX
     Reaction ID:                  8619548
     Reactant BRN:                 203413, 3588525
     Reactant:                     2-phenothiazin-10-yl-ethanol, 2-cyanoethyl
                                   diisopropylchlorophosphoramidite
     Product BRN:                  8645640
     Product:                      diisopropyl-phosphoramidous acid
                                   2-cyano-ethyl ester 2-phenothiazin-10-yl-
                                   ethyl ester
     No. of Reaction Details:      2
```

Reaction Identification Data

- Reactions are defined by reactants and products
- Reactant and Product name given
- Reactant and Product BRN given
- Number of Reaction Details gives the total number of reaction variations

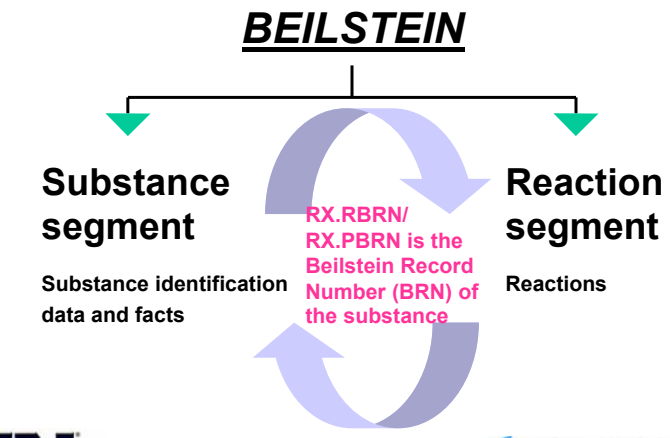
Reaction sample record

```
Reaction Details:
RX
     Reaction RID:                 8619548.1
     Reaction Classification:      Preparation
     Yield:                        95 percent (BRN=8645640)
     Reagent:                      diisopropylethylamine
     Solvent:                      CH2Cl2
     Temperature:                  25 Cel
     Reaction Type:                Substitution
     Reference(s):
     1. Tierney, Mark T.; Grinstaff, Mark W., J.Org.Chem., CODEN: JOCEAH,
        65(17), <2000>, 5355 - 5359; BABS-6262693
RX
     Reaction RID:                 8619548.2
     Reaction Classification:      Preparation
     Yield:                        89 percent (BRN=8645640)
     Reagent:                      DIPEA
     Solvent:                      acetonitrile
     Reaction Type:                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-6255887
```

Reaction Detail 1

Reaction Detail 2

BEILSTEIN file segments



STN

FIZ KARLSRUHE

BRN link between file segments

Substance File Segment

```
Beilstein Records (BRN):      1209327
Beilstein Pref. RN (BPR):     108-05-4
CAS Reg. No. (RN):            108-05-4
Chemical Name (CN):           acetoxyethene, acetic acid vinyl ester,
                              Essigsaeure-vinylester, acetic acid ethenyl
                              ester, vinyl acetate
Autonom Name (AUN):           acetic acid vinyl ester
Molec. Formula (MF):          C4 H6 O2 ...
```

BRN

Reaction File Segment

```
Reaction:
RX
     Reaction ID:             8743437
     Reactant BRN:            1209327
     Reactant:                acetoxyethene
     Product BRN:             506007
     Product:                 acetic acid
     No. of Reaction Details: 4 ...
```

RX.RBRN

BRN link between file segments

Substance File Segment

```
Beilstein Records (BRN):      1209327
Beilstein Pref. RN (BPR):     108-05-4
CAS Reg. No. (RN):            108-05-4
Chemical Name (CN):           acetoxyethene, acetic acid vinyl ester,
                              Essigsaeure-vinylester, acetic acid ethenyl
                              ester, vinyl acetate
Autonom Name (AUN):           acetic acid vinyl ester
Molec. Formula (MF):          C4 H6 O2 ...
```

BRN

Reaction File Segment

```
Reaction:
RX
     Reaction ID:             5801739
     Reactant BRN:            506007, 906677
     Reactant:                acetic acid, zinc acetate alumini   e,
                              ethyne
     Product BRN:             1209327
     Product:                 acetoxyethene ...
```

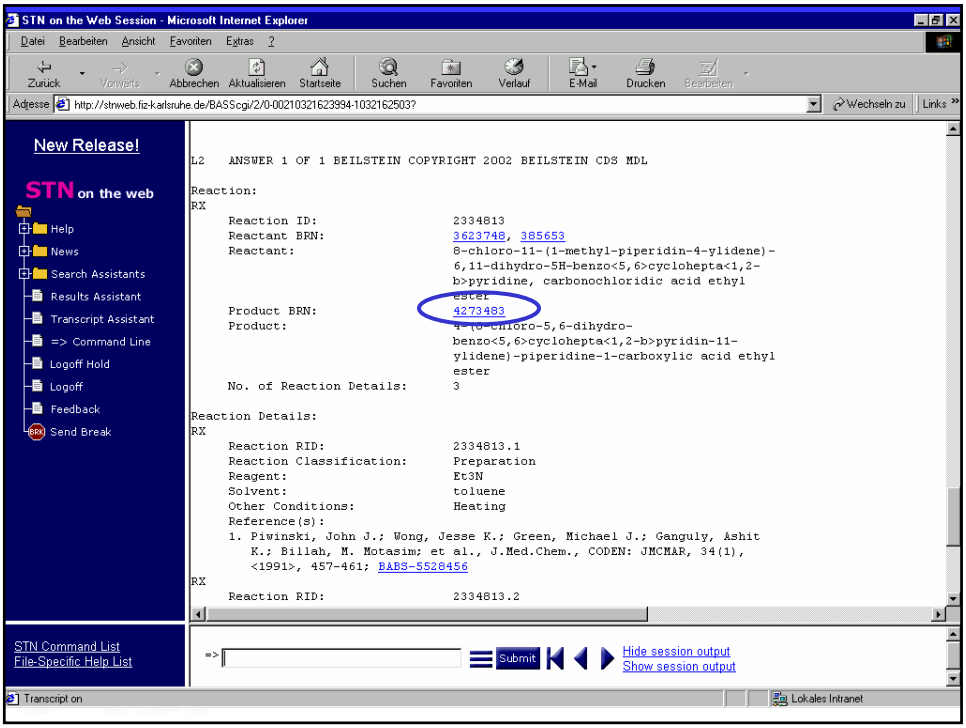
RX.PBRN

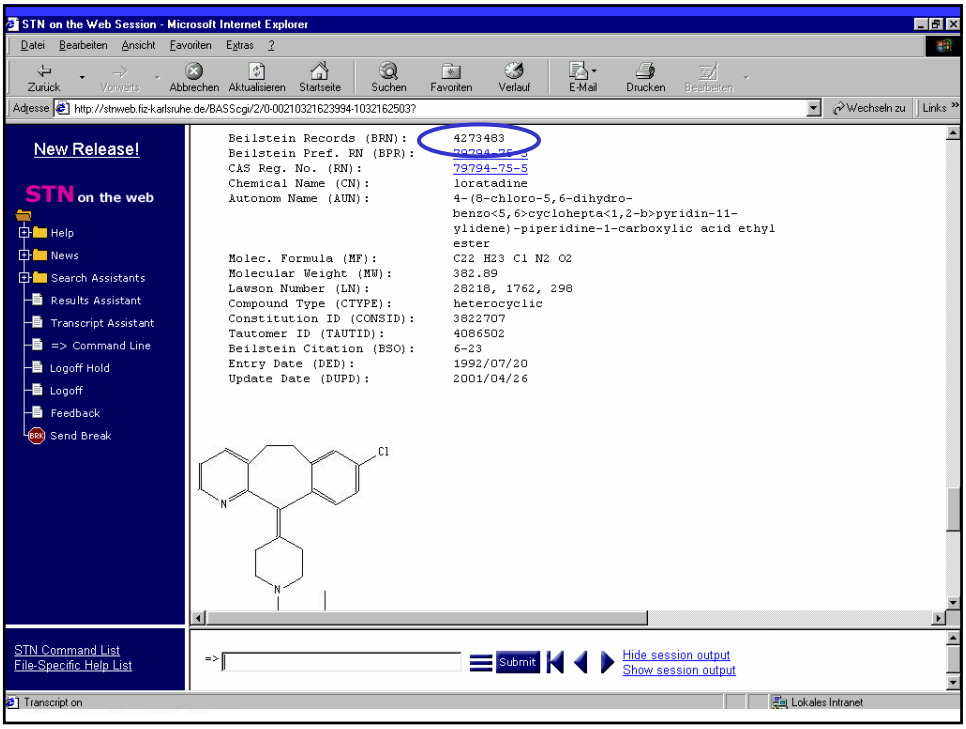
STN on the Web BRN links

- Click on the Product BRN or Reactant BRN for the IDE display of the substance record

STN

FIZ KARLSRUHE


STN on the Web Session - Microsoft Internet Explorer
Datei Bearbeiten Ansicht Favoriten Extras ?
Zurück Vorwärts Abbrechen Aktualisieren Startseite Suchen Favoriten Verlauf E-Mail Drucken Bearbeiten
Adresse http://stnweb.fiz-karlsruhe.de/BASScgi/2/0-00210321623994-1032162503?
Wechseln zu Links
New Release!
STN on the web
Help
News
Search Assistants
Results Assistant
Transcript Assistant
=> Command Line
Logoff Hold
Logoff
Feedback
Send Break
L2 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL
Reaction:
RX
Reaction ID: 2334813
Reactant BRN: 3623748, 385653
Reactant: 8-chloro-11-(1-methyl-piperidin-4-ylidene)-6,11-dihydro-5H-benzo<5,6>cyclohepta<1,2-b>pyridine, carbonochloridic acid ethyl ester
Product BRN: 4273483
Product: 4-(8-chloro-5,6-dihydro-benzo<5,6>cyclohepta<1,2-b>pyridin-11-ylidene)-piperidine-1-carboxylic acid ethyl ester
No. of Reaction Details: 3
Reaction Details:
RX
Reaction RID: 2334813.1
Reaction Classification: Preparation
Reagent: Et3N
Solvent: toluene
Other Conditions: Heating
Reference(s):
1. Piwinski, John J.; Wong, Jesse K.; Green, Michael J.; Ganguly, Ashit K.; Billah, M. Motasim; et al., J.Med.Chem., CODEN: JMCMAR, 34(1), <1991>, 457-461; BABS-5528456
RX
Reaction RID: 2334813.2
STN Command List
File-Specific Help List
=>
Submit
Hide session output
Show session output
Transcript on
Lokales Intranet


STN on the Web Session - Microsoft Internet Explorer
Datei Bearbeiten Ansicht Favoriten Extras ?
Zurück Vorwärts Abbrechen Aktualisieren Startseite Suchen Favoriten Verlauf E-Mail Drucken Bearbeiten
Adresse http://stnweb.fiz-karlsruhe.de/BASScgi/2/0-00210321623994-1032162503?
Wechseln zu Links
New Release!
STN on the web
Help
News
Search Assistants
Results Assistant
Transcript Assistant
=> Command Line
Logoff Hold
Logoff
Feedback
Send Break
Beilstein Records (BRN): 4273483
Beilstein Pref. RN (BPR): 79794-75-5
CAS Reg. No. (RN): 79794-75-5
Chemical Name (CN): loratadine
Autonom Name (AUN): 4-(8-chloro-5,6-dihydro-benzo<5,6>cyclohepta<1,2-b>pyridin-11-ylidene)-piperidine-1-carboxylic acid ethyl ester
Molec. Formula (MF): C22 H23 Cl N2 O2
Molecular Weight (MW): 382.89
Lawson Number (LN): 28218, 1762, 298
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 3822707
Tautomer ID (TAUTID): 4086502
Beilstein Citation (BSO): 6-23
Entry Date (DED): 1992/07/20
Update Date (DUPD): 2001/04/26
Cl
N
N
STN Command List
File-Specific Help List
=>
Submit
Hide session output
Show session output
Transcript on
Lokales Intranet

Reaction display from the *substance* file segment

Display codes

First 20 reaction references or prefix "F" for full list

- RX / **F**RX
  - All reactions of a compound
- RX**PRO** / **F**RXPRO (*or* PRE / **F**PRE)
  - Reactions in which the compound is a *product*
- RX**REA** / **F**RXREA (or REA / **F**REA)
  - Reactions in which the compound is a *reactant*

Searching for substances with reaction references

- S RXREA/FA for substances which are *reactants* in reaction records
- S RXPRO/FA for substances which are *products* in reaction records
- S RX/FA for substances which are *reactants* and/or *products* in reaction records

Example: display RX for a substance

```
=> S 4481-62-3/RN
L1            1 4481-62-3/RN

=> D

L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

     Beilstein Records (BRN):        3087311
     Beilstein Pref. RN (BPR):       4481-62-3
     CAS Reg. No. (RN):              4481-62-3
     Chemical Name (CN):             betulonic acid
     Autonom Name (AUN):             1-isopropenyl-5a,5b,8,8,11a-pentamethyl-9-
                                     oxo-eicosahydro-cyclopenta<a>chrysene-3a-
                                     carboxylic acid
     Molec. Formula (MF):            C30 H46 O3
     Molecular Weight (MW):          454.69
     Lawson Number (LN):             12950
     ...
```

Search in Substance File Segment

Display QRD

Example: display RX for a substance

```
Field Availability:

   Code      Name                                        Occurrence
   ========================================================
   BRN       Beilstein Records                                1
   BPR       Beilstein Preferred RN                           1
   RN        CAS Registry Number                              1
   CN        Chemical Name                                    1
   AUN       Autonomname                                      1
   MF        Molecular Formula                                1
   .
   .
   .

 This substance also occurs in Reaction Documents:

   Code      Name                                        Occurrence
   ========================================================
   RX        Reaction Documents                              21
   RXREA     Substance is Reaction Reactant                  15
   RXPRO     Substance is Reaction Product                    6
```

FA table

Indication of reactions

Example: display RX for a substance

```
=> D FRX

L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN

Reaction:
RX
     Reaction ID (.ID):              7912186
     Reactant BRN (.RBRN):           103233, 2570928
     Reactant (.RCT):                KMnO4, pyridine,
                                     (28)
     Product BRN (.PBRN):            3087311
     Product (.PRO):                 betulonic acid
     No. of React. Details (.NVAR):  1
     :
     :
Reaction:
RX
     Reaction ID (.ID):              8925047
     Reactant BRN (.RBRN):           3087311, 906769
     Reactant (.RCT):                betulonic acid, formic acid ethyl ester
     Product BRN (.PBRN):            8959459
     Product (.PRO):                 2-hydroxymethylenebetulonic acid

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

*Display all reactions with FRX, **or...***

*Compound is product with FRX**PRO***

*Compound is reactant with FRX**REA***

Example: display RX for a substance

```
=> D COS FULL

FILE & COST CENTER                 QUANTITY @    RATE      ESTIMATED COST
                                                                 DOLLARS

HOME FILE           COST=
  CONNECT HOURS                      0.01 @   25,00
  INTERNET                           0.01 @    5,00
BEILSTEIN FILE      COST=
  SFE SESSION CONNECT HOURS          0.04 @    0,00
  INTERNET                           0.04 @    5,00                0,20
  IDENTIFICATION OF SUBSTANCE        1    @    8,37                8,37
  REACTION DATA                      1    @    8,37                8,37
...


BEILSTEIN FILE      COST=
  SFE SESSION CONNECT HOURS          0.02 @    0.00
  INTERNET                           0.02 @    5.00                0.10
  REACTION DATA                     21    @    8.37              175.77
...
```

Display costs

Display RX records from substance segment for one charge

Displaying each RX individually is much more expensive!!

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

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 BRN	/RX.SRBRN
Stage Reactant	/RX.SRCT
Number of Stages	/RX.SNR

Reactions: Helpful search fields

- The Reaction Supersearchfield (/RX)
- The Reaction Basic Index (/BIRX)

The Supersearchfield RX

```
=> S CHCL3/RX
            53 CHCL3/RX.RCT
          7145 CHCL3/RX.RGT
            90 CHCL3/RX.PRO
             0 CHCL3/RX.SUBJ
         96093 CHCL3/RX.SOL
             3 CHCL3/RX.CAT
             0 CHCL3/RX.TYP
             0 CHCL3/RX.PRT
             0 CHCL3/RX.SRCT
L1      103237 CHCL3/RX

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

Content of RX

The Basic Index for Reactions

- **BIRX** contains **single terms** from the following fields
- All fields containing chemical names (Products, Reactants, Catalysts, Solvents)
- BRNs of Reactants and Products
- Text fields (Subject Studied, Type, Other Conditions, Classification and Note)

```
=> S KNOEVENAGEL/BIRX
L1          1022 KNOEVENAGEL/BIRX
```


Search strategy: reactants

```
=> S ACETYLCYSTEINE/CN
L1            1 ACETYLCYSTEINE/CN

=> SELECT L1 1- BRN
E1 THROUGH E1 ASSIGNED

=> S E1/RX.RBRN
L2          296 1724426/RX.RBRN
=> D

L2   ANSWER 1 OF 296 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction:
RX
     Reaction ID (.ID):              8871529
     Reactant BRN (.RBRN):           8952862, 1724426
     Reactant (.RCT):                clofibryl-S-acyl-glutathione,
                                     N-acetyl-L-cysteine
     ...
```

Search for a substance

Select BRN and search the E-number in /RX.RBRN

Search strategy: preparations

```
=> S ACETYLCYSTEINE/CN
L1            1 ACETYLCYSTEINE/CN

=> SELECT L1 1- BRN
E1 THROUGH E1 ASSIGNED

=> S E1/RX.PBRN
L2            7 1724426/RX.PBRN

=> S L2 AND (PREPARATION OR MULTISTAGE)/RX.CL
       7722342 PREPARATION/RX.CL
         56513 MULTISTAGE/RX.CL
L3            5 L2 AND (PREPARATION OR MULTISTAGE)/RX.CL
```

Search for a substance

Select BRN and search the E-number in /RX.PBRN

Refine the results to studies focused on preparation

Refining with reaction details

```
=> S ANILINE/CN
L1            2 ANILINE/CN

=> SELECT L1 1- BRN
E1 THROUGH E2 ASSIGNED

=> S E1-E2/RX.PBRN
          2800 605631/RX.PBRN
             0 6121979/RX.PBRN
L2        2800 (605631/RX.PBRN OR 6121979/RX.PBRN)

=> S L2 AND RX.YD>90 (P) (PREPARATION OR MULTISTAGE)/RX.CL
        366396 RX.YD>90 %
       7722342 PREPARATION/RX.CL
         56513 MULTISTAGE/RX.CL
        363779 RX.YD>90 % (P) (PREPARATION OR MULTISTAGE)/RX.CL
L3          26 L2 AND RX.YD>90 % (P) (PREPARATION OR MULTISTAGE)/RX.CL
```

Search for reaction detail data

Use the (P) operator to restrict terms to one reaction detail

Multi-step reactions

- Structures of intermediates are not known
  - Reaction Classification “Multistage” assigned
  - All starting materials for all steps entered together in the Reactant field
  - Reaction conditions are listed for single steps
- Structures of intermediates are known
  - Multistep synthesis is split into several single step preparations

Multistage Reaction

```
Reaction:
RX
     Reaction ID:                  8700547
     Reactant BRN:                 8685258, 605969
     Reactant:                     3-trifluoromethyl-5,6-dihydro-<1,4>dioxine-2-
                                   carbonyl chloride, 3-chloro-aniline
     Product BRN:                  8704888
     Product:                      3-trifluoromethyl-5,6-dihydro-<1,4>dioxine-2-
                                   carboxylic acid (3-chloro-phenyl)-amide
     No. of Reaction Details:      1
```

Reactants for all stages listed in the Reactant field

Multistage Reaction

```
Reaction Details:
RX
     Reaction RID:                 8700547.1
     Reaction Classification:      Multistage
     Yield:                        100 percent (BRN=8704888)
     Nr. of Stages:                2
     Stage 1
     Reagent:                      polystyrene-bound 4-hydroxy-3-
                                   nitrobenzophenone, pyridine
     Solvent:                      CH2Cl2
     Time:                         24 hour(s)
     Temperature:                  20 Cel
     Reaction Type:                Condensation
     Stage 2
     Reagent:                      Et3N
     Stage reactant:               3-chloro-aniline
     Stage Reactant BRN:           605969
     Solvent:                      acetonitrile
     Time:                         14 hour(s)
     Other Conditions:             Heating
     Reaction Type:                Condensation
     Reference(s):  ...
```

Reaction Detail

Stage 1

Stage 2

Reactions: search example

- Reactions of malonic acid diethyl ester with urea

```
=> S MALONIC ACID DIETHYL ESTER/CN
L1            1 MALONIC ACID DIETHYL ESTER/CN

=> SELECT L1 1- BRN
E1 THROUGH E1 ASSIGNED

=> S E1/RX.RBRN
L2         7329 774687/RX.RBRN

=> S UREA/CN
L3            3 UREA/CN

=> SELECT L3 1- BRN
E2 THROUGH E4 ASSIGNED

=> S E2-4/RX.RBRN
               0 5327343/RX.RBRN
            5798 635724/RX.RBRN
               1 773698/RX.RBRN
L4          5799 (5327343/RX.RBRN OR 635724/RX.RBRN OR 773698/RX.RBRN)
```

Search for both chemical names, select and search the RX.RBRN

Reaction: search example

Search for both RX.RBRN in one reaction

Display reactions

```
=> S L2 AND L4
L5           3 L2 AND L4

=> D RX 1-3

L5   ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction:
RX
     Reaction ID:                  3533123
     Reactant BRN:                 4987685, 774687, 635724
     Reactant:                     adamantan-2-ylidene-acetaldehyde, malonic
                                   acid diethyl ester, urea
     Product BRN:                  5115960
     Product:                      5-(2-adamantan-2-ylidene-ethylidene)-
                                   pyrimidine-2,4,6-trione
     No. of Reaction Details:      1

Reaction Details:                  ...
```


Reactions: search example

```
L5   ANSWER 2 OF 3 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction:
RX
     Reaction ID:                  748385
     Reactant BRN:                 774687, 635724
     Reactant:                     malonic acid diethyl ester, urea
     Product BRN:                  120502
     Product:                      pyrimidine-2,4,6-trione
     No. of Reaction Details:      6

Reaction Details:
RX
     Reaction RID:                 748385.1
     Reaction Classification:      Preparation
     Reagent:                      sodium pentylate
     Note(s):                      Handbook
     Reference(s):
     1. Patent: Wacker,A. DE 593673 1932, Fortschr.Teerfarbenfabr.Verw.Industri
        ezweige, 20, 792 ...
```

Search for references

Bibliographic information

Journal reference searching

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

Super-searchfield AJT

Search bibliography with (S)-operator

```
=> S OLAH?/AU (S) J.ORG.CHEM./JT
         12259 OLAH?/AU
       1439837 J.ORG.CHEM./JT
L1        3817 OLAH?/AU (S) J.ORG.CHEM./JT
=> D HIT

L1   ANSWER 1 OF 3817 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction Details:
RX
     Reaction RID (.RID):            8776654.1
     Reaction Classification (.CL):  Preparation
     Yield (.YDT):                   60 percent (BRN=1934803)
     Reagent (.RGT):                 H2O2
     Solvent (.SOL):                 H2O
     Temperature (.T):               20
     Reference(s):
     1. Simon, Juergen; salzbrunn, Stefan; Prakash, G. K. Surya; Petasis, Nicos
        A.; Olah, George A., J.Org.Chem., CODEN: JOCEAH, 66(2), <2001>, 633 -
        634; BABS-6278639
```

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

Searching bibliography in file segments

Substance file segment

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

Reaction file segment

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

File segment specific search

```
=> S SHARPLESS?/AU
L1          3522 SHARPLESS?/AU

=> S SHARPLESS?/AU.SUB
            3522 SHARPLESS?/AU
         8374887 ALL/FA
L2          1150 SHARPLESS?/AU.SUB
                 (SHARPLESS?/AU AND ALL/FA)
=> D HIT

L2   ANSWER 1 OF 1150 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Melting Point:
 Value      |Ref.
 (MP)       |
 (Cel)      |
===========+====
 182 - 183 | 1

Reference(s):
 1. Converse, Antonella; Burow, Kristina; Marzinzik, Andreas; Sharpless, K.
    Barry; Finn, M. G., J.Org.Chem., CODEN: JOCEAH, 66(12), <2001>, 4386 -
    4392; BABS-6290981
```

Search for author in both file segments

Search for author in substance file segment

Hit: Reference in substance data

File segment specific search

```
=> S SHARPLESS?/AU.RX
            3522 SHARPLESS?/AU
         8374887 ALL/FA
L3          2372 SHARPLESS?/AU.RX
                 (SHARPLESS?/AU NOT ALL/FA)

=> D HIT

L3   ANSWER 1 OF 2372 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction Details:
RX
     Reaction RID (.RID):              8859825.1
     Reaction Classification (.CL):    Preparation
     Yield (.YDT):                     75 percent (BRN=8850588)
     Reagent (.RGT):                   K2CO3
     Solvent (.SOL):                   acetonitrile
     Time (.TIM):                      16 hour(s)
     Temperature (.T):                 20
     Reference(s):
     1. Converse, Antonella; Burow, Kristina; Marzinzik, Andreas; Sharpless, K.
        Barry; Finn, M. G., J.Org.Chem., CODEN: JOCEAH, 66(12), <2001>, 4386 -
        4392; BABS-6290981
```

Search for author in reaction file segment

Hit: Reference in reaction data

Patents in BEILSTEIN

- Earliest patent 1869 and most recent 1981
- Primarily from literature period 1925-1980
- Some unique patent data ~ 1930-1960
- Mainly US and DE patents

Patent reference searching

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

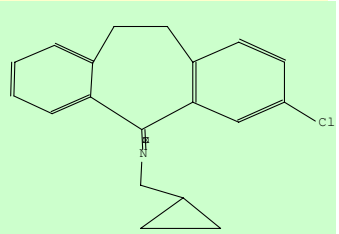
Example: DuPont patents

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

=> D QRD
L1   ANSWER 1 OF 36 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CRN MDL ON STN

     Beilstein Records (BRN):        2874357
     Beilstein Pref. RN (BPR):       59864-49-2
     CAS Reg. No. (RN):              59864-49-2
     Chemical Name (CN):             3-Chloro-N-cyclopropylmethyl-10,11-
                                     dihydro-5H-dibenzocyclohepten-5-imine
     Autonom Name (AUN):             . . .
     Molec. Formula (MF):            C19 H18 Cl N
     Molecular Weight (MW):          295.81
     Lawson Number (LN):             14006, 7475
     File Segment (FS):              Stereo compound
     Compound Type (CTYPE):          isocyclic
     Constitution ID (CONSID):       2613369
     Tautomer ID (TAUTID):           2775007
     Beilstein Citation (BSO):       5-12
     Entry Date (DED):               1989/07/11
     Update Date (DUPD):             1989/07/26
```

DuPont patents with Boiling Point references for cyclopropyl containing compounds



Example: DuPont patents

```
Field Availability:

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


Boiling Point:
 Value       | Press.      |Ref.
 (BP)        | (.P)        |
 (Cel)       | (Torr)      |
=============+=============+====
 140 - 150   | 0.2         |1

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

Hit: Patent reference with boiling point data

CAPLUS reference: S 85:46269/DN

New EcoPharm data

Ecological and pharmacological data

EcoPharm Data

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

Typical EcoPharm Queries

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

EcoPharm topics

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

New Journals for EcoPharm

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

STN

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EcoPharm: Related Physical Data

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

STN

FIZ KARLSRUHE

Old versus new structure

Old	New
Toxicity (TOX)	Pharmacological Data (PHARM)
Biological Function (BF)	Pharmacological Data (PHARM)
Ecological Data (ECOL)	Ecological Data (ECO)
Use (USC)	Laboratory Use and Handling (USC)

Pharmacological Data

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

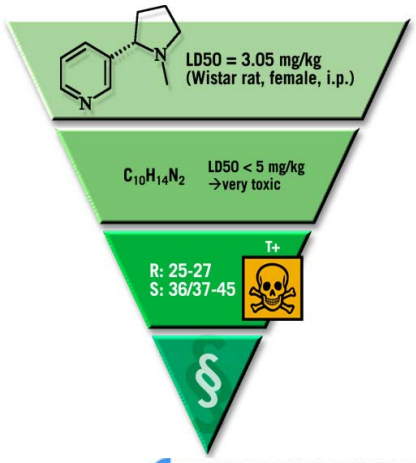
Toxicological Data

1 **Level 1**
Basic Scientific Data

2 **Level 2**
Evaluation and Classification

3 **Level 3**
Regulation

4 **Level 4**
Risk Assessment



STN

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Detailed datastructure for PHARM

Effect	Test System	Test Method
- Acute toxicity - Chronic toxicity. . .	- Escheria coli - Lumbricus terrestris	- in vitro - Amersham kit

Endpoint of Effect	Metabolite	Type of Data/Values
- Mortality - Luminescence	- Chemical name - BRN	- MTD - LD50

STN

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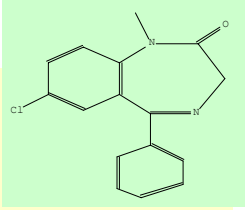
Search Fields: PHARM

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

STN FIZ KARLSRUHE

Pharmacological Data

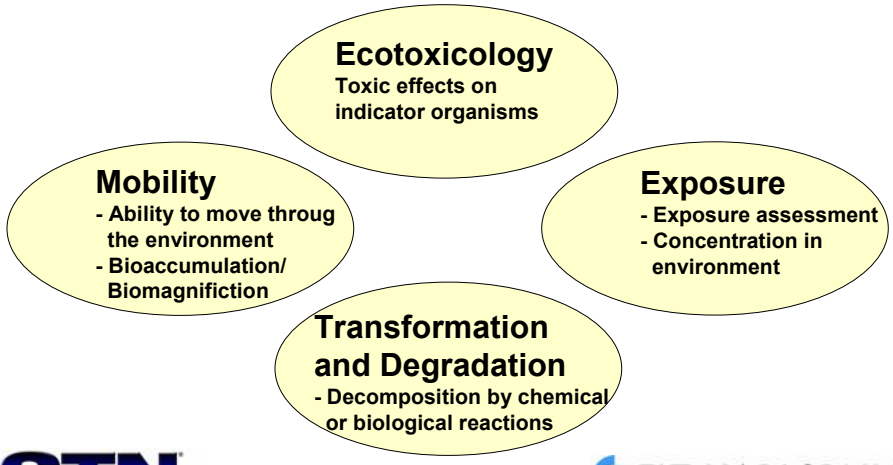


Chemical Name (CN):	..., diazepam
PHARM	
Effect:	biotransformation
Species or Test-System:	human liver microsomes
Concentration:	200 .my.mol/l
Method, Remarks:	in vitro; title comp. as substrate; potassium phosphate buffer, pH 7.4; 37 deg C; NADPH; incub. for 20 min; formation of TMZ and NDZ measured by HPLC
Further Details:	TMZ: temazepam; NDZ: N-desmethyldiazepam
Results:	title comp. was metabolized to TMZ and NDZ with the rate of 9.2 and 2 nmol/min/nmol of P450, respectively
Metabolite BRN:	759300, 751823
Metabolite:	7-chloro-3-hydroxy-1-methyl-5-phenyl-1,3-dihydro-benzo<e><1,4>diazepin-2-one, 7-chloro-5-phenyl-1,3-dihydro-benzo<e><1,4>diazepin-2-one
Reference(s):	...

Ecological Data

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

Ecological data



Ecological data

Subjects

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

Ecological data

Hint:
Use display code ECO to display all available Ecological Data

Subjects (continued)

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

DEGRADATION

Ecological data: ECTOX

```
Chemical Name (CN):                ..., diazepam

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


EcoPharm Basic Index (/BIPED)

- Content: All fields from EcoPharm data

```
=> S ENDOCRINE/BIPED
L7          151 ENDOCRINE/BIPED
=> D HIT
L1   ANSWER 1 OF 151 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL
ECTOX
     Effect:                       endocrine system effects
     Species or Test-System:       Carassius auratus gibelio, Crucian Carp
     Sex:                          male and female
     Exposure Period:              2 week(s)
     Method, Remarks:              200/sex one-year old fish with ca. 12-15 cm
                                   lenght and 150 g body weight; temperature of
                                   water 20 deg C; 12:12 light-dark rhythm; fed
                                   daily with commercial fish pellets; test
                                   solution water changed every other day; fish
                                   ...
```

EcoPharm: search examples

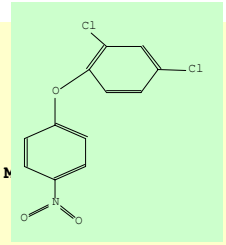
- Find toxicological data for nitrofen

```
 => S NITROFEN/CN
L1            1 NITROFEN/CN

=> D


L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS M

     Beilstein Records (BRN):        1887356
     Beilstein Pref. RN (BPR):       1836-75-5
     CAS Reg. No. (RN):              1836-75-5
     Chemical Name (CN):             (2,4-dichloro-phenyl)-(4-nitro-phenyl)-
                                     ether, nitrofen
     Molec. Formula (MF):            C12 H7 Cl2 N O3
     Molecular Weight (MW):          284.10
     Lawson Number (LN):             5221, 5220
     Compound Type (CTYPE):          isocyclic
     ...
```



EcoPharm: search examples

```
 => D PHARM


L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Pharmacological Data:
PHARM
     Effect (.E):                    mutagenic (microorganism)
     Species or Test-System (.SP):   Escherichia coli, strain WP2s (lambda)
     Concentration (.C):             0.279 - 35.71 mmol/l
     .
     .
     .
PHARM
     Effect (.E):                    cytotoxicity
     Species or Test-System (.SP):   hepatocytes from Wistar rat
     .
     .
     .
Only first 20 entries are displayed. Total number of entries = 23.
     Use "DIS F<prop>" for full format, e.g. FCPD instead of CPD.
```

STN

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EcoPharm: search examples

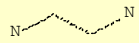
- Find antihistamines which are not ethylenediamine derivatives

```
=> S ANTIHISTAMINIC/PHARM.E
L1          139 ANTIHISTAMINIC/PHARM.E

=>
Uploading C:\STNEXP\QUERIES\ethylendiamin.str

L2       STRUCTURE UPLOADED

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




```
Structure attributes must be viewed using STN Express query preparation.
```

Search for the pharmacological effect

Build and upload ethylenediamine structure

EcoPharm: search examples

```
=> S L2 SSS SUBSET
ENTER SUBSET L# OR (END):L1
ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):FULL
FULL SUBSET SEARCH INITIATED 13:13:46 FILE 'BEILSTEIN'
FULL SUBSET SCREEN SEARCH COMPLETED -     49 TO ITERATE

100.0% PROCESSED      49 ITERATIONS                          49 ANSWERS
SEARCH TIME: 00.00.01

L3           49 SEA SUB=L2 SSS FUL L1

=> S L1 NOT L3
L4           90 L1 NOT L3
```

Conduct structure search in subset

Exclude all records retrieved by substructure search

STN

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EcoPharm: search examples

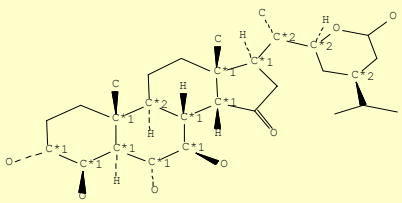
```
=> D HIT, STR
```

Display hit and structure

```
L4   ANSWER 1 OF 90 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Pharmacological Data:
PHARM
     Effect:                        antihistaminic
     Species or Test-System:        rat peritoneal mast cell
     Method, Remarks:               inhibitory activity against histamine
                                    release
     Type:                          IC50
     Value of Type:                 800 nmol/l
     Reference(s):
     1. Jung, Michael E.; Johnson, Ted W., Tetrahedron
        , CODEN: TETRAB, 57(8), <2001>, 1449 - 1482; BABS-6279539
```


EcoPharm: search examples



```
Atom/Bond Notes:
     1. CIP Descriptor: R
     2. CIP Descriptor: S
```

Laboratory Use and Handling

Focus on

- Application or handling of the substance
- Use of the substance in preparative chemistry and laboratory

Example: laboratory use and handling

```
Use of Compound:
USC
     Use Pattern (.PT):              flame retardant
     Reference(s):
     1. Sjoedin, Andreas; Carlsson, Hakan; Thuresson, Kaj; Sjoelin, Sverker;
        Bergman, Ake; Oestman, Conny, Environ.Sci.Technol., CODEN: ESTHAG,
        35(3), <2001>, 448 - 454; BABS-6284379
```

```
Use of Compound:
USC
     Laboratory Use and Handling (.LH): phase-transfer catalyst for
                                        enantioselective C-alkylation
     Reference(s):
     1. Casas, Jesus; Najera, Carmen; Sansano, Jose M.; Gonzalez, Jose; Saa,
        Jose M.; Vega, Manuel, Tetrahedron: Asymmetry, CODEN: TASYE3, 12(5),
        <2001>, 699 - 702; BABS-6277639
```

Physical properties

Keywords and numeric searching

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 UV/VIS 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

Example: mass spectrum

```
Mass Spectrum:
MS
     Description (.KW):              chemical ionization (CI), spectrum
     Reference(s):
     1. Lorenz, Volker; Spoida, Marlies; Fischer, Axel; Edelmann, Frank T.,
        J.Organomet.Chem., CODEN: JORCAI, 625(1), <2001>, 1 - 6; BABS-6301532
```

Example: melting point

```
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  | 1
```

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

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

Comparative Operators

Examples: numeric searching

- Value
  => S 100/BP
  (=> S 100=BP)

```
Boiling Point:
 Value       | Press.      |Ref.
 (BP)        | (.P)        |
 (Cel)       | (Torr)      |
=============+=============+====

 100         | 1           | 1
```

- Range
  => S BP>100

```
Boiling Point:
 Value       | Press.      |Ref.
 (BP)        | (.P)        |
 (Cel)       | (Torr)      |
=============+=============+====

 126         | 0.2         | 1
```

  => S 100-110/BP

```
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
```

```
=> D HIT

L2   ANSWER 1 OF 856 BEILSTEIN ...
Melting Point:
 Value    |Ref.
 (MP)     |
 (Cel)    |
==========+====
 0        | 1
```

- 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 BEILSTEIN ...
Melting Point:
 Value    |Ref.
 (MP)     |
 (Cel)    |
==========+====
 0        | 1
```

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STN Units System

- General Information on the STN Units system
  www.cas.org/ONLINE/STN/units.html
- HELP UNIT for units in BEILSTEIN
  - 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 BEILSTEIN property
  - D UNIT ALL to see the complete list
- SET UNIT to change units in BEILSTEIN
  - HELP SET UNIT for instructions

Proximity searching

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

Example

- Find a substance with a sublimation point of 100 Cel measured at 0.1 Torr.

Example: proximity searching

```
=> S 100/SP (P) 0.1/SP.P
           722 100 CEL /SP
           771 0.1 TORR /SP.P
L1          70 100 CEL /SP (P) 0.1 TORR /SP.P

=> S 100/SP AND 0.1/SP.P
           722 100 CEL /SP
           771 0.1 TORR /SP.P
L2          72 100 CEL /SP AND 0.1 TORR /SP.P

=> S L2 NOT L1
L3           2 L2 NOT L1

=> D HIT

L3   ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Sublimation Point:
 Value       | Press.      |Ref.
 (SP)        | (.P)        |
 (Cel)       | (Torr)      |
=============+=============+====
 100         | 2.000001    | 1

 60          | 0.1         | 2
```

The (P)-operator must be used!

Property keywords

- Present for numerous physical properties, e.g. MEC.KW, ENEM.KW
- All Keywords (/AKW) contains keywords from all individual xxx.KW fields (as a bound phrase)

```
=> 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
```

Example: mechanical property 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 ****
```


Property Hierarchy (/PH)

- All property field names and associated codes indexed as bound phrase
- All keywords indexed as bound phrase
- Browse /PH when for topics you are unsure will be a property field or a keyword term
- Remember that BEILSTEIN is a zero connection hour file

Example: Property Hierarchy

```
=> 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 field codes

Field Availability (/FA)

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

```
=> E NMR/FA

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

=> S MIXTURE?/CTYPE AND NMR/FA
         20072 MIXTURE?/CTYPE
       3104245 NMR/FA
L1          57 MIXTURE?/CTYPE AND NMR/FA
```

Field Not Available (/FNA)

Use of FA

```
=> S ANILINE/CNS AND PHARM/FA
         21614 ANILINE/CNS
         505614 PHARM/FA
L1         429 ANILINE/CNS AND PHARM/FA
```

Use of FNA

```
=> S ANILINE/CNS AND (MP<0 OR MP/FNA)
         21614 ANILINE/CNS
          8510 MP<0 CEL
       8374887 ALL/FA
       3992891 MP/FA
       4381996 MP/FNA
                  (ALL/FA NOT MP/FA)
L1        5737 ANILINE/CNS AND (MP<0 OR MP/FNA)
```


Physical properties

- 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)

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)

Crystal properties

- 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)

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)
- ...

Search examples: physical data

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

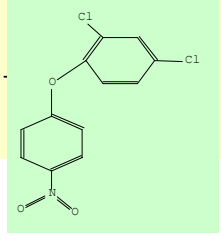
```
=> S NITROFEN/CN
L1            1 NITROFEN/CN

=> D

L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

     Beilstein Records (BRN):        1887356
     Beilstein Pref. RN (BPR):       1836-75-5
     CAS Reg. No. (RN):              1836-75-5
     Chemical Name (CN):             (2,4-dichloro-phenyl)-
                                     ether, nitrofen
     Molec. Formula (MF):            C12 H7 Cl2 N O3
     ...
```

Search for the chemical name and display IDE data



Search examples: physical data

```
Field Availability:

     Code      Name                                        Occurrence
     ========================================================
     BRN       Beilstein Records                                1
     BPR       Beilstein Preferred RN                           1
     RN        CAS Registry Number                              1
     CN        Chemical Name                                    2
     .
     .
     .
     SLB       Solubility (MCS)                                 1
     USC       Use of Compound                                  6
     UVS       UV and Visible Spectrum                          2
     XREF      Crossfile Reference                              3
     .
     .
     .
```


Search examples: physical data

```
=> D UVS

L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS

UV and Visible Spectrum:
 Description       |Solvent | Absorption    |Ref.| Note
                   |        | Maxima        |    |
 (.KW)             |(.SOL)  | (.AM)         |    |
                   |        | (nm)          |    |
==================+========+===============+====+=======
 Absorption maxima |ethanol | 292           | 1  | 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

Notes(s):
1. Handbook
```

Display information on UV and Visible Spectrum

Search examples: physical data

- Find pyrole derivatives with a boiling point lower than or equal to 30 Celsius?

```
=> S BP<=30
L1          5481 BP<=30 CEL

=>
Uploading C:\STNEXP\QUERIES\Pyrol.str

L2       STRUCTURE UPLOADED

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

```
Structure attributes must be viewed using STN Express query preparation.
```

Search for the boiling point range lower than or equal to 30 CEL

Build and upload the structure of pyrol and conduct a substructure search in subset L1

Search examples: physical data

```
=> S L2 SSS SUBSET
ENTER SUBSET L# OR (END):L1
ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):FULL
FULL SUBSET SEARCH INITIATED 17:53:18 FILE 'BEILSTEIN'
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
```

Search examples: physical data

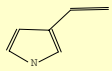
```
=> D IDE BP
```

Display IDE and Boiling Point information

```
L3   ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

     Beilstein Records (BRN):        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
     Tautomer ID (TAUTID):           6267819
     Beilstein Citation (BSO):       6-20
     Entry Date (DED):               1994/07/18
     Update Date (DUPD):             2000/02/29
```


Search examples: physical data



```
...

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
```

Search examples: physical data

Boiling Point data can also be tabulated from multiple records

```
=> D L3 1-3 BPTAB

L3   3 ANSWERS  BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Boiling Point:
 ANS | BRN      | Value          | Press.      |Ref.     | Note
     |          | (BP)           | (.P)        |         |
     |          | (Cel)          | (Torr)      |         |
=====+==========+================+=============+=========+=======
   1 | 6642346 | 30             | 0.006       |1        |
   2 | 4402618 | 30             | 0.5         |2        |
   3 | 1159    | 30             |             |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. Muir et al., J.Chem.Soc.Perkin Trans.2, CODEN: JCPKBH, <1975>,
    1316,1317,1318
```


Search examples: physical data

- What is the density of vitamin-c crystals?

Search for the chemical name and display IDE data

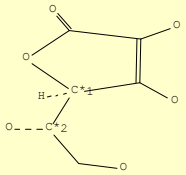
```
=> S VITAMIN-C/CN
L1            1 VITAMIN-C/CN

=> D

L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

     Beilstein Records (BRN):        84272
     Beilstein Pref. RN (BPR):       50-81-7
     CAS Reg. No. (RN):              50-81-7, 89-65-6, 5776-48-7, 10504-35-5,
                                     26094-91-7, 34562-78-2, 62624-30-0,
                                     76094-61-6
     Chemical Name (CN):             (R)-5-((S)-1,2-dihydroxy-ethyl)-3,4-
                                     dihydroxy-5H-furan-2-one, L-ascorbic acid,
                                     L-Ascorbinsaeure, L(+)ascorbic acid,
                                     ascorbic acid, vitamin-C,
                                     ...
```

Search examples: physical data



```
Atom/Bond Notes:
       1. CIP Descriptor: R
       2. CIP Descriptor: S

  Field Availability:

    Code     Name                                      Occurrence
    ========================================================
    BRN       Beilstein Records                              1
    BPR       Beilstein Preferred RN                         1
...
```


Search examples: physical data

```
    BIO       Biological Behaviour                           1
    CDEN      Density (Crystal)                              4
    CDER      Chemical Derivative                           35
    CDIC      Circular Dichroism                             2
    CNF       Conformation                                   2
    COEV      Concentration in Environment                   1
    CRYPH     Crystal Phase                                  4
    CSG       Crystal Space Group                            2
    CSYS      Crystal System                                 1
    DE        Dissociation Exponent                         31
    DEN       Density (Liquid)                               1
    DM        Dipole Moment                                  3
    ...
    MP        Melting Point                                 13
    MS        Mass Spectrum                                  3
    MSUS      Magnetic Susceptibility                        1
    NMR       Nuclear Magnetic Resonance                    31
    OPT       Optics                                         4
    ORD       Optical Rotatory Dispersion                    8
...
```

Crystal data

Search examples: physical data

```
=> D CDEN
L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILS
Crystal Density:
 Value       |Ref.| Note
 (CDEN)      |    |
 (g/cm**3)   |    |
=============+====+=======
             | 1  |
 1.714       | 2  | 1, 2
 1.74        | 3  | 2
 1.696       | 4  | 2
Reference(s):
 1. Hvoslef, Acta Crystallogr.Sect.B, CODEN: ACBCAR, 24, <1968>,
    23,24,29-31,33,34
 2. Beck, 46, <1943>, 18, 21
 3. Cox; Goodwin, J.Chem.Soc., CODEN: JCSOA9, <1936>, 769, 774
 4. Armour Research Foundation, Anal.Chem., CODEN: ANCHAM, 20, <1948>, 986
Notes(s):
1. bei 8grad.
2. Handbook
```

Display Crystal Density data

Hint:
Use "D CRY" to display all available crystal data for ONE display fee

Chemical data

Derivatives, natural sources and purification of substances

Chemical data

- Chemical Derivative

  Derivative name, BRN and comment may be given. Derivatives for characterization are recorded as individual compounds.

- Isolation from Natural Product

  Names of natural sources from which compound has been isolated in scientific nomenclature.

- Purification

  Description of purification method.

- Related Structure

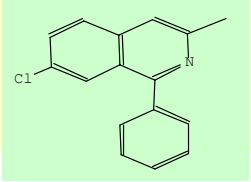
  Indicates differences in structure (constituion, configuration) given in former literature references. Contains new BRN assigned to compound.

Search example: chemical data

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

IDE data of 7-chloro-3-methyl-1-phenyl-isochinoline

Beilstein Records (BRN):	1345900
Beilstein Pref. RN (BPR):	21158-93-0
CAS Reg. No. (RN):	21158-93-0
Chemical Name (CN):	7-chloro-3-methyl-1-phenyl-isoquinoline
Autonom Name (AUN):	7-chloro-3-methyl-1-phenyl-isoquinoline
Molec. Formula (MF):	C16 H12 Cl N
Molecular Weight (MW):	253.73
Lawson Number (LN):	24514
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	1251297
Tautomer ID (TAUTID):	1302015
Beilstein Citation (BSO):	5-20-08-00385, 6-20
Entry Date (DED):	1988/11/29
Update Date (DUPD):	1996/01/03



Search example: chemical data

```
Field Availability:

     Code      Name                                        Occurrence
     ========================================================
     BRN       Beilstein Records                                  1
     BPR       Beilstein Preferred RN                             1
     RN        CAS Registry Number                                1
     CN        Chemical Name                                      1
     AUN       Autonomname                                        1
     MF        Molecular Formula                                  1
     FW        Formular Weight                                    1
     LN        Lawson Number                                      1
     CTYPE     Compound Type                                      1
     CONSID    Constitution ID                                    1
     TAUTID    Tautomer ID                                        1
     BSO       Beilstein Citation                                 2
     ED        Entry Date                                         1
     UPD       Update Date                                        1
     CDER      Chemical Derivative                                2
     ...
```


Search example: chemical data

```
=> D CDER

Chemical Derivative:
CDER
     (CDER):                          C16H12ClN*C6H3N3O7
     Derivative BRN (.BRN):           6468957
     Reference(s):
     1. Zielinski, Wojciech, Pol.J.Chem., CODEN: PJCHDQ, 54(11/12), <1980>,
        2209-2215; BABS-5804357
CDER
     Note(s) (.COM):                  Pikrat C16H12ClN*C6H3N3O7: F: 193-194grad
                                      (aus A.)
     Reference(s):
     1. Bhattacharya, Indian J.Chem., CODEN: IJOCAP, 6, <1968>, 341,343
```

Search example: chemical data

Search for the BRN of the derivative (picrate)

```
=> S 6468957/BRN
L2            1 6468957/BRN

=> D

L2   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

     Beilstein Records (BRN):          6468957
     Fragm. Molec. Formula (FMF):      C16 H12 Cl N , C6 H3 N3 O7
     Molecular Formula (MF):           C16 H12 Cl N . C6 H3 N3 O7
     Molecular Weight (MW):            253.73, 229.11
     Fragment BRN (FBRN):              1345900, 423400
     Lawson Number (LN):               24514, 5222
     Compound Type (CTYPE):            heterocyclic
     Constitution ID (CONSID):         5627885
     Tautomer ID (TAUTID):             6160544
     ...
```


Search example: chemical data

```
Field Availability:

     Code      Name                                      Occurrence
     ========================================================
     BRN       Beilstein Records                                1
     FMF       Fragment Molecular Formula                       2
     MF        Molecular Formula                                1
     FW        Formular Weight                                  2
     CBRN      Fragment BRN                                     2
     LN        Lawson Number                                    2
     CTYPE     Compound Type                                    1
     CONSID    Constitution ID                                  1
     TAUTID    Tautomer ID                                      1
     BSO       Beilstein Citation                               1
     ED        Entry Date                                       1
     UPD       Update Date                                      1
     MP        Melting Point                                    1
```

Search example: chemical data

```
=> D MP

L2   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Melting Point:
 Value      |Ref.
 (MP)       |
 (Cel)      |
============+====
 190 - 191  | 1

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

Characterization of derivative

STN

FIZ KARLSRUHE

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BEILSTEIN on STN

Tips for managing display costs

Tips for managing display costs

- BEISLTEIN pricing model
  - No connection hour charges
  - No search term charges
  - No structure search charges
  - No SELECT charges
  - Per *field* display charge (currently $8.37)
  - No *free-of-charge* display formats

Basic tips for managing display costs

- Always think twice about the ALL format
- IDE already includes the FA table
- HIT does not necessarily give a full field display
- QRD (default) is IDE + HIT
- F<field> for more than 20 references
- Display RX from substance segment
- Use *super display fields* for a single charge

Basic tips for managing display costs

Super display fields

IDE	Identification of substance	OPTP	Optical
CRY	Crystals	SEP	Structure and energy
ECB	Electrochemical behavior	SF	Safety
ECO	Ecological	SOL	Solution behavior
ELEP	Electrical	THE	Thermodynamic
GAS	Gases	TRA	Transport phenomena
LIQ	Liquids	CHE	Chemical
MAGP	Magnetic	LVS	Liquid/Vapor system
MECP	Physical and mechanical		

STN

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Appendix – New Topics

New topics

- Conformation (CNF) in ***Structure and Energy Parameter***
- Luminescence (LUM) in ***Spectral Data***
- Electrical Data (ELE) and Magnetic Data (MAG) in ***Electrical and Magnetic Properties***
- Henry Constant (HNC), Partition Constant Octan-1-ol/Water (POW), Complex Phase Equilibria (CPEM), Electrical Data (EDM), Optical Data (ODM) in ***Multi-Component Systems***

Conformation (CNF)

- " Conformations are defined as spatial arrangements of the atoms in a molecule, which can be interconverted by rotation about a single bond."
- "You find associated information about thermochemical data in the field Object of Investigation (/CNF. OBJ)."

```
=> E A/CNF.OBJ
**** START OF FIELD ****
E3           0 --> A/CNF.OBJ
E4       63062     CONFORMATION/CNF.OBJ
E5       10153     CONFORMER EQUILIBRIUM/CNF.OBJ
E6        6128     ENERGY DIFFERENCE BETWEEN THE CONFORMERS/CNF.OBJ
E7        5597     THE AUTHOR INVESTIGATED THE CONFORMATION/CNF.OBJ
**** END OF FIELD ****
```

Luminescence (LUM)

- The field Luminescence Description (LUM.KW) contains keywords from a list of controlled terms:
- ...
- Radioluminscence
- Electroluminescence
- Luminescence
- X-ray emission spectrum
- ...

Electrical Data (ELE)

- Field contains keywords from a list of controlled terms:
- ...
- Dielectric anisotropy
- Dielectric relaxation time
- Piezoelectricity
- Photovoltaic effect
- ...

Magnetic Data (MAG)

- Field contains keywords from a list of controlled terms:
- ...
- Anisotropy of magnetic susceptibility
- paramagnetic
- Rotational magnetic moment
- ...

Henry Constant (HNC)

- "The Henry Constant is the ratio of the concentration in an aqueous solution at equilibrium."

```
Henry Constant (MCS):
 Value          | Temp.   | Solvent   |Ref.
 (HNC)          | (.T)    | (.SOL)    |
 (Pa*m**3/mol)  | (Cel)   |           |
================+=========+===========+====
 12.9           | 25      | H2O       | 1

Reference(s):
 1. Sacchetti, Mark, J.Pharm.Sci., CODEN: JPMSAE, 87(8), <1998>, 982 -
    986; BABS-6142975
```

Partition Coefficient Octan-1-ol/Water (POW)

- "The partition coefficient POW describes the equilibrium distribution of a substance between n-octanol and water phases."

```
Partition octan-1-ol/water (MCS):
 Value       | Log POW    | Temp.   |Ref.
 (POW)       | (.LOG)     | (.T)    |
 (--)        | (--)       |   (Cel) |
=============+============+=========+====
             | 1.5        | 37      | 1

Reference(s):
 1. Shafiee, M.; Deferme, S.; Villard, A.-L.; Egron, D.; Gosselin, G.;
    Imbach, J.-L.; Lioux, T.; Pompon, A.; Varray, S.; Aubertin, A.-M.;
    Mooter, G. van den; et al., J.Pharm.Sci., CODEN: JPMSAE, 90(4),
    <2001>, 448 - 463; BABS-6304541
```


Complex Phase Equilibria (CPEM)

- Field contains keywords from a list of controlled terms:

```
=> E A/CPEM.KW
**** START OF FIELD ****
E3           0 --> A/CPEM.KW
E4           4     LIQUID-SOLID-VAPOUR PHASE EQUILIBRIUM/CPEM.KW
E5         128     PHASE EQUILIBRIUM/CPEM.KW
E6           6     SOLID-VAPOUR PHASE EQUILIBRIUM/CPEM.KW
E7           8     TRIPLE POINT/CPEM.KW
**** END OF FIELD ****
. . .
Complex Phase Equilibria:
CPEM
     Description (.KW):              Phase equilibrium
     Partner BRN (.PABRN):           8972812, 776019
     Partner (.PA):                  poly(ethylene oxide), Mn=500,
                                     Mw/Mn=1.1, density 1.07 g/ml;
                                     Monomer(s): ethylene oxide,
                                     2,6,10,15,19,23-hexamethyl-
                                     tetracosane
     Temperature (.T):               85 - 195 Cel
     Note(s) (.COM):                 neutron scattering
```

Electrical Data (EDM)

- Field contains keywords from a list of controlled terms:

```
**** START OF FIELD ****
E3           0 --> A/EDM.KW
E4          61     DIELECTRIC CONSTANT/EDM.KW
E5          19     DIELECTRIC LOSS/EDM.KW
**** END OF FIELD ****
```

```
Electrical Data:
EDM
     Description (.KW):              Dielectric constant
     Partner BRN (.PABRN):           505945
     Partner (.PA):                  ethane-1,2-diol
     Temperature (.T):               25 - 120 Cel
     Reference(s):
     1. Smits, A. L. M.; Wuebbenhorst, M.; Kruiskamp, P. H.; Soest, J. J.
        G. van; Vliegenthart, J. F. G.; Turnhout, J. van, J.Phys.Chem.B,
        CODEN: JPCBFK, 105(24), <2001>, 5630 - 5636; BABS-6312330
```


Optical Data (ODM)

- Field contains only one keyword:

```
**** START OF FIELD ****
E3           0 --> A/ODM.KW
E4          26     KERR CONSTANT/ODM.KW
**** END OF FIELD ****
```

```
ODM
     Description (.KW):              Kerr constant
     Partner BRN (.PABRN):           1305151
     Partner (.PA):                  4-methyl-phenol
     Reference(s):
     1. Prezhdo, V. V.; Vashchenko, E. V.; Prezhdo, O. V.,
        Russ.J.Gen.Chem., CODEN: RJGCEK, 70(1), <2000>, 121 - 129,
        Zh.Obshch.Khim., CODEN: ZOKHA4, 70(1), <2000>, 128 - 136; BABS-
        6250485
```

Multicomponent Systems

Equilibrium Systems

Property is cross-indexed at all partners

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

Examples: Azeotropes, Eutectics, Liquid/Vapour Equilibria

Examples: Solubility, Adsorption, Critical Micelle Concentration

STN

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Multicomponent Systems

Equilibrium Systems

Property is cross-indexed at all partners

Examples: Azeotropes, Eutectics, Liquid/Vapour Equilibria

EXAMPLE: Eutectic Vanillin/Salicylic Acid

```
=> s vanillin/cn and 774890/lssm.pabrn
L3    1 VANILLIN/CN AND 774890/LSSM.PABRN
=> d lssm
```

```
=> s 774890/brn and 472792/lssm.pabrn
L4    1 774890/BRN AND 472792/LSSM.PABRN
=> d lssm
```

STN

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Multicomponent Systems

```
LSSM
     Description:                Eutectic
     Partner BRN:                472792
     Partner:                    4-hydroxy-3-methoxy-benzaldehyde
     Note(s):                    Handbook
     Reference(s):
     1. Opfer-Schaum; Piristi, Z. Lebensm.-Unters., 87, <1944>, 65, 66
```

Salicylic Acid

```
LSSM
     Description:                Eutectic
     Partner BRN:                774890
     Partner:                    2-hydroxy-benzoic acid
     Note(s):                    Handbook
     Reference(s):
     1. Opfer-Schaum; Piristi, Z.Lebensm.Unters., 87, <1944>, 65,66
```

Vanillin

Multicomponent Systems

EXAMPLE:

```
=> s 20-30/cmc and octane/cmc.sol

L6    1 20 G/L - 30 G/L /CMC AND
      OCTANE/CMC.SOL
```

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

Examples:
Solubility, Adsorption, Critical Micelle Concentration

Multicomponent Systems

```
Critical Micelle Concentration:
 Value        | Temp.   | Solvent                  |Ref.
 (CMC)        | (.T)    | (.SOL)                   |
 (g/L)        | (Cel)   |                          |
==============+=========+==========================+====
 4.32112e+09 | 29.85   | heptane                  | 1
 2.48064e+09 | 29.85   | octane                   | 1
 6.80177e+09 | 29.85   | 2,2,4-trimethyl-pentane  | 1
 1.78269e+09 | 29.85   | decane                   | 1
 4.48116e+09 | 29.85   | various solvent(s)       | 1

Reference(s):
 1. Majhi, Pinaki R.; Moulik, Satya P., J.Phys.Chem.B, CODEN: JPCBFK, 103(29),
    <1999>, 5977 - 5983; BABS-6192892
```

STN

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STN®

Appendix – Patent Coverage

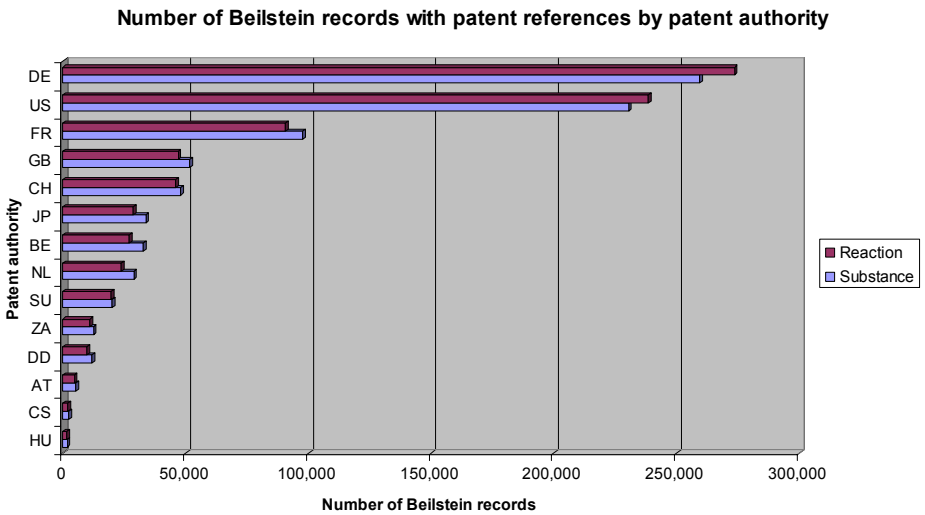
Patents in BEILSTEIN

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

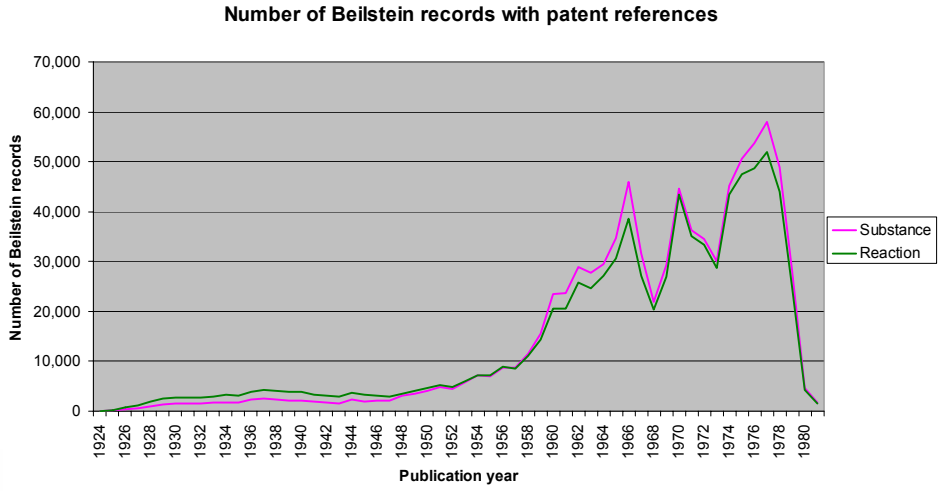
STN

FIZ KARLSRUHE

Patents in Beilstein



Patents in Beilstein



Example: DuPont reaction patents

```
=> S (DUPONT? OR DU(S)PONT?)/PA (S) US/PC (S) 1930-1934/PY
L1         1626 (DUPONT? OR DU(S)PONT?)/PA (S) US/PC (S) 1930-1934/PY

=> S L1 NOT ALL/FA
L2         1216 L1 NOT ALL/FA

=> D RX
L2   ANSWER 1 OF 1216 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL
Reaction:
RX
     Reaction ID (.ID):              8288020
     Reactant BRN (.RBRN):           3144247
     Reactant (.RCT):                air, 2.6-dichloro-1.4-dihydro-
                                     anthracenediol-(9.10)
     Product (.PRO):                 substance of mp: 273-274 degree
     No. of React. Details (.NVAR):  1

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

Limit to Reaction Records with NOT ALL/FA

Hit: Patent reference with reaction data

BEILSTEIN on STN

www.stn-international.com

The reloaded BEILSTEIN file

More data, easier to navigate

The BEILSTEIN File is a most important structure and factual database, containing fully searchable chemical structures and associated properties from the literature period 1779 to present. After reloading and updating, the file now contains more than 8.1 million substances and will be updated quaterly.

There are three different data sources for the file:

- a) The Beilstein Handbook from the Basic Series to Supplement 4 covering the literature from 1779 to 1959. For more than 1.1 million compounds the complete Handbook information is available. These evaluated data are indicated as "Handbook Data" in the notes of literature references.
- b) Primary literature from 1960 to 1979: this data source contains appr. 3 million substances. Specific data are available for melting point (/MP), boiling point (/BP), density (/DEN), refractive index (/RI), optical rotatory power (/ORP), isolation from natural product (/INP) and chemical derivative (/CDER). All other physical and chemical properties are available as keywords together with corresponding references to the original literature. This part of the file is being continuously updated to provide entries for more data fields.
- c) Primary literature data > 1979: in contrast to source b) detailed information for all physical and chemical properties have been abstracted from the literature. All data fields contain references as well as data.

New subject area

As a part of a major upgrade an entirely new Pharmacological and Ecological subject area has been added, as well as a number of new topics and new fields. The four already existing pharmacological and ecological topics (Use (/USC), Toxicity (/TOX), Biological Function (/BF), Ecological Data (/ECOL)) have been moved into the new structure.

Uncovering the extra detail demanded by this new subject area caused BEILSTEIN to increase journal coverage by nearly 45%, and all of the 180 journals now included are indexed in their entirety, not just for the additional information needed for EcoPharm.

Information on the influence of chemical substances and their behaviour in the environment (man, animal, plant) is of vital importance in drug research as well as in the protection of the environment. For example, it helps to plan the synthesis and evaluation of new therapeutic agents more efficiently with regard to health and environmental effects.

The influence of chemical substances on the living species can have desired therapeutic effects as well as adverse toxic results.

The Beilstein file now contains chemical structures and associated properties for more than 8.1 million substances

This property is described in Pharmacological Data and Ecotoxicology. The behaviour in non-living ecosystems such as air, soil, and water are rather more complex and are described in several properties of Ecological Data.

Basically, the EcoPharm segment consists of two main disciplines:

- Ecological and Environmental Data

Here you find information on e.g. the accumulation of insecticides in plants which are finally eaten by animals and humans

- Pharmaco-related Data

Are you interested in substances that exhibit particular bioactive effects ?
Or are you looking for potential candidates for pharmacological screening?

BEILSTEIN provides you with scientific and empirical data, e.g. test results such as Acute Toxicity as well as descriptive information like skin and eye irritation.

Search Example:
What are the bacteriostatic/bactericidal effects of GENTAMICIN
(MIC minimal inhibition concentration; MBC minimal bactericidal concentration)?

```
=> s gentamicin/cn and pharm/fa
L1           24 GENTAMICIN/CN AND PHARM/FA

d . . .

=> s gentamicin/cn and mic/pharm.typ and mbc/pharm.typ
L3            3 GENTAMICIN/CN AND MIC/PHARM.TYP AND MBC/PHARM.TYP

=> d


L3   ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

      Beilstein Records (BRN):        8826628
      Chemical Name (CN):             gentamicin, gentamicin C1;
                                      gentamicin C2; gentamicin C1A; mixture of
      Compound Type (CTYPE):          mixture (composition partially given)
      Compos.: Comp. Brn (COMPBRN):   8812655, 8813379, 8813470
      Compos.: Comp. Name (COMPN):    gentamicin C1a, gentamicin C2, gentamicin C1
      Entry Date (DED):               2001/07/25
      Update Date (DUPD):             2001/07/25

Pharmacological Data:

PHARM
      Effect:                         bactericidic
      Species or Test-System:         Enterococcus faecalis J4
      Method, Remarks:                strain isolated from the blood of a patients
                                      with endocarditis; microdilution method;
                                      Mueller-Hinton broth with 5  percent of
                                      sheep blood; incubated at 37 deg C for 48h;
                                      colony reading
      Further Details:                control strain: Staphylococcus aureus ATCC
                                      25923; MBC defined as the lowest conc. of
                                      the title comp. that killed at least 99.9
                                      percent of the original inoculum
      Type:                           MBC
      Value of Type:                  64 mg/l
      Reference(s):
      1. Gavalda, Joan; Cardona, Pere Joan; Almirante, Benito; Capdevila, Josep
         Anton; Laguarda, Montserrat; Pou, Leonor; Crespo, Ernesto; Pigrau,
         Carles; Pahissa, Albert, Antimicrob.Agents & Chemother., CODEN: AMACCQ,
         40(1), <1996>, 173 - 178
PHARM
      Effect:                         bacteriostatic
      Species or Test-System:         Enterococcus faecalis J4
      Method, Remarks:                strain isolated from the blood of a patients
                                      with endocarditis; microdilution method;
                                      inoculum 1E5 CFU/ml; serial twofold
                                      dilutions of the title comp.; Mueller-Hinton
                                      broth with 3  percent lysed sheep blood;
                                      incubated at 37 deg C for 24h; colony
                                      reading
      Further Details:                control strain: Staphylococcus aureus ATCC
      Type:                           MIC
      Value of Type:                  16 mg/l
      Reference(s):
      1. Gavalda, Joan; Cardona, Pere Joan; Almirante, Benito; Capdevila, Josep
         Anton; Laguarda, Montserrat; Pou, Leonor; Crespo, Ernesto; Pigrau,
         Carles; Pahissa, Albert, Antimicrob.Agents & Chemother., CODEN: AMACCQ,
         40(1), <1996>, 173 - 178
```

PHARM data focus on human and mammalian pharmacology and toxicology, i.e. both therapeutic and toxic effects of substances as well as studies on pharmacodynamics and pharmacokinetics are included.

Several subfields are available for specification e.g.:

/PHARM.E (Effect)
/PHARM.TYP (Typ)
/PHARM.V (Value of Type)
/PHARM.META (Metabolite)
/PHARM.MR (Method)
/PHARM.SP (Species, Test System)

Default Display Format is QRD (Query Related Display): IDE plus requested fields

Reorganization of existing fields

The reload also led to a reorganization of existing fields, resulting in a more userfriendly and easier-to-use data structure. Management of specific searches (for example from spectral origin) will be more systematic. In the old data structure, e.g. information about NMR data were spread over various topics and fields. Due to the reorganization, these topics are grouped together into one new topic "NMR". All entries concerning NMR data are not only clearly arranged, but also extended in depth (new fields: temperature and frequency).

The following topics are grouped analogous to NMR: IR, RAMAN, UV/VIS, Fluorescence, Phosphorescence.

Numerical specifications about the previous topics IR Spectrum, IR Bands, Raman Spectrum, Raman Bands, UV/VIS Spectrum, Absorption Maxima, Fluorescence Spectrum, Fluorescence Maxima, Phosphorescence Spectrum, and Phosphorescence Maxima have been transferred into the Comment Field. No previous information concerning numerical specifications got lost, but non-specific numeric values for spectra scanning ranges will no longer be input from the primary literature. Some topics in the old data structure have been reassigned to keywords (e.g. the former independent topic "Quadrupole Moment" was placed as keyword at the topic "Electrical Moment").

Example: NMR Data

```
NMR
      Coupling Nuclei:     1H-1H,31P-1H
      Solvents:            D2O, various solvent(s)
      Temperature:         4 - 40 Cel
      Frequency:           500 MHz
      Note(s):             temperature dependence
      Reference(s):
      1. Zachova, J.; Cisarova, I.; Budesinsky, M.; Liboska, R.; Tocik, Z.;
      Rosenberg, I., Nucleosides Nucleotides, CODEN: NUNUD5, 18(11-12),
      <1999>, 2581 - 2600; BABS-6222605
NMR
      Description:         Chemical shifts
      Nucleus:             1H
      Solvents:            D2O, various solvent(s)
      Temperature:         4 - 40 Cel
      Frequency:           500 MHz
      Note(s):             temperature dependence
      Reference(s):
      1. Zachova, J.; Cisarova, I.; Budesinsky, M.; Liboska, R.; Tocik, Z.;
      Rosenberg, I., Nucleosides Nucleotides, CODEN: NUNUD5, 18(11-12),
      <1999>, 2581 - 2600; BABS-6222605
```

The reorganization of existing fields resulted in a more user-friendly and easier-to-use data structure

The following topics have been added to the BEILSTEIN File:

- Safety Data (Flash Point, Autoignition)
- Conformation, Electrical Moment
- Luminescence
- Electrochemical Characteristics, Cross-Section
- Henry Constant, Partition Octanol-Water
- Complex Phase Equilibria
- Additional optical and electrical data for MCS

New compound types added

Up to now, BEILSTEIN was virtually exclusively a database of "small and pure" molecules:

- small:
  less than 255 "heavy" atoms
- pure:
  stoicheometrically defined

These substances are the classical Beilstein compounds.

This definition has been lifted: the following new compound types have been added:

- Biomolecules (carbohydrates, enzymes, hormones etc.)
- Mixtures (composed of components)
- Polymers (monomers given, monomers not given)

These compounds may be described by means of names or information about the components.

New compound types have been added: biomolecules, mixtures, and polymers

Example: Compound Type "Biomolecule"

```
Beilstein Records (BRN):        8388571
Chemical Name (CN):             S-(1,2-dicarboxyethyl)
                                glutathione-
                                synthesizing enzyme
Compound Type (CTYPE):          biomolecule
Entry Date (DED):               2000/03/08
Update Date (DUPD):             2000/03/08

No structure diagram available for this BRN

Field Availability:

Code     Name                                Occurrence
================================================
BRN      Beilstein Records                            1
CN       Chemical Name                                1
CTYPE    Compound Type                                1
ED       Entry Date                                   1
UPD      Update Date                                  1
INP      Isolation from Natural Product               1
PHARM    Pharmacological Data                         2
```

Many substances classified as "Biomolecules" have Pharmacological Data.

Using BEILSTEIN you have access to high-quality data for mostly all chemistry-related areas !

BEILSTEIN – Searching for reactions and preparations

See STNews 3/2002
Coming in June 2002

Reactions in the reloaded BEILSTEIN file

BEILSTEIN contains the largest collection of chemical facts and with its 9 million reactions, is one of the most important reaction databases.

Fully searchable chemical structures, comprehensive information on chemical and physical properties as well as pharmacological and ecological data make it an indispensable device for conducting chemical or pharmaceutical research and development. The BEILSTEIN database provides citations from the organic chemistry literature.
One of its main applications is the planning of synthetic routes. For improvements in data structure and extended data coverage a complete reload of the BEILSTEIN file was realized. In this context advantageous changes for the reaction data were implemented.

All reactions are self-contained documents and no longer part of substance documents. BEILSTEIN on STN provides a convenient source of information on reactants and reaction products which are included in the database as fully indexed substances.

New structure of reaction data

In the reloaded BEILSTEIN file reaction data possess a new user-friendly structure. Compared to the old BEILSTEIN version more valuable data were added. For example, "Catalyst", "Solvent" or "Reaction Type" are now available in separate search fields. In addition, reaction displays are much more concise and convenient to handle. In the new file all reaction information is concentrated under the subject "Reaction Data". "Reactions" (REA) and "Preparations" (PRE) present in the former BEILSTEIN version were reorganized, and the complete information is now available in the new "Reaction Data" (RX).

Reaction data are clearly separated in two parts, Reaction Identification Data and Reaction Details, as shown in the example below. All reactions possessing identical Reaction Identification Data, which means reactions with exactly the same reactants and products, are combined under one Reaction ID. The total number of reaction variations is given in the field "Number of Reaction Details" (RX.NVAR). Particular facts of a distinct way to carry out a reaction are given in the Reaction Details.

Example Structure of reaction data

```
RX
      Reaction ID:                    5347186
      Reactant BRN:                   8496283
      Reactant:                       2-iodo-benzoic acid 4-methoxy-
                                      naphthalen-1-yl ester
      Product BRN:                    8493514
      Product:                        12-methoxy-dibenzo<c,h>chromen-6-one
      No. of Reaction Details:        2

Reaction Details:
RX
      Reaction RID:                   5347186.1
      Reaction Classification:        Preparation
      Yield:                          58 percent (BRN=8493514)
      Reagent:                        NaOAc
      Catalyst:                       PdCl2(PPH3)2
      Solvent:                        N,N-dimethyl-acetamide
      Time:                           24 hour(s)
      Temperature:                    130 Cel
      Reaction Type:                  Cyclization
      Reference(s):
      1. Qabaja, Ghassan; Jones, Graham B., J.Org.Chem., CODEN: JOCEAH,
      65(21), <2000>, 7187 - 7194
RX
      Reaction RID:                   5347186.2
      Reaction Classification:        Preparation
      Yield:                          65 percent (BRN=8493514)
      Reagent:                        NaOAc
      Catalyst:                       PdCl2(PPh3)2
      Solvent:                        N,N-dimethyl-acetamide
      Reaction Type:                  Cyclization
      Reference(s):
      1. Qabaja, Ghassan; Perchellet, Elisabeth M.; Perchellet, Jean-Pierre;
         Jones, Graham B., Tetrahedron Lett., CODEN: TELEAY, 41(17), <2000>,
         3007 - 3010; BABS-6220208
```

Reaction Identification Data

Reaction Data

Reaction Detail

Reaction Identification Data

Reaction Identification Data include Reaction ID, which is the unique registry number of the reaction, Reactant Name, Reactant BEILSTEIN Record Number (Reactant BRN), Product Name, and Product BEILSTEIN Record Number (Product BRN). The data give information on reactants and products which are usually registered organic compounds.

In the reaction documents the BRN, which identifies an indexed title compound, appears in the Reactant BRN (RX.RBRN) field for a reactant, while the one of a product is listed in the Product BRN (RX.PBRN) field.

Reaction Details

Reaction Details provide explicit information about reaction conditions. If quoted in the literature, further information such as yield, reagent, catalyst, solvent, time, temperature, pressure, pH value or reaction type are indexed. Important information which can not be attributed to other parameter fields, e.g. heating, UV irradiation or description of biological methods are stored in the "Other Conditions" field.

Depending on the aim of investigation, each Reaction Detail is classified either as "Preparation" or as "Chemical Behaviour" in the Reaction Classification field (RX.CL). A reaction is ranked as "Preparation" if the investigation focused on the preparative method. "Chemical Behaviour" is assigned to data concentrating on thermodynamic or kinetic studies of a reaction.

"Multistage" reactions are a special type of preparations where the structures of intermediates are unknown. In this case starting materials for all steps are entered together in the corresponding fields and details for each reaction step are given individually in the single stages

Table Reaction data and their search codes

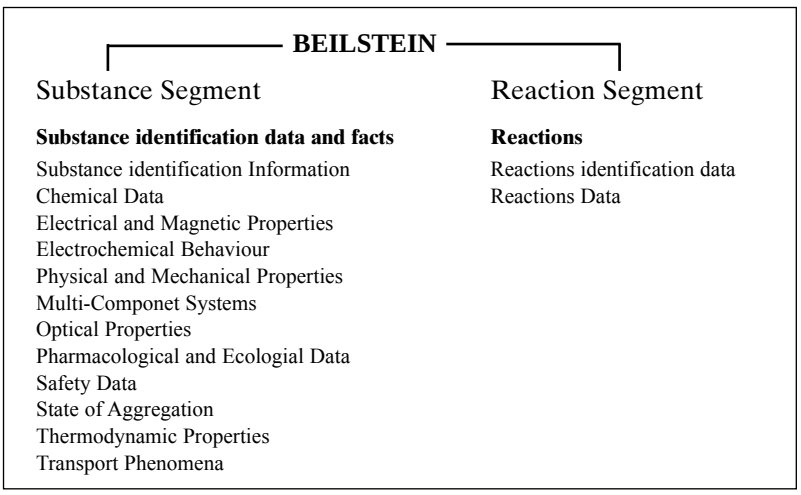
Field	Search code
Reaction Identification Data	
Reaction ID	RX.ID
Reactant BRN	RX.RBRN
Reactant	RX.RCT
Product BRN	RX.PBRN
Product	RX.PBRN
No. of Reaction Details	RX.NVAR
Reaction Details	
Reaction ID	RX.ID
Reaction Classification	RX.CL
Yield	RX.YD
Reagent	RX.RGT
Catalyst	RX.CAT
Solvent	RX.SOL
Time	RX.TIM
Temperature	RX.T
Pressure	RX.P
pH Value	RX.PH
Reaction Type	RX.TYP
Subject Studied	RX.SUBJ
Prototype Reaction	RX.PRT
Other Conditions	RX.COND
Note	RX.COM

Different ways to gain reactions

The BEILSTEIN file consists of the two independent file segments: substances and reactions. Search in substance documents, e.g. for identification data or chemical or physical facts results in a substance answer set.

Retrieval in the reaction data, e.g. for reactants, products, reagents, catalysts, reaction type or reaction classification leads to reaction documents. In order to achieve reactions, two strategies are offered: The cost-effective display out of a substance document, or the specific detailed search for reaction data.

Figure BEILSTEIN file structure



Display reactions of a compound from the substance document

Displaying reaction data from the substance document offers the opportunity of showing identification data and reactions for a compound at a glance. In the "Field Availability" table included in the display format "IDE" existing reaction documents of a compound are indicated. To display all reactions of the compound the "RX" format can be used. If you are interested in reactions that lead to the searched compound as the reaction product, "RXPRO" is the suitable format. All reactions with the compound acting as a reactant are indicated by "RXREA". Employing the display formats "RX", "RXPRO" or "RXREA" from a substance document represents a cost-effective method to show all desired reaction data of a compound for one display fee.

The display formats "RXPRO" and "RXREA" were established exclusively for substance answer sets and are not valid in the reaction file segment. Only the 20 first reaction documents are displayed with the described codes. In order to show all reactions the full formats "FRX", "FRPRO" or "FRXREA" have to be used.

Search for reactions of compounds

To confine the search for reactions, the choice of reaction data can be used.

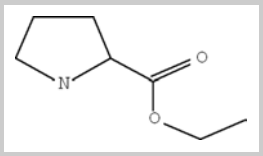
Reactants and products are searchable by name and BRN but in most cases a retrieval will start in the substance file segment. Due to the file organization, substance and reaction data can not be concatenated in one query. For a comfortable shift to the reaction data, select the BRN from the substance answer set.

Example *Display of reactions for a compound out of the substance document*

```
=> S PROLIN-ETHYL ESTER/CN
L1             1 PROLIN-ETHYL ESTER/CN

=> D IDE


L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

   Beilstein Records (BRN):    81263
   CAS Reg. No. (RN):          5817-26-5, 60169-67-7, 96163-72-3
   Chemical Name (CN):         prolin-ethyl ester
   Autonom Name (AUN):         pyrrolidine-2-carboxylic acid ethyl ester
   Molec. Formula (MF):        C7 H13 N O2
   .
   .
```

Search for a compound in the chemical name field

Display Identification Data of the compound



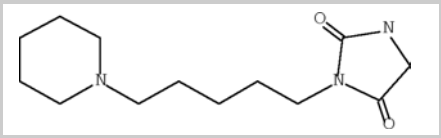
```
 Field Availability:

   Code      Name                                      Occurrence
   ========================================================
   BRN       Beilstein Records                                1
   RN        CAS Registry Number                              3
   CN        Chemical Name                                    1
   .
   .
   .

    This substance also occurs in Reaction Documents:

   Code      Name                                      Occurrence
   ========================================================
   RX        Reaction Documents                               6
   RXREA     Substance is Reaction Reactant                   3
   RXPRO     Substance is Reaction Product                    3

=> D RXREA

L1 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction:
RX
   Reaction ID:                3821611
   Reactant BRN:               81263, 396343
   Reactant:                   prolin-ethyl ester, (3,4-dimethoxy-
                               phenyl)-acetyl chloride
   Product BRN:                4547445
   Product:                    1-<(3,4-dimethoxy-phenyl)-acetyl>-
                               pyrrolidine-2-carboxylic acid ethyl ester
   No. of Reaction Details:    1

Reaction Details:
RX
   Reaction RID:               3821611.1
   Reaction Classification:    Preparation
   Yield:    89 percent (BRN=4547445)
   Reference(s):
   1. Yasuda, Shingo; Yamada, Toru; Hanaoka, Miyoji, Tetrahedron Lett.,
      CODEN: TELEAY, 27(18), <1986>, 2023-2026; BABS-5546862
   .
   .
   .
```

Indication of Reaction Documents

Display reactions "D RXREA": Reactions where the substance is the reaction reactant.

Example Search for reaction data starting in the substance file segment

```
L1       STRUCTURE UPLOADED

=> D
L1 HAS NO ANSWERS
L1                STR
```



```
...

=> S L1 SSS FULL
FULL SEARCH INITIATED 11:05:19 FILE 'BEILSTEIN'
FULL SCREEN SEARCH COMPLETED -     219 TO ITERATE

100.0% PROCESSED     219 ITERATIONS                4 ANSWERS
SEARCH TIME: 00.00.07

L2            4 SEA SSS FUL L1

=> SELECT L2 1- RX.PBRN
E1 THROUGH E4 ASSIGNED

=> S E1-E4
              1 5837132/RX.PBRN
              0 6040826/RX.PBRN
              1 6079220/RX.PBRN
              1 8645556/RX.PBRN
L3            3 (5837132/RX.PBRN OR 6040826/RX.PBRN OR
              6079220/RX.PBRN OR 8645556/RX.PBRN)


=> S L3 AND (PREPARATION? OR MULTISTAGE)/RX.CL
         7722342 PREPARATION/RX.CL
           56513 MULTISTAGE/RX.CL
L4             3 L3 AND (PREPARATION OR MULTISTAG

=> D RX


L4   ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction:
RX
    Reaction ID:                8613445
    Reactant BRN:               8620409, 132339
    Reactant:                   3-(5-chloro-pentyl)-imidazolidine-
                                2,4-4-benzyl-piperidine
    Product BRN:                8645556
    Product:                    3-<5-(4-benzyl-piperidin-1-yl)-
                                pentyl>-imidazolidine-2,4-dione
    No. of Reaction Details:    1

Reaction Details:
RX
    Reaction RID:               8613445.1
    Reaction Classification:    Preparation
    Yield:                      76 percent (BRN=8645556)
    Reagent:                    NaI, K2CO3
    Solvent:                    acetonitrile
    Time:                       18 hour(s)
    Other Conditions:           Heating
    Reaction Type:              Condensation
    Reference(s):
1. Schelkun, Robert M.; Yuen, Po-wai; Serpa, Kevin; Meltzer,
Leonard T.; Wise, Lawrence D.; Whittemore, Edward R.; Woodward,
Richard M., J.Med.Chem., CODEN: JMCMAR, 43(9), <2000>, 1892 -
1897; BABS-6252946
```

Conduct a structure search

Reaction search for the retrieved compounds

Search reactions which lead to the desired compounds: Select RX.PBRN

Search selected terms

Focus on preparations by employing the Reaction Classification field (RX.CL)

Display reactions

If it is intended to find reactions where the substance is employed as reactant, the "Reaction Reactant BRN" (RX.RBRN) has to be selected. To gain reactions for those compounds of the answer set that lead to the substances as reaction products, select the "Reaction Product BRN" (RX.PBRN).

After searching for the selected terms, display reactions inclusive reaction details with "D RX". The default display format QRD (Query Related Data) includes only Reaction Identification Data unless Reaction Details are looked for.

If you want to retrieve proporation data and exclude reactions which lead to the desired compound but possess the Reaction Classification "Chemical Behaviour", narrow the answer set by concatenating with "(PREPARATION? OR MULTISTAGE)/ RX. CL".

BEILSTEIN – EcoPharm Data

See STNews 4/2002
Coming in August 2002

BEILSTEIN's new subject: EcoPharm Data

In the domain of factual and bibliographic databases of organic substances BEILSTEIN and BEILSTEIN Abstracts (BABS) are outstanding in providing structures, facts, reactions with nearly unlimited combinations of search possibilities.

In the past, scientists would turn to BEILSTEIN for questions such as "What happens when organic compound A reacts with organic compound B?" Today, where the scope of BEILSTEIN has been enhanced, searchers can retrieve answers to questions beyond the above theme, for example "What happens to an organic chemical compound when it reacts with something else, e.g. any test system, animal or human beings, environmental compartments, etc.?"

Information on the influence of chemical substances and their behaviour in the environment is of vital importance in drug research as well as in the protection of the environment. For example, it helps to plan the synthesis and evaluation of new therapeutic agents more efficiently with regard to health and environmental effects.
The influence of chemical substances on the living species can have desired therapeutic effects as well as toxic adverse effects. This property is described in Pharmacological Data and Ecotoxicology. The behaviour of chemical substances in the non-living ecosystems such as air, soil, and water are rather more complex and is described in several properties of Ecological Data.
This new topic "EcoPharm Data" replaces the segment titled "Physiological Behaviour" (with its four properties Toxicity, Biological Function, Ecological Data, and Use) in the old data structure. The already existing factual data have been moved into the new structure (see Example 1).

The journal base for the new subject EcoPharm is a further 60 journals (in total now 180 journals) added to the former coverage. The data input for this section started in 1994 with a detailed data structure containing several main and subfields (see Examples 2 and 3). EcoPharm provides greater depth of compound information in the areas of ecotoxicology, pharmacology, and biodegradation. These important biological data augment the amount of physical properties and reference data already available for compounds in BEILSTEIN.

In combination with corresponding physicochemical properties such as Henry Constant, Partition Coefficient (n-octanol/water) Solubility, etc. the database now enables chemists and scientists in related fields to get instant access to the entire scope of pharmacological and environmental sciences. Whether you are interested in synthesis planning, in pharmacological evaluation of existing or new therapeutic agents, or in exposure assessment of chemicals: BEILSTEIN is the right place to gather the necessary information!

Pharmacological Data

Pharmacological (and toxicological) Data in BEILSTEIN focus on human and mammalian pharmacology and toxicology, i.e. both therapeutic and toxic effects of chemical substances as well as studies on pharmacodynamics and pharmacokinetics are included. Examinations with bacteria or enzymes concerning human pathology are also regarded.

Example 1: Sample record for "old" Pharmacological Data in the reloaded BEILSTEIN

```
Beilstein Records (BRN):     164808

Pharmacological Data:
PHARM
     Note(s):                antitumor activity against L1210 leukemia,
                             mice (in vivo)
     Reference(s):
     1. Wang, Yuqiang; Liu, Mao-Chin; Lin, Tai-Shun; Sartorelli, Alan C.,
         J.Med.Chem., CODEN: JMCMAR, 35(20), <1992>, 3667-3671;
         BABS-5705413
```

No subfields available; this substance was mentioned in a "traditional" journal excerpted for the database

Search Example 2: Pharmacological Data

```
=> file beilstein
=> s human/pharm.sp (p) anti-inflammatory/pharm.e and inp/fa
L1        21 HUMAN/PHARM.SP (P) ANTI-INFLAMMATORY/PHARM.E AND INP/FA

=> d

L1 ANSWER 1 OF 21 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

. . .

Pharmacological Data:
PHARM
   Effect:                      anti-inflammatory
   Species or Test-System:      TPA activated human granular white blood
                                cells
   Method, Remarks:             nitro blue tetrazolium chloride reduction
                                system
   Type:                        IC50
   Value of Type:               1.05 mg/l
   Reference(s):
   1. Koyama, Junko; Morita, Izumi; Tagahara, Kiyoshi; Hirai, Kei-Ichi,
      Phytochemistry, CODEN: PYTCAS, 53(8), <2000>, 869 - 872; BABS-6238195
PHARM
   Effect:                      anti-inflammatory
   Species or Test-System:      TPA activated human granular white blood
                                cells
   Method, Remarks:             nitro blue tetrazolium chloride reduction
                                system
   Type:                        IC100
   Value of Type:               4.0 mg/l
   Reference(s):
   1. Koyama, Junko; Morita, Izumi; Tagahara, Kiyoshi; Hirai, Kei-Ichi,
      Phytochemistry, CODEN: PYTCAS, 53(8), <2000>, 869 - 872; BABS-6238195
```

Search for substances isolated from natural product(s) which exhibit an anti-inflammatory effect on humans.

Effect: covers all kind of effects, therapeutic like anti-inflammatory or toxic like genetic toxicity
Species: like human, mammals, and their isolated organs. Information on sex of species is also included
Type: such as LD50, EC50, LOEC
Value: numeric value of type

Toxicological Data

In principle, we can distinguish between four levels of data:

Level 1:
Scientific and empirical data, e.g. test results such as Acute Toxicity (Lethal Dose, LD50)

Level 2:
Evaluated and classified data, e.g. LD50>5mg/kg is very toxic

Level 3:
Regulation concerning handling, storage, transport etc.

Level 4:
Risk assessment, i.e. the collection of information in order to deal with the risk.

Data of LEVEL 1 are facts and therefore independent of any critical evaluation or legislation; this level is the source for the Toxicology Data in BEILSTEIN. LEVELs 2-4 include data which have been evaluated and can be country- dependent. Data of LEVEL 2 and 3 can be retrieved in the MSDS Databases.

Ecological Data

(Ecotoxicological and Ecological Chemistry Data)

Ecological Data are concerned with effects and interactions of chemical substances, especially environmental chemicals, with living and non-living nature.

Their behaviour in the environment for instance, their distribution, accumulation potentials and transformation are also focal points of research in ecological chemistry.

Biological Behaviour: This property contains bioaccumulation, biomagnification and biomoni-

Important Search Fields (for a complete list see Summary Sheet)

Pharmacological and Toxicological Data	
Effect	/PHARM.E
Species or Test system	/PHARM.SP
Route of Application	/PHARM.RA
Type	/PHARM.TYP
Value	/PHARM.V
Result	/PHARM.RE
Method	/PHARM.MR

Ecological Data	
Biological Behaviour	/BIO
Biodegradation	/BIOD
Concentration in Environment	/COEV
Degradation	/ECDH, ECDP
Stability in Soil	/ECS
Exposure Assessment	/EXCA
Ecotoxicology	/ECTOX
Laboratory Use	/USC

Search Example 3: Ecotoxicological Data

```
=> file beilstein

Uploading C:\Programme\stnexp\Queries\strychnine.str

L6       STRUCTURE UPLOADED

L7            733 SEA SSS FUL L6


=> s l7 and toxicity/ectox.e (p) oryzias/ectox.sp
L16           1 L7 AND TOXICITY/ECTOX.E (P) ORYZIAS/ECTOX.SP

=> d
. . .

Ecotoxicology:
ECTOX
    Effect:                  behavioral symtoms
    Species or Test-System:  Oryzias latipes, Japanese medaka
    Concentration:           1 - 10 mg/l
    Exposure Period:         48 hour(s)
    Method, Remarks:         30-d-old juvenile fish, 12 mm mean length;
                             aqueous solution of test comp. added to
                             aquaria; observation of behavioral and
                             morphological response, methods by Drummond
                             (1986, 1991)
    Further Details:         25 deg C; five behavioral and morphological
                             indicators: loss of equlibrium, general
                             activity, startle response, hemorrhage,
                             deformity
    Results:                 sign of stress occurred at 2 and 24 h for 10
                             and 1 mg/l, respectively; behavioral
                             effects: loss of equilibrium, hypoactive
                             swimming, convulsions and tetany,
                             underreactive to startle stimuli
    Reference(s):
    1. Rice, Patricia J.; Drewes, Charles D.; Klubertanz, Theresa M.;
       Bradbury, Steven P.; Coats, Joel R., Environ.Toxicol.Chem., CODEN:
       ETOCDK, 16(4), <1997>, 696 - 704; BABS-6147046

ECTOX
    Effect:                  toxicity to fish (acute)
    Endpoint of Effect:      mortality
    Species or Test-System:  Oryzias latipes, Japanese medaka
    Exposure Period:         48 hour(s)
    Method, Remarks:         30-d-old juvenile fish, 12 mm mean length;
                             acute toxicity test according to American
                             . . .
```

Search for substances with strychnine substructure and information on toxic effects on Oryzias species

Species: Species in ECTOX are aquatic, terrestrial and aerial non-mammalian representatives of the food chain, which are used as indicators for the pollution degree of ecosystems
Method: This field contains a comprehensive summary of the test procedure

Notice the bibliographic part: Environ. Toxicol. Chem. was not a traditional journal for BEILSTEIN

toring data. Bioaccumulation is the ability of organisms to concentrate substances within themselves. Bioaccumulation is the result ot two processes: accumulation and elimination.

Biomagnification is a sequence of processes in an ecosystem by which higher concentrations of chemical substances are attained in organisms at higher trophic level in the food chain.

Biomonitoring has the objective that the appearance of substances is comprehensively monitored.

Degradation contains the subdivisions Biodegradation, Abiotic Degradation and Stability in Soil. Biodegradation describes the degradation of an organic substance to smaller molecules or to inorganic substances by microorganisms. This can occur by means of aerobic or anaerobic degradation. The property Stability in Soil characterizes the resistance or stability of a substance in soil. Standardized soils are often used for measurement of specific dissipation times.

Concentration in Environment gives information on the degree of pollution by hazardous chemicals in living organisms or non-living environmental compartments.

Exposure Assessment describes the spread of pollution originating from natural or synthetic substances or sources, e.g. the contamination of hen feed with dioxins and PCBs due to careless handling.

Ecotoxicology is a subdivision of toxicology. It concentrates on the toxic effects of chemical substances on organisms, which are indicators for the degree of pollution in an ecosystem (air, soil, water).Typical species are fish and daphnia for water, earthworms for soil and birds for air. Its aim is to reveal structural and functional changes in the ecosystem due to effects of chemical substances.

Use and Handling describes the use of a substance in the preparative chemistry, in the laboratory and contains information on safety aspects or the attainment of the desired effect, such as phase transfer catalysis, reduction, quenching, etc.

Find physical properties in the reloaded BEILSTEIN file

BEILSTEIN, a major structure searchable database in organic chemistry, now contains more than 8.3 million substances. BEILSTEIN is not only an important reaction database, but also has the largest collection of chemical factual data.

For indexed substances BEILSTEIN offers comprehensive information including pharmacological and ecological data as well as chemical data and physical properties. Storage of this information in more than 100 different topics each comprising numerous search fields enables precise retrieval for specific information. Various physical properties are described by controlled terms or are numerically searchable.

The reloaded file offers several improvements for property data searching:

- More properties added, including Henry Constant, Partition Coefficient Octanol/ Water, Luminescence
- New data fields for existing topics: ESR data enhanced for more precise searching based on coupling nuclei, solvents, and temperature
- Systematic grouping of spectroscopic properties for NMR, IR, Raman, UV/VIS spectrum, fluorescence, and phosphorescence
- Controlled terms extended and transferred to individual keyword fields

Together with the excellent numerical search facilities on STN, the new BEILSTEIN file offers convenient access to a wide range of physical facts for organic compounds.

Manifold physical property data

The selection of relevant physical data for the file is enormously diverse. Single and multi-component systems are considered. The huge number of about 90 physical topics can be summarized under the following 11 subjects. Use the predefined display codes, given in brackets, to display all data for a subject at once.

Single-component systems

Information on physical properties of the pure title substance

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

Multi-component systems

Information on physical properties of the title substance in a multi-component system

- Multi-Component Systems (MCS)

A subject comprises numerous properties. For instance the subject Spectroscopic Data contains ESR Data (ESR), Fluorescence Data (FLU), Infrared Spectrum (IR), Luminescence (LUM), Mass Spectrum (MS), Nuclear Magnetic Resonance (NMR), Nuclear Quadrupole Resonance (NQR), Other Spectroscopic Methods (OSM), Phosphorescence (PHO), Raman Spectrum (RAS), Rotational Spectrum (ROT), UV and Visible Spectrum (UVS).

Details on all property fields can be found in the Database Summary Sheet available at www.stn-international.de/stndatabases/databases/beilstei.html

Handle property data with helpful search fields

Several search fields were generated to enhance user-friendliness in dealing with property information:

- All Keywords (/AKW)

In the /AKW field all keywords of the different properties are concentrated. The field corresponds to the former Controlled Terms field (/CT) and may be used to search for a keyword independent of the superordinated topic.

- Property Hierarchy (/PH)

The /PH field gives an alphabetic order of names and field codes for all chemical and physical property fields as well as all available keywords.

Example: Use of a predefined display code to show all available data of a subject for one compound at one time

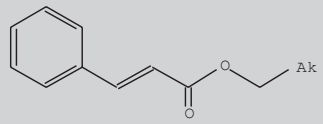
Display all Physical and Mechanical Properties for a compound (e.g. phenanthrene) with the display format MECP

```
=> D MECP

L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL


Liquid Density:
 Value          | Temp.      | Ref. Temp.| Ref.      | Note
 (DEN)          | (.T)       | (.RT)     |           |
 (g/cm**3)      | (Cel)      | (Cel)     |           |
=============== +============ +===========+========== +=======
                |            |           | 1, 2, 3   |
 1.176          |            |           | 4         | 1
 1.203          |            |           | 5         | 1
 1.213          | 0          | 4         | 6         | 2
 1.175          | 17         |           | 7         | 1
 1.182          | 20         |           | 8         | 1
 1.179          | 25         |           | 9         | 1
 1.063          | 100.5      |           | 10        | 1
 1.066          | 101        |           | 11        | 1
 1.058 - 1.018  | 110 - 170  |           | 12        | 1
 1.037          | 120        |           | 13        | 1
 1.044          | 130        |           | 14        | 1
 1.0412         | 131.1      | 4         | 15        | 2
 1.035          | 148        |           | 16        | 1
 1.025          | 160        |           | 16        | 1
 1.009          | 180        |           | 14        | 1
 0.965          | 240        |           | 14        | 1
 0.919          | 300        |           | 14        | 1

Reference(s):
  1. Gurevich; Bednov, Russ.J.Phys.Chem.(Engl.Transl.), CODEN: RJPCAR, 46,
     <1972>, 1532, 2673
  2. Lin; Lin, J.Chin.Chem.Soc.(Taipei), CODEN: JCCTAC, 12, <1965>, 25,29,34
...

Notes(s):
1. g/cm**3
2. Handbook


Mechanical Property:
MEC
     Description (.KW):              Specific volume
     Note(s) (.COM):                 bei 20-95grad., Handbook
     Reference(s):
     1. Ueberreiter; Orthmann, Z.Naturforsch., CODEN: ZNTFA2, 5a, <1950>,
        101, 107
...

Acoustic Property:
SOUND
     Description (.KW):              Ultrasonic properties
     Reference(s):
     1. Kartha et al., Indian J.Pure Appl.Phys., CODEN: IJOPAU, 12, <1974>,
        648



Surface Tension:
 Value     | Temp.  | Ref. |  Note
 (ST)      | (.T)   |      |
 (g/s**2)  | (Cel)  |      |
===========+======== +=====  +======
           |        | 1    |
 37.24     | 100.5  | 2    |  1
 36.34     | 120    | 3    |  1

Reference(s):
 1. Biswas, Spectrochim.Acta, CODEN: SPACA5, 21, <1965>, 1979
 ...
```

Example: Search for melting points of cinnamic acid alkyl esters

```
L1       STRUCTURE UPLOADED

=> D
L1 HAS NO ANSWERS
L1                STR
```

Build and upload structure of cinnamic acid alkyl esters

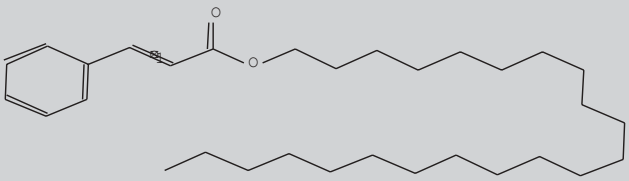



```
Structure attributes must be viewed using STN Express query preparation.

=> S L1 CSS FULL
FULL SEARCH INITIATED 13:13:44 FILE 'BEILSTEIN'
SCREENING
SCREENING
SCREENING
FULL SCREEN SEARCH COMPLETED -  34625 TO ITERATE

 30.7% PROCESSED   10631 ITERATIONS                      10 ANSWERS

 75.8% PROCESSED   26250 ITERATIONS                      30 ANSWERS

100.0% PROCESSED   34625 ITERATIONS                      44 ANSWERS
SEARCH TIME: 00.01.34

L2            44 SEA CSS FUL L1
```

Conduct a Closed Substructure Search to find cinnamic acid alkyl esters

```
=> S L2 AND MP/FA
        3992891 MP/FA
L3            11 L2 AND MP/FA

=> D CN STR HIT

L3   ANSWER 1 OF 11 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

     Chemical Name (CN):          docosanoic cinnamate
     Autonom Name (AUN):          3-phenyl-acrylic acid docosyl ester
```

Confine hits to records with available data for Melting Point (/MP) by concatenating with MP/FA




```
Atom/Bond Notes:
        1. CIP Descriptor: E


Melting Point:
 Value   | Ref.
 (MP)    |
 (Cel)   |
=========+====
 54 - 56 | 1

Reference(s):
 1. Ruecker, Gerhard; Shenkel, Eloir; Manns, Detlef; Falkenberg, Miriam;
Marek, Anne, Phytochemistry, CODEN: PYTCAS, 41(1), <1996>, 297-300; BABS-
6009005
```

The /PH field can be used to search for the presence of a property, whether a specific value is recorded in the file or whether the information is recorded as a controlled term.

- Field Availability (/FA)

Indicated in /FA are all display fields available for a record; they are indexed with names and codes. The FA table for a title compound lists all data, including all property data accessible for the compound in the database. The use of /FA is advisable if only records with information for a special property are desired from a hit record set.

Property search

Physical data may contain numerical and non-numerical search fields as well as keywords. Mostly a property will be given together with property conditions, description or notes. Use the (P) operator to combine a property with corresponding property conditions and restrict data to the same experiment. Numerous fields in the physical properties are numerically searchable, like boiling point (/BP) or critical pressure (/CRP). On STN, numerical search fields are loaded with a default unit, which is Cel for temperatures and Torr for pressures in the BEILSTEIN file. If a search command is entered without specifying the unit for a property, the default unit is assumed. Numerical data might be given in the original literature as distinct values or as ranges. Both are searchable in the BEILSTEIN database with the numerical operators provided on STN. In order to learn whether a search field is numerically searchable or not, or about the default unit for a numerical property, see the BEILSTEIN Database Summary Sheet.

Example: Search for compounds with a boiling point within the range 99-101 Cel measured at a pressure of 760 Torr

Search for Quadrupole Moment using the Expand list

```
=> E QUADRUPOLE MOMENT/PH
E1        26946      PURIFICATION/PH
E2          401      PVT RELATIONSHIP/PH
E3          196 -->  QUADRUPOLE MOMENT/PH
E4          298      RADIAL DISTRIBUTION FUNCTION/PH
E5            3      RADICAL CONTACT SHIFTS/PH
E6          184      RADIOLUMINESCENCE/PH
E7         4955      RAMAN/PH
E8         2175      RAMAN INTENSITIES/PH
E9          919      RAMAN RESONANCE EFFECT/PH
E10       24069      RAMAN SPECTRUM/PH
E11       24069      RAS/PH
E12         102      RATE OF ADSORPTION/PH

=> S E3
L1           196 "QUADRUPOLE MOMENT"/PH

=> D HIT

L1  ANSWER 1 OF 196 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Dipole Moment:
 Value    | Description         |Ref.
 (DM)     | (.KW)               |
 (D)      |                     |
==========+=====================+====
          | Quadrupole moment   | 1

Reference(s):
 1. Sham, J.Chem.Phys., CODEN: JCPSA6, 71, <1979>, 3744
```

Quadrupole Moment is a Keyword for the topic Dipole Moment

Search for the temperature range in the Boiling Point field (/BP) and the corresponding pressure (/BP.P).
Use (P) operator to combine property values with property conditions

```
=> S 99-101/BP (P) 760/BP.P
         36402 99 CEL - 101 CEL /BP
         18684 760 TORR /BP.P
L1         436 99 CEL - 101 CEL /BP (P) 760

=> D

L1 ANSWER 1 OF 436 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

  Beilstein Records (BRN): 8899478
  Chemical Name (CN):      2-bromo-2-chloro-1-difluoromethoxy-
                            1,1-difluoro-ethane
  Autonom Name (AUN):      2-bromo-2-chloro-1-difluoromethoxy-
                            1,1-difluoro-ethane
  Molec. Formula (MF):     C3 H2 Br Cl F4 O
  Molecular Weight (MW):   245.40

...

Boiling Point:
 Value       | Press.      |Ref.
 (BP)        | (.P)        |
 (Cel)       | (Torr)      |
============ +=============+====
 100         | 760         | 1

Reference(s):
 1. Horvath, Ari L., Chemosphere, CODEN: CMSHAF, 44(4),
<2001>, 897 - 906;
    BABS-6311562
```

2003 – The Year of Chemistry

Chemistry has become an integral part of our lives. We come across it with almost every step we take - but who will actually think of chemistry when buying fresh rolls, admiring sparkling diamonds or kissing his or her partner?

These examples already show the various manifestations of chemistry and therefore the chemical organizations in Germany have, together with the Bundesministerium für Bildung und Forschung (BMBF) – Federal Ministry of Education and Research –, named the year 2003 "Year of Chemistry", thus continuing the tradition of the former subject-related years (e.g. 2002: "The Year of Geosciences") . The goal of this initiative is to encourage the dialog between scientists and the interested public. (More information at www.jahr-der-chemie.de)

STN International takes the "Year of Chemistry" as an opportunity to present milestones of chemistry together with the corresponding databases. The first article is dedicated to the history of dyestuff synthesis, also showing some old existing patents relating to this subject which are contained in BEILSTEIN. STNews 2/2003 will feature an article on "Leopold Gmelin – a Pioneer of Physiological Chemistry".

BEILSTEIN's Hidden Treasures: Old Patents

Old patents in organic chemistry are closely related to the synthesis of dyes. Until the middle of the 19th century, all dyes available to man came from natural sources. Most of these were plant extracts or minerals and a few were animal products. The range of colours was limited, and so was the usability of dyes. It was not until the 19th century that the pace of advancement quickened into a gallop. With the progress of organic chemistry inevitably came the first widespread marketing of a synthetic dye.

In 1856, while searching for a cure for Malaria, William Henry Perkin discovered the first synthetic dyestuff "Mauvein", which resulted in the build-up of a completely new branch of industry in Europe. It was a brilliant fuchsia type colour, belonging to the class of Aniline dyes. The field of synthetic dye chemistry was now exploding, since the increasing textile production of the late 19th century industrial revolution led to a growing demand for inexpensive dyes. Soon Germany became the leader in the synthetic dye industry as chemists educated in the spirit of Justus LIEBIG and Friedrich WÖHLER dominated the synthesis of "coal-tar" dyes. These chemists discovered dozens of new dyes a year.

One area of early synthetic dye chemistry, azo dyes, remains one of the largest and most important to the industry. The birth of the azo dyes came in 1858, the same year in which PERKIN started the production of "Mauvein", although their value was not appreciated until P. BÖTTIGER produced "Congo Red", the first direct cotton dye, in 1884.

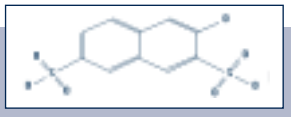
During the last 125 years synthetic dyes have been prepared in an amazing number and variety. Also the possibilities of further synthesis are unlimited. Methods of synthesis have been the precursor of the upcoming pharmaceutical industry. Many dyestuff producing companies adopted the processes also for isolating drugs from medical plants.

Most of the promising dyes were protected by patents; in former times, and even more today, the knowledge about already existing patents is very important. In order to determine whether an invention is patentable, it is necessary to know what has already been invented or published (known as the "prior art"). The prior art includes all previously issued patents, as well as technical reports, journal articles and even non-written physical material.

The BEILSTEIN File is a most important structure and factual database, containing fully searchable chemical structures and associated properties from the literature period ranging from 1779 to present. Patents are covered until 1980 (approx. 160,000 patents). There is a substantial number of unique patent data esp. from 1930-1940.
Many of the old patents have the main focus on preparative methods: laboratory synthesis, purification, technical synthesis, biochemical preparation.

Preparation of Acid Chrome Black V

Preparation Product



```
Reaction:
RX
   Reaction ID (.ID):              674868
   Reactant BRN (.RBRN):           521151
   Reactant (.RCT):                6-hydroxy-naphthalene-2-sulfonic acid
   Product BRN (.PBRN):            623734
   Product (.PRO):                 3-hydroxy-naphthalene-2,7- disulfonic acid
   No. of React. Details (.NVAR): 1

Reaction Details:
RX
   Reaction RID (.RID):            674868.1
   Reaction Classification (.CL): Preparation
   Reagent (.RGT):                 sulfuric acid, potassium pyrosulfate
   Note(s) (.COM):                 Handbook
   Reference(s):
   1.Patent: Baum 1883, Fortschr.Teerfarbenfabr.Verw.Industriezweige,
             1, 384
```

Acid Chrome Black V belongs to the class of Mordant Dyes, suitable for application on wool after chrome methods. Mordant Dyes vary in their constitution, all of which possess an acid character. Because of the presence of hydroxyl or carboxyl groups in their molecules they are capable of forming lakes with metallic mordants.

Synthetic Preparation of Indigo

```
Reaction:
RX
   Reaction ID (.ID):              5712118
   Reactant (.RCT):                in the side-chain brominated
                                         2-acetylamino-acetophenone
   Product BRN (.PBRN):            88275
   Product (.PRO):                 1H,1'H-<2,2'>biindolylidene-3,3'-dione
   No. of React. Details (.NVAR): 1
```

Preparation Product

```
Reaction Details:
RX
   Reaction RID (.RID):            5712118.1
   Reaction Classification (.CL): Preparation (half reaction)
   Note(s) (.COM):                 Handbook
   Reference(s):
   1.Patent: BASF DE 21592, Fortschr.Teerfarbenfabr.
   verw.Industriezweige, 1,138
   2.Baeyer; Bloem, Chem.Ber., CODEN: CHBEAM, 17, <1884>, 966
```

One of the most cited journals for old patents is the so-called "coal tar dye" journal: "P. Friedländers Fortschritte der Teerfarbenfabrikation und Verwandte Industriezweige"

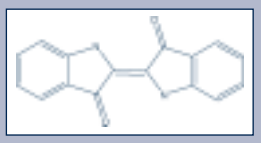
Experts say that Egyptian mummy clothes from the third millennium BC had borders of indigo dyed stripes. The name Indigo is derived from the Greek Indikon and the Latin Indicum, meaning a substance from India.
In 1880 Adolph von Bayer first synthesized artificial Indigo, chemically identical to the natural product but missing the associated impurities. By 1897 the production methods had improved to the point that synthetic Indigo could commercially compete with natural Indigo and by 1920 synthetic Indigo had almost completely replaced the natural product.

One of the most cited journals for old patents is the so-called "coal tar dye" journal: "P. Friedländers Fortschritte der Teerfarbenfabrikation und Verwandte Industriezweige" published from volume 1 (1877) to 24 (1937). This journal is a collection of important old patents related to dye chemistry.

Search Example: Which substances with an indigo substructure are mentioned in old patents?

Note: The publication date of a patent reference in BEILSTEIN may fall outside the cut-off date of a given series; e.g. some parts of Suppl. IV (1950-1959) were not published until 1980.

```
=>
Uploading C:\Programme\stnexp\Queries\indigo1.str

L10      STRUCTURE UPLOADED


=> s l5
SAMPLE SEARCH INITIATED 16:35:10
SAMPLE SCREEN SEARCH COMPLETED -      24 TO ITERATE

100.0% PROCESSED       24 ITERATIONS   22 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:   ONLINE   **COMPLETE**
                         BATCH    **COMPLETE**
PROJECTED ITERATIONS:          187 TO       773
PROJECTED ANSWERS:             159 TO       721

L11           22 SEA SSS SAM L5

=> s l5 full
FULL SEARCH INITIATED 16:35:16
FULL SCREEN SEARCH COMPLETED -     402 TO ITERATE

100.0% PROCESSED      402 ITERATIONS   372 ANSWERS
SEARCH TIME: 00.00.01

L12          372 SEA SSS FUL L5

=> s l12 and p/dt
L13            3 L12 AND P/DT

=> d 1-3 hit


L13  ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Crystal Property Description:
CPD
      Reference(s):
      1.Patent: Minnesota Mining Co. US 3981859 1976,
         Chem.Abstract, 86(6391)


L13  ANSWER 2 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Chemical Derivative:
CDER
      Note(s) (.COM):     dibromide, Further Data see Handbook
                         (Preparation), Handbook
      Reference(s):
      1.Patent: Hoechster Farbw. DE 242030, Fortschr.Teerfarbenfabr.Verw.
        Industriezweige, 10, 377
      2.Patent: Hoechster Farbw. DE 230596, Fortschr.Teerfarbenfabr.Verw.
        Industriezweige, 10, 374
      3.Patent: Hoechster Farbw. DE 224809, Fortschr.Teerfarbenfabr.Verw.
        Industriezweige, 10, 370

Crystal Property Description:
CPD
      (CPD):                          kupferglaenzend, violett
      Note(s) (.COM):                  Handbook
      Reference(s):
      1. Grandmougin, Chem.Ber., CODEN: CHBEAM, 42, <1909>, 4408
      2.Danaila, C.R.Hebd.Seances Acad.Sci., CODEN: COREAF,
         149, <1909>, 1385
      3.Patent: Ges. f. chemical Ind. DE 193438
CPD
      (CPD):                          blau
      Note(s) (.COM):                  Handbook
      Reference(s):
      1.Patent: Hoechster Farbw. DE 228960, Fortschr.Teerfarbenfabr.Verw.
        Industriezweige, 10, 383
```



Take advantage of the structure search capability in BEILSTEIN to find early patent data.

```
Melting Point:
 Value    |Solvent          |Reference    | Note
 (MP)     |(.SOL)           |             |
 (Cel)    |                 |             |
========= +=================+=============+=======
          |nitrobenzene     | 1,  2,  3   | 1
          |methyl benzoate  | 4           | 1

Reference(s):
 1. Grandmougin, Chem.Ber., CODEN: CHBEAM, 42, <1909>, 4408
 2. Danaila, C.R.Hebd.Seances Acad.Sci., CODEN: COREAF, 149, <1909>, 1385
 3. Patent: Ges. f. chemical Ind. DE 193438
 4. Patent: Hoechster Farbw. DE 228960,
    Fortschr.Teerfarbenfabr.Verw.Industriezweige, 10, 383

Notes(s):
1. Handbook


L13  ANSWER 3 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Isolation from Natural Product:
INP(INP):                           von reinem Indigo aus Naturindigo
                                    Durch Behandlung mit Eisessig-
                                    Schwefelsaeure und Hydrolyse des
                                    entstandenen Sulfats
     Note(s) (.COM):                Handbook
     Reference(s):
     1. Patent: Ullmann,G. DE 156829,Fortschr.Teerfarbenfabr.Verw.Industrie
        zweige, 8, 441
     2. Binz; Kufferath, Justus Liebigs Ann. Chemical, CODEN: JLACBF, 325,
        <1902>,199
     3. Bloxam, J.Chem.Society, CODEN: JCSOA9, 87, <1905>, 977


Note: The publication date of a patent reference in BEILSTEIN may fall outside the cut-
off date of a given series; e.g. some parts of Suppl. IV (1950-1959) were not published
until 1980.
```

Patent references may occur in numeric fields as well as in reaction records.

Examples for old journals cited in BEILSTEIN

- Fortschritte der Teerfarben-fabrikation und Verwandte Industriezweige
- Justus Liebigs Annalen der Chemie
- Crells Chemisches Journal/ Crells Neueste Entdeckungen
- Buchners Neues Repertorium für Pharmacie
- Die Pflanzenstoffe
- Fresenius Zeitschrift für Analytische Chemie
- Monatshefte Chemie
- Ann.Chim. (Paris)
- Chemische Berichte

Important search fields for patents in BEILSTEIN:

- Document Type (/DT)
- Journal Title (/JT)
- Patent Assignee (/PA)
- Patent Country(/PC)
- Patent Number (/PN)
- Publication Year (/PY)
- Citation (unresolved) (/URES)

Note: The country coverage is not sytematic (e.g. Main Series and 1. Suppl. Series only cover German patents); it is recommended to use the EXPAND command for /PC.

BEILSTEIN - all STNews articles and STNotes at a glance

In response to many customer questions a series of STNews articles and two detailed STNotes were published.

All this material is now available in a single reference document at

www.stn-international.com/training_center/chemistry/beilstein/all_beilstein.pdf

Back to the Roots – Potential Drugs from Natural Products

Natural products are increasingly used as a resource for potential drugs. Despite promising achievements accomplished in the field of genetically engineered synthetic drugs, extracts from plants and animals remain a basic source for many pharmaceuticals. Approximately half of the world's medicines originate from natural resources, are synthetic analogs of natural products, or were developed on the basis of structural leads gained from natural products. The importance of natural products is both good and bad news for medical researchers. The good news is that remedies for the treatment of cancer and other diseases may be literally "growing on trees". The bad news is that a lot of plants are in scarce and dwindling supply.

New Life for Old Remedies

In many parts of the world, herbal medicines are a major part of pharmaceutical care. The foundations of modern pharmacology are based largely on the knowledge gained from remedies isolated from plants. Many popular drugs derive from early uses of crude plant drugs, e.g. willow and cinchona barks for fever, foxglove for congestive heart failure, or opium for pains.

For a time there was a trend in the pharmaceutical industry to move away from natural products. Synthetic chemicals made successful entries into the therapeutic area, but the need for structurally novel therapeutic categories continues. Plants are accomplished "chemists", they synthesize complicated chemicals with a broad range of activities. Many of these compounds are difficult or impossible to manufacture in the laboratory, and companies are returning to those "natural chemists". In recent years, success stories such as the development of taxol, an anti-cancer agent extracted from the yew tree, have attracted attention to the potential of plants as a source of new drugs.

BEILSTEIN's extensive data collection offers you an array of capabilities; a pharmacist or medical researcher interested in extracts of natural products with associated pharmacological data will find BEILSTEIN an invaluable source of information. Information on Isolation from Natural Product (/INP) is available for more than 131,000 substances, more than 26,000 of these have Pharmacological Data (/PHARM).

Isolation from Natural Product contains names of the source in nature (plant, fungus, animal etc.) or an industrial grade natural product from which compounds have been isolated. Sources are only recorded when a compound has been isolated. The identification of well-known compounds by instrumental methods (e.g. GLC, TLC) as components of natural or synthetic products is not recorded here (e.g. the identification of pentan-2-one in tobacco smoke or limonene in the ethereal oils of a rare plant or saccharose as a component of a tree-bark extract). Terms do not belong to a controlled vocabulary, specific names (e.g. the systematic name of the plant or animal) are used when they are available.

Pharmacological (and toxicological) Data in BEILSTEIN focus on human and mammalian pharmacology and toxicology, i.e. both therapeutic and toxic effects of chemical substances as well as studies on pharmacodynamics and pharmacokinetics are included. Examinations with bacteria or enzymes concerning human pathology are also regarded. All indexed data are stored in a very detailed way.

Pharmacological Data fields

Pharmacological Data are stored in the following fields:

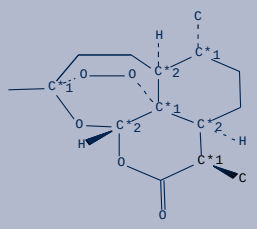
PHARM.E (Effect)
contains effects from the areas of pharmacodynamics, pharmacokinetics, and human toxicology. Both therapeutic and adverse effects are considered.

PHARM.EP (Endpoint of Effect)
The investigation endpoint at which the effect was recorded is entered in this field. It is an observable or measurable biological or chemical event used as an index of the effect on a cell, tissue, organ, organism, etc.

PHARM.SP (Species or Test Systems)
In general mammals, humans or their isolated organs or cells. Microorganisms or enzymes concerning human pathology are also considered. Species are entered by means of the systematic (Latin) names and, if available, the English trivial name. For the entry of a test system the author's designation is used.

While searching for new and effective drugs for the treatment of malaria, researchers rummaged in the "poison cabinet" of nature. They came across the Chinese medicinal herb Quinghaosu (Artemisia annua). This example shows available pharmacological information.

```
=> file beilstein

=> s artemisia annua/inp and antimalar?/pharm.e
...
=> d
L1   ANSWER 1 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

      Beilstein Records (BRN):      4194670
      Beilstein Pref. RN (BPR):     63968-64-9
      CAS Reg. Number (RN):         63968-64-9, 113472-97-2, 119241-68-8
      Chemical Name (CN):           artemisinin
      Molec. Formula (MF):          C15 H22 O5
      Molecular Weight (MW):        282.34
      Lawson Number (LN):           23913
      File Segment (FS):            Stereo compound
      Compound Type (CTYPE):        heterocyclic
      Constitution ID (CONSID):     3149255
      Tautomer ID (TAUTID):         3983360
      Beilstein Citation (BSO):     6-19
      Entry Date (DED):             1991/10/23
      Update Date (DUPD):           2003/01/18
```



Stereo Information

- *Chiral centers (*)*
- *Cahn-Ingold-Prolog (CIP) descriptors : E, Z, R, S*

```
 Atom/Bond Notes:
        1. CIP Descriptor: R
        2. CIP Descriptor: S

   Field Availability:

      Code    Name                                  Occurrence
      ========================================================
      BRN     Beilstein Records                            1
      BPR     Beilstein Preferred RN                       1
      RN      CAS Registry Number                          3
      CN      Chemical Name                                1
      MF      Molecular Formula                            1
      FW      Formular Weight                              1
      ...
      INP     Isolation from Natural Product               8
      ...
      PHARM   Pharmacological Data                        92
      ...

Isolation from Natural Product:
INP
      (INP):                              Artemisia annua
      Reference(s):
      1.Rafatro, Herintsoa; Ramanitrahasimbola, David; Rasoanaivo,
      Philippe; Ratsimamanga-Urverg, Suzanne; Rakoto-Ratsimamanga, Albert;
      Frappier, Francois, Biochem.Pharmacol., CODEN: BCPCA6, 59, <2000>,
      1053 - 1062; BABS-6357224
INP
      ...

Pharmacological Data:
PHARM
      Effect (.E):                    antimalarial
      Endpoint of Effect (.EP):       <3H>hypoxanthine incorporation
      Species or Test-System (.SP):   Plasmodium falciparum 3D7R/actD2.3
                                      strain
      Concentration (.C):             Ca. 0.01 - 5 .my.mol/l
      Method, Remarks (.MR):          parasitized RBCs of 1E-1 percent
                                      parasitemia in 2 percent haematocrit
                                      were incubated in the absence or
                                      presence of increasing title comp.
                                      concentrations for 3 d at 37 deg C; on
                                      day 7 of experiment the incorporation
                                      of <3H>hypoxanthine was determined
      Further Details (.FD):          twice synchronized culture of
                                      actD-resistant strain selected from a
                                      chloroquine-susceptible strain, 3D7,
                                      was used; reference: P. falciparum,
                                      3D7 strain; RBCs = red blood cells;
                                      actD = actinimycin D
      Results (.RE):                  IC50 value for 3D7R/actD2.3 strain was
                                      significantly higher than for
                                      reference strain (plots)
      Reference(s):
      1. Abrahem, Abrahem; Certad, Gabriela; Pan, Xing-Qing; Georges, Elias,
         Biochem.Pharmacol., CODEN: BCPCA6, 59, <2000>, 1123 - 1132;
         BABS-6356986 ...
```

PHARM.S (Sex)
Information on the sex of the test species is entered in this field.

PHARM.RA (Route of Application)
Provides information relating to the method of application of the substances under investigation such as oral, subcutaneous, intravenous, etc.

PHARM.C (Concentration)
The administered test concentration or starting concentration is entered in this field.

PHARM.KD (Kind of Dosing)
Contains special or explanatory information on the dosing, e.g. twice a day for the first 2 days then once a day for the following 3 days.

PHARM.EX (Exposure Period)
Generally describes the whole period of examination starting from the moment of administration of the test substance. Other time-periods like incubation times, pre- or post-observation times, if available, are entered in the field "Method".

PHARM.MR (Method, Remarks)
Contains a comprehensive summary of the test procedure. It gives details about the method of investigation (e.g. hot plate test, Ames test, Western Blot) as well as explanatory information on test parameters such as number of animals exposed, age, weight, housing and feeding conditions, etc. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

PHARM.FD (Further Details)
This field offers further details about the investigated effect and test method as well as explanations for abbreviations used in other free-text fields.

PHARM.H (Half-life Time)
The time required for the initial concentration of a test substance present in an organism to decrease by one half through biological processes such as metabolism and excretion.

PHARM.TYP (Type)
Contains specific dose designations derived from dose-response curves like LD50, EC50, LOEC, etc. Such numerical parameters are particularly useful for comparing the potency of different substances causing the same effect on the same species or the potency of the same substance on different species.

- LD 50: the quantity of a substance that causes the death of 50% of the subjects examined (lethal dose/kg weight).
- EC 50: the concentration of a substance (measured in air or water) that causes a specific effect/reaction on 50% of the subjects examined.
- LOEC: abbreviation for "lowest observed effect concentration". It indicates the lowest concentration at which an effect is observable.
- IC50: inhibitory concentration on 50% of the species

PHARM.V (Value of Type)
The numerical value of the corresponding type is entered in this field.

PHARM.RE (Results)
Results which are not available in numerical form, or other information related to numerical entries are entered as free-text in this field. If no effects have been detected from the investigation this (negative) result is entered in the field "Comment".

PHARM.BRN (Metabolite BRN)
Information on metabolites from pharmacokinetic studies is given in form of the inked BRN numbers (PHARM.BRN) together with the related chemical names (PHARM.META).

PHARM.META (Metabolite)
Information on metabolites from pharmacokinetic studies is given in form of the BRN numbers together with the related chemical names.

PHARM.COM (Comment)
Data of the properties "Biological Function" and "Toxicity" of the previous data structure are stored in this field.

PHARM.E	Effect
PHARM.EP	Endpoint of Effect
PHARM.SP	Species or Test System
PHARM.S	Sex
PHARM.RA	Route of Application
PHARM.C	Concentration
PHARM.KD	Kind of Dosing
PHARM.EX	Exposure Period
PHARM.MR	Method, Remarks
PHARM.FD	Further Details
PHARM.H	Half-life Time
PHARM.TYP	Type
PHARM.V	Value of Type
PHARM.RE	Results
PHARM.BRN	Metabolite BRN
PHARM.META	Metabolite
PHARM.COM	Comment

Find titles and abstracts of BEILSTEIN citations in BABS – the BEILSTEIN Abstracts Database

BEILSTEIN has been synonymous with high-quality, organic chemistry data for two centuries. This comprehensive information source on organic compounds, including the BEILSTEIN database and the BEILSTEIN Abstracts database (BABS), is offered on STN.

Evaluated BEILSTEIN data come from the top journals in organic and related chemistry, ecology and pharmacology. Currently about 180 journals are covered.

BEILSTEIN contains fully searchable structures, reactions, associated physical and chemical properties, as well as detailed pharmacological and ecological data. Each fact in the BEILSTEIN database is displayed with its corresponding literature reference. All citations from 1980 to the present referenced in BEILSTEIN are indexed with title and abstract in BABS. The BABS Accession Number, given at the end of each citation in BEILSTEIN serves as a link between a certain BEILSTEIN reference and the corresponding BABS record.

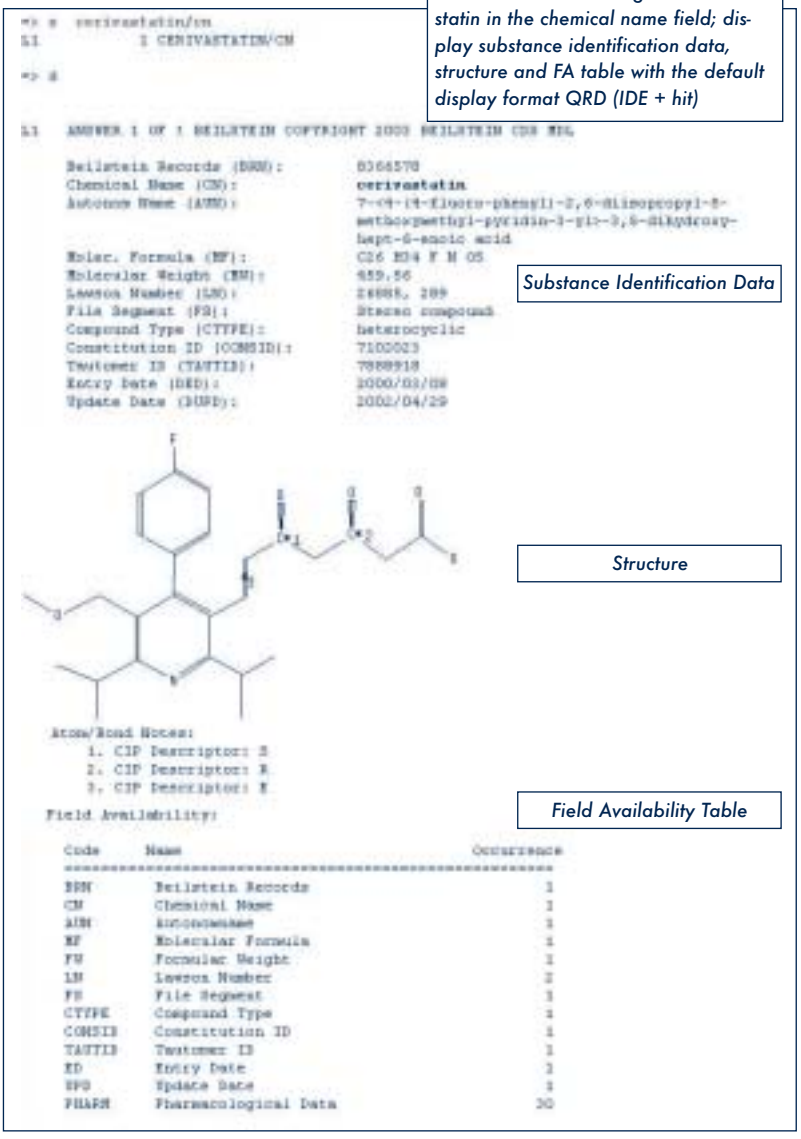
When you have displayed a BEILSTEIN fact, e.g. a property, and wish to gain more information on the focus of the original literature, you can easily access the corresponding BABS record via the BABS Accession Number. Use the convenient way in STN on the Web and simply click on the BABS Accession Number. The active link will lead you directly to the relevant, full BABS record including bibliographic data, title and abstract.

As BABS is connected to the STN Full-Text Solution, you can access the full-text for a citation of interest directly via ChemPort. If the document is not available in electronic form you may order it at FIZ AutoDoc, FIZ Karlsruhe's document delivery broker service which is part of the STN Full-Text Solution.

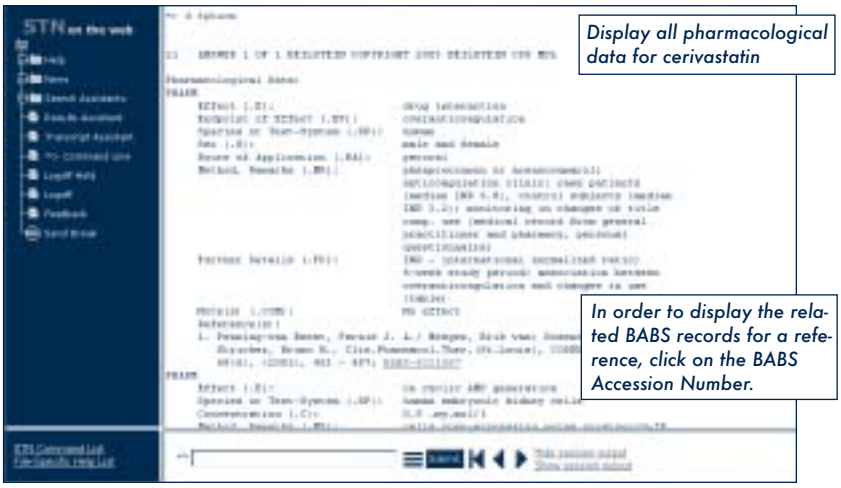
STN, your one-stop information shop, offers a continuous information chain for organic compounds. Go non-stop all the way from a retrieved BEILSTEIN fact, via title and abstract of the reference in BABS, to the original chemical literature.

1. Search and display compound record

Search for the active ingredient cerivastatin in the chemical name field; display substance identification data, structure and FA table with the default display format QRD (IDE + hit)



2. Display facts for the compound and access the related BABS record



3. Automatic display of BABS data

BEILSTEIN - all STNews articles and STNotes at a glance

In response to many customer questions a series of STNews articles and two detailed STNotes were published.

All this material is now available in one single reference document at

www.stn-international.com/training_center/chemistry/beilstein/all_beilstein.pdf

Searching Spectroscopic Data in BEILSTEIN

The BEILSTEIN file with its more than 8 million substances is a most important structure and factual database, containing fully searchable chemical structures and associated properties from the literature period 1779 to present.

Spectroscopy is an important type of chemical analysis; it is the study of the interaction of electromagnetic radiation with matter. Many 20th century chemistry discoveries depend on spectroscopic evidence, e.g. protein structures or the Buckyballs. On the other hand, advances in spectroscopic techniques often lead to revolutions in chemical and biological sciences, e.g. X-ray crystallography, NMR, MRI. If a data set on one molecule from different types of spectroscopic measurement can be collected, we have a unique fingerprint of the molecule.

BEILSTEIN is an excellent source for spectral information with several search fields to search spectroscopic data (see Table 1).

To increase precision all these fields have a Comment (/xxx.COM) and a Keyword (/xxx.KW) subfield; in addition, for some spectroscopic properties Solvent, Temperature or information on Coupling Nuclei are available.

Additional search and display fields are available to enhance user-friendliness when dealing with spectroscopic information:

- All Keywords (/AKW)
- Property Hierarchy (/PH)
- Field Availability (/FA)

In the AKW field all keywords of the different properties are gathered. The field corresponds to the former Controlled Terms field (/CT) and may be used to search for a keyword independent of the superordinated topic.

Examples for Keywords are listed in Table 2. For a complete list use EXPAND A/XXX. KW, where XXX stands for one of the field codes listed in Table 1.

Nuclear Magnetic Resonance	/NMR
Electron Spin Resonance	/ESR
Nuclear Quadrupole Resonance	/NQR
Rotational Spectrum	/ROT
Infrared Spectrum	/IR
Raman Spectrum	/RAS
Ultraviolet Spectrum	/UVS
Luminescence	/LUM
Fluorescence	/FLU
Phosphorescence	/PHO
Mass Spectrum	/MS
Other Spectroscopic Methods	/OSM

Table 1: Search Fields belonging to "Spectra"

Table 2: Examples for Keywords

NMR:
- Chemical shifts
- Dynamic NMR
- Spin-spin relaxation time
- Double resonance

...

ESR:
- Signals
- G-factor
- ENDOR
- ESR line width

...

IR:
- Fine structure of IR bands
- Intensity of IR bands
- Far IR spectrum
- Fermi resonance

...

UVS:
- Absorption Maxima
- Reflection Spectrum
- Triplet-triplet band
- Band anisotropy

...

MS:
- Electron Impact
- Fragmentation pattern
- Laser desorption
- Metastable ions

...

The PH field gives an alphabetic order of names and field codes from all chemical and physical property fields as well as all available keywords.
The /PH field can be used to search for the presence of a property, whether a specific value is recorded in the file or the information is recorded as a controlled term.

Indicated in FA are all display fields available for a record; they are indexed with names and codes. The FA table for a title compound lists all data,

including all property data accessible for the compound in the database. The use of FA is advisable if only records with information for a special property are desired from a hit record set. For complex numeric searches the additional use of "FIELD NOT AVAILABLE" (/FNA) is recommended, e.g.:

```
=> s benzoic(w)acid/cns and (200-250/bp or bp/fna) and orp/fa and de/fa
```

```
=> s gentiana/inp and ms/fa and uvs/fa and nmr/fa and ir/fa

L15          48 GENTIANA/INP AND MS/FA AND UVS/FA AND NMR/FA AND IR/FA

=> d ide hit


L15  ANSWER 1 OF 48 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

   . . .

     Chemical Name (CN):              isovitexin-6-O"-.beta.-D-glucoside

   . . .

Infrared Spectrum:
 Descript | Solvent  |Ref.| Note
 ion      |          |    |
 (.KW)    | (.SOL)   |    |
==========+==========+====+=======
 Bands    | KBr      | 1  | 1

Reference(s):
 1.  Lin, Chun-Nan; Kuo, Shih-Hsien; Chung, Mei-Ing; Ko, Feng-Nien; Teng,
     Che-Ming, J.Nat.Prod., CODEN: JNPRDF, 60(8), <1997>, 851-853;
     BABS-6073790

Notes(s):
1. 3500 - 1640 cm**(-1)


Mass Spectrum:
MS
     Description (.KW):               spectrum
     Note(s) (.COM):                  FAB (fast atom bombardment)
     Reference(s):
     1.Lin, Chun-Nan; Kuo, Shih-Hsien; Chung, Mei-Ing; Ko,
     Feng-Nien; Teng, Che-Ming, J.Nat.Prod., CODEN: JNPRDF, 60(8),
     <1997>, 851-853; BABS-6073790

Nuclear Magnetic Resonance:
NMR
     Description (.KW):               Chemical shifts
     Nucleus (.NUC):                  1H
     Solvents (.SOL):                 dimethylsulfoxide-d6
     Reference(s):
     1. Haribal, Meena; Renwick, J. Alan A., Phytochemistry, CO
        47(7), <1998>, 1237-1240; BABS-6089245
NMR
     Description (.KW):               Chemical shifts
     Nucleus (.NUC):                  13C
     Solvents (.SOL):                 dimethylsulfoxide-d6
     Reference(s):
     1. Haribal, Meena; Renwick, J. Alan A., Phytochemistry, CODEN: PYTCAS,
        47(7), <1998>, 1237-1240; BABS-6089245
     . . .


UV and Visible Spectrum:
 Description       |Solvent   | Absorption    |Ref.
                   |          | Maxima        |
 (.KW)             |(.SOL)    | (.AM)         |
                   |          | (nm)          |
===================+=========+===============+====
 Absorption maxima |methanol  | 318           | 1
 Absorption maxima |methanol  | 268, 330      | 1
 Absorption maxima |methanol  | 268.8, 390    | 1
 ...
```

Available Subfields:
- *Comment /IR.COM*
- *Description /IR.KW*
- *Solvent /IR.SOL*
- *Temperature /IR.T*

Available Subfields:
- *Comment /MS.COM*
- *Description /MS.KW*

Available Subfields:
- *Frequency /NMR.F*
- *Description /NMR.KW*
- *Comment /NMR.COM*
- *Nucleus /NMR.NUC*
- *Coupling Nuclei /NMR.NUI*
- *Solvent /NMR.SOL*
- *Temperature /NMR.T*

Available Subfields:
- *Absorption Maxima /UVS.AM*
- *Comment /UVS.COM*
- *Ext./Abs. Coefficient /UVS.EAC*
- *Description /UVS.KW*
- *Solvent /UVS.SOL*

Search for gentiana ingredients with information on ms, uvs, nmr, and ir spectra

Chemical Abstracts Service
provides access to STN International
in North America

STNotes

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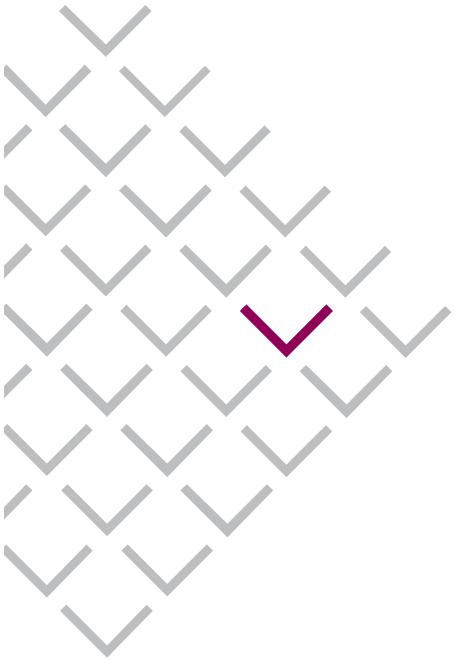


The New BEILSTEIN File on STN - Reaction Data

With the reload of the BEILSTEIN file, searching and displaying of reaction data have changed.

BEILSTEIN, a major structure and factual database, has been reloaded. The file now contains more than 8.1 million substances.

The following new content has been added:

- Pharmacological data
- Ecological data
- Biomolecules, polymers, and mixtures
- Additional properties

In addition, the data structure has been modified for:

- Precise searching of properties
- Searching and displaying of reaction data

This STNote highlights and illustrates the changes to searching and displaying of reaction data in the reloaded Beilstein file.

In response to customer requests for more detailed information on new and enhanced system features, we have created STNotes. STNotes give you the in-depth technical details you need for efficient use of STN. We hope you find this information useful. Please let us know how we can continue to improve in meeting your technical information needs.

Reaction data for substances

There are now two separate search file segments: substance data and reaction data. Search in the substance file segment for information such as substance identification data, chemical or physical data. Answers are records for substances and factual data such as properties. Search in the reaction segment for information such as reactants, products, reagents, catalysts or reaction type. Answers to reaction queries are records with reaction information; substance information is not included.

Because the substance and reaction data are searchable in separate file segments, you may not combine substance information and reaction data search terms in the same search query. However, you may restrict substance or property search results to the answers containing reaction data.

There are now two ways to obtain reaction information for a compound or a set of compounds:

- Display reaction data for a substance or a set of substances after a search of substance information or other substance data
- Search the reaction data, for example by searching a Beilstein Record Number (BRN) as a product or a reactant.

Content of the Substance File Segment

Substance identifying information

Chemical data

Electrical and magnetic properties

Electrochemical behavior

Physical and mechanical properties

Multi-component systems

Optical properties

Pharmacological data

Ecological data

Safety data

Spectral data

State of aggregation data

Thermodynamic properties

Transport phenomena

Content of the Reaction File Segment

Reaction identification data

Reaction details

Displaying reaction data in the substance file

To display reaction data after searching substance or property information, follow these steps:

1. Search substance or property information, e.g., a substance name. Combine the substance search with RX/FA to restrict answers to those containing reaction data.
2. Display a substance record in the default display format QRD, consisting of the Substance Identifying Information (IDE) and HIT. The IDE format now includes information on the availability of reaction data in the Field Availability (FA) table.
3. Display the reaction information.

The cost of displaying reaction information for a substance in the substance file segment is the same, regardless of how many reactions are displayed.

Search a substance name and display reaction data

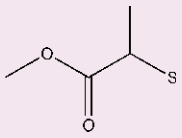
```
=> FILE BEILSTEIN
=> S THIOLACTIC ACID METHYL ESTER/CN AND RX/FA

L1           1 "THIOLACTIC ACID METHYL ESTER"/CN AND
                RX/FA

=> D QRD

L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN
     CDS MDL

     Beilstein Records (BRN):      1902427
     Beilstein Pref. RN (BPR):     53907-46-3
     CAS Reg. No. (RN):            53907-46-3, 82031-
                                   68-3, 105368-24-9,
                                   132958-63-5
     Chemical Name (CN):           2-mercapto-propionic
                                   acid methyl ester,
                                   2-mercapto-propanoic
                                   acid, methyl ester,
                                   methyl 2-
                                   mercaptopropionate,
                                   thiolactic acid
                                   methyl ester
                    .
                    .
                    .
```




```
   Field Availability:

     Code     Name                                Occurrence
   ========================================================
     BRN      Beilstein Records                        1
     BPR      Beilstein Preferred RN                   1
     RN       CAS Registry Number                      4
     CN       Chemical Name                            4
     AUN      Autonomname                              1
     MF       Molecular Formula                        1
     FW       Formular Weight                          1
     LN       Lawson Number                            2
     CTYPE    Compound Type                            1
     CONSID   Constitution ID                          1
     TAUTID   Tautomer ID                              1
     BSO      Beilstein Citation                       2
     ED       Entry Date                               1
     UPD      Update Date                              1
     BP       Boiling Point                            1
     XREF     Crossfile Reference                      3

 This substance also occurs in Reaction Documents:

     Code     Name                                Occurrence
   ========================================================
     RX       Reaction Documents                      21
     RXREA    Substance is Reaction Reactant          20
     RXPRO    Substance is Reaction Product            1
```

Search the substance name in the Chemical Name (/CN) field and combine with RX/FA to ensure that reaction data are available.

Display QRD, the default display format.

The QRD format includes the Field Availability data as well as availability of reaction data.

Use one of the following formats for displaying reaction information in the substance search file:

- RX (the first 20 reaction records for each substance)
- FRX (all reactions for the substance)
- RXPRO (the first 20 reactions in which the substance is a product
- FRPRO (all the reactions in which the substance is a product)
- RXREA (the first 20 reactions in which the substance is a reactant)
- FRXREA (all the reactions in which the substance is a reactant)

The display formats RXPRO, FRPRO, RXREA, and FRXREA are special formats available only in the substance file segment for displaying reaction data. These formats are not available for displaying reaction data in the reaction file segment.

All reaction information is now labeled Reaction (RX). The Reaction data are clearly separated into two parts, Reaction Identification Data and Reaction Details.

All reactions possessing identical Reaction Identification Data are combined under one Reaction ID. The total number of reaction variations is given in the field Number of Reaction Details. The Reaction Details section includes information needed to carry out a reaction. Additional information such as pH and Type of Reaction may be included. References from which the reactions were indexed are included.

```
=> D FRX

L1   ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2002 BEILSTEIN
     CDS MDL

Reaction:
RX
     Reaction ID:                  7042916
     Product BRN:                  1902427
     Product:                      2-mercapto-propionic
                                   acid methyl ester
     No. of Reaction Details:      1

Reaction Details:
RX
     Reaction RID:                 7042916.1
     Reaction Classification:      Preparation (half
                                   reaction)
     Reference(s):
     1. Eugster; Allner, Helv.Chim.Acta, CODEN: HCACAV,
     45, <1962>, 1750,1760
                    .
                    .
                    .
Reaction:
RX
     Reaction ID:                  896983
     Reactant BRN:                 1902427, 108582
     Reactant:                     2-mercapto-propionic
                                   acid methyl ester,
                                   phenyl-oxirane
     Product BRN:                  1978090
     Product:                      2-(2-hydroxy-
                                   2-phenyl-
                                   ethylsulfanyl)-
                                   propionic acid methyl
                                   ester
     No. of Reaction Details:      1

Reaction Details:
RX
     Reaction RID:                 896983.1
     Reaction Classification:      Preparation
     Reagent:                      Py
     Solvent:                      benzene
     Time:                         8 hour(s)
     Other Conditions:             Heating
     Reference(s):
     1. Jankowski,K. et al., Bull.Acad.Pol.Sci.Ser.
     Sci.Chim., CODEN: BAPCAQ, 19, <1971>, 661-671

=> D COST FULL

BEILSTEIN FILE     COST=
  SESSION CONNECT HOURS         0.03 @    0.00      0.00
  INTERNET HOURS                0.03 @    6.00      0.18
  IDENTIFICATION OF SUBSTANCE   1    @    7.78      7.78
  REACTION DATA                 1    @    7.78      7.78
```

Use the FRX format to display all the reactions, if there are more than 20 reactions.

There is only one charge for each FRX or RX display in the substance file segment, regardless of how many reactions are displayed.

Searching reaction data

Another way to find reaction information is by searching the reaction data explicitly in the reaction search file segment.

With the improved and additional reaction data, you may now conduct more precise reaction searches.

See the table for a list of search fields you may use.

Use the AND operator to combine terms from the Reaction Identification or from the Reaction Identification and Reaction Details search fields.

Use the (P) operator to restrict terms to one reaction detail.

Search fields for reaction data

Reaction Identification Data	Search field
Reaction ID	/RX.ID
Reactant BRN	/RX.RBRN
Reactant	/RX.RCT
Product BRN	/RX.PBRN
Product	/RX.PBRN
Number of Reaction Details	/RX.NVAR

Reaction Details	Search field
Reaction Detail ID	/RX.RID
Reaction Classification	/RX.CL
Number of Stages	/RX.SNR
Stage Reactant	/RX.SRCT
Stage Reactant BRN	/RX.SRBRN
Yield	/RX.YD
Reagent	/RX.RGT
Catalyst	/RX.CAT
Solvent	/RX.SOL
Time	/RX.TIM
Temperature	/RX.T
Pressure	/RX.P
pH Value	/RX.PH
Reaction Type	/RX.TYP
Subject Studied	/RX.SUBJ
Prototype Reaction	/RX.PRT
Other Conditions	/RX.COND
Comment	/RX.COM

Using the (P) operator

```
=> S (DIELS(W)ALDER)/RX.TYP (P) (PREPARATION OR
     MULTISTAGE)/RX.CL (P) H2O/RX.SOL
L1          92 (DIELS(W)ALDER)/RX.TYP (P) (PREPARATION
               OR MULTISTAGE)/RX.CL (P) H2O/RX.SOL

=> D 8 HIT

L1   ANSWER 8 OF 92 BEILSTEIN COPYRIGHT 2002 BEILSTEIN
     CDS MDL

Reaction Details:
RX
     Reaction RID:                 8760756.1
     Reaction Classification:      Preparation
     Reagent:                      Cu(dDP)2
     Solvent:                      H2O
     Temperature:                  25
     Reaction Type:                Diels-Alder reaction
                        .
                        .
                        .
```

To illustrate how a typical reaction search might be conducted, the following is a list of steps to find reactions using a particular substance as a reactant:

1. Search a substance name in the /CN field.
2. Select the Beilstein Record Number (BRN) from the substance answer set.
3. Search the E-number for the extracted BRN in the Reaction Reactant BRN (/RX.RBRN) field.
4. Restrict to a special type of reaction or by another parameter.

An example of a reactant search

```
=> E TRIPHENYL-VINYL-SILANE/CN 5
E1           1     TRIPHENYL-VINYL-PHOSPHONIUM;
                   BROMIDE/CN
E2           1     TRIPHENYL-VINYL-PLUMBANE/CN
E3           1 --> TRIPHENYL-VINYL-SILANE/CN
E4           1     TRIPHENYL-VINYL-STANNANE/CN
E5           1     TRIPHENYL-VINYL-TOSYLAT/CN

=> S E3
L3           1 TRIPHENYL-VINYL-SILANE/CN

=> SELECT L3 1 BRN
E1 THROUGH E1 ASSIGNED

=> S E1/RX.RBRN
L4          62 913423/RX.RBRN

=> S L4 AND (MICHAEL(W)ADDITION)/RX.TYP
         2391 MICHAEL/RX.TYP
        33019 ADDITION/RX.TYP
         1698 (MICHAEL(W)ADDITION)/RX.TYP
L5           2 L4 AND (MICHAEL(W)ADDITION)/RX.TYP

=> D RX 1

L5   ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2002 BEILSTEIN
     CDS MDL

Reaction:
RX
     Reaction ID:                  8796796
     Reactant BRN:                 1863524, 913423
     Reactant:                     2-phenyl-
                                   butyronitrile,
                                   triphenyl-vinyl-
                                   silane
     Product BRN:                  8792635
     Product:                      2-ethyl-2-phenyl-4-
                                   triphenylsilanyl-
                                   butyronitrile
     No. of Reaction Details:      1

Reaction Details:
RX
     Reaction RID:                 8796796.1
     Reaction Classification:      Preparation
     Yield:                        60 percent
                                   (BRN=8792635)
     Reagent:                      t-BuOK
     Solvent:                      dimethylsulfoxide
     Time:                         12 hour(s)
     Temperature:                  40 Cel
     Reaction Type:                Michael addition
     Reference(s):
     1. Bunlaksananusorn, Tanasri; Rodriguez, Alain
     Louis; Knochel, Paul, Chem.Commun.
        , CODEN: CHCOFS(8), <2001>, 745 - 746; BABS-
        6282908
```

EXPAND and search the substance name in the Chemical Name (/CN) field.

SELECT BRN.

Search the E-number in the /RX.RBRN field.

Restrict to a special reaction type in the /RX.TYP field.

Display the reaction information (RX).

Searching for preparation

When searching for preparation, you may also use the Reaction Classification field (RX.CL) to restrict a search to records that focus on a preparative method.

Each reaction is classified in the Reaction Classification field as Preparation, Chemical Behaviour, or Multistage. A reaction is classified as Preparation when the investigation focuses on the preparative method. Chemical Behaviour is assigned when thermodynamic or kinetic aspects of a reaction are emphasized. Multistage reactions are a special type of preparations in which the structures of intermediates are unknown.

An example of a preparation search

```
=> E GALANTHAMINE/CN
E1           1     GALANTERIN/CN
E2           1     GALANTHAMIN/CN
E3           5 --> GALANTHAMINE/CN
E4           1     GALANTHAMINE A-NAPHTYLCARBAMATE/CN
E5           1     GALANTHAMINE 1-D/CN
E6           1     GALANTHAMINE CARBONATE/CN
E7           1     GALANTHAMINE HYDROBROMIDE/CN
E8           1     GALANTHAMINE HYDROCHLORIDE/CN
E9           1     GALANTHAMINE N-BUTYLCARBAMATE/CN
E10          3     GALANTHAMINE N-OXIDE/CN
E11          1     GALANTHAMINE PHENYLCARBAMATE/CN
E12          1     GALANTHAMINE; HYDROBROMIDE/CN

=> S E2-E12 AND RX/FA
       5873847 RX/FA
                 (RX/FA.RX OR REAX/FA)
L1           8 (GALANTHAMIN/CN OR GALANTHAMINE/CN OR
                    .
                    .
                    .
               HYDROBROMIDE"/CN) AND RX/FA

=> SELECT L1 BRN 1-
E1 THROUGH E8 ASSIGNED

=> S E1-E8/RX.PBRN
L2          17 (3787265/RX.PBRN OR 4329423/RX.PBRN OR
               5299810/RX.PBRN OR 583597 8/RX.PBRN OR
               5837313/RX.PBRN OR 5839627/RX.PBRN OR
               8079609/RX.PB RN OR 93736/RX.PBRN)

=> S L2 AND (PREPARATION OR MULTISTAGE)/RX.CL
L3          17 L2 AND (PREPARATION OR MULTISTAGE)/RX.CL

=> D 4

L3   ANSWER 4 OF 17 BEILSTEIN COPYRIGHT 2002 BEILSTEIN
     CDS MDL

Reaction:
RX
     Reaction ID:                  5008528
     Reactant BRN:                 569492
     Reactant:                     6-methoxy-10-methyl-
                                   galantham-1-en-3-one
     Product BRN:                  8079609
     Product:                      galanthamine 1-d
     No. of Reaction Details:      1

Reaction Details:
RX
     Reaction RID:                 5008528.1
     Reaction Classification:      Preparation
     Yield:                        37 percent
                                   (BRN=8079609)
     Reagent:                      NaBD4, CH3OD
     Time:                         1 hour(s)
     Temperature:                  0 - 10 Cel
     Reference(s):
     1. Lee, Thomas B. K.; Goering, Keith E.; Ma,
     Zhenkun, J.Org.Chem., CODEN:
        JOCEAH, 63(13), <1998>, 4535-4538; BABS-6124889
```

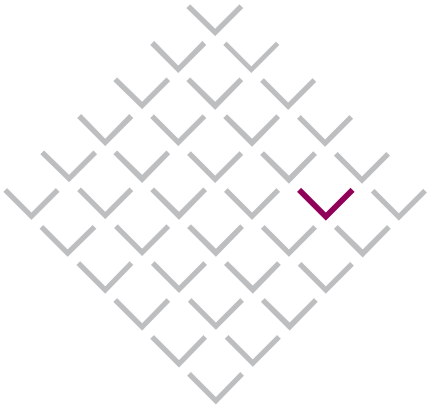
EXPAND the names for the substances of interest.

Search the names for the substances of interest. Combine with RX/FA to require availability of reaction data.

SELECT the BRNs and search the E-numbers in the Product BRN (/RX.PBRN) field.

Refine the results to studies emphasizing preparation.

The default display format in the reaction file segment is QRD which includes Reaction Identification Data and HIT.



Searching bibliographic information

When searching for bibliographic information you can now restrict your search to the reaction or substance search file segment. Simply append the file segment (/XXX.RX or /XXX.SUB) when you search for the following bibliographic information: Author (AU), International Standard Number (ISN), Journal Title (JT) Patent Assignee (PA) and Patent Number (PN). For example, to search an author's name in the reaction file segment, follow the name by /AU.RX. To search an author's name in the substance segment, follow the name by /AU.SUB.

Cost

Enter HELP COST at an arrow prompt in the Beilstein file for information on the cost of displaying records in the file. There are no connect hour charges in the file. There is a charge for each display.

Search for an author's name in a reaction file segment

```
=> S SHARPLESS?/AU.RX
L1        2313 SHARPLESS?/AU.RX
               (SHARPLESS?/AU NOT ALL/FA)

=> D HIT

L1   ANSWER 1 OF 2313 BEILSTEIN COPYRIGHT 2002
     BEILSTEIN CDS MDL

Reaction Details:
RX
     Reaction RID:                 8782653.1
     Reaction Classification:      Preparation
     Reagent:                      NH2NH2*H2O
     Solvent:                      methanol, CHCl3
     Time:                         12 hour(s)
     Temperature:                  20
     Reference(s):
     1. Petrassi, H. Michael; Sharpless, K. Barry;
     Kelly, Jeffery W., Org.Lett.
        , CODEN: ORLEF7, 3(1), <2001>, 139 - 142;
        BABS-6278633
```

For more information

For more information on searching in the reloaded Beilstein file, refer to the revised Beilstein database summary sheet available in print, online in the STNGUIDE file, and on the web at:

http://info.cas.org/ONLINE/DBSS/beilsteinss.html

Enter HELP RXS at an arrow prompt in the Beilstein file for information and examples of reaction searches. Enter HELP PRE at an arrow prompt in the Beilstein file for information on searching for preparation records. Enter HELP DIRECTORY for a complete list of online help messages for the file.

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STNotes

DECEMBER 2002 No. 32

The New BEILSTEIN File on STN - Physical Properties

With the reload of the Beilstein file, searching and displaying of physical property data have improved.

Beilstein, a major structure and factual database, has been reloaded.

STNote 29 - *The New Beilstein File on STN – Reaction Data* focused on how searching and displaying of reaction data have changed as a result of the reload.

This STNote highlights and illustrates the following improvements in searching and displaying of physical properties in the reloaded Beilstein file on STN:

- Additional search fields
- Using Field Availability (/FA)
- Searching Property Hierarchy (/PH)
- Searching property values and conditions
- Searching keywords
- Display enhancements.

In response to customer requests for more detailed information on new and enhanced system features, we have created STNotes. STNotes give you the in-depth technical details you need for efficient use of STN. We hope you find this information useful. Please let us know how we can continue to improve in meeting your technical information needs.

Additional search fields

Data and search fields were added for the following properties in these categories.

Multi-Component Systems properties
- Henry Constant
- Partition Constant Octan-1-ol/Water
- Complex Phase Equilibrium
- Electrical Data
- Optical Data

Safety
- Flash Point

Structure and Energy Parameter
- Conformation

Spectral Data
- Luminescence

Electrical and Magnetic Properties
- Electrical Data
- Magnetic Data

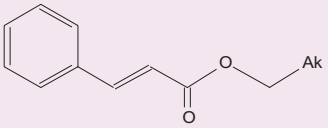
For more in-depth searching of property data, new search fields for existing properties were also added. For example, for ESR data you can now search Coupling Nuclei, Solvents, Temperature and Comment.

Using Field Availability (/FA)

The Field Availability (/FA) index contains all display fields, both names and codes, available in Beilstein. The FA table for a compound lists all data, including all property data, accessible for the compound. The /FA field is very useful when you want to retrieve and display only records with information for a special property.

Find melting points of cinnamic acid alkyl esters.

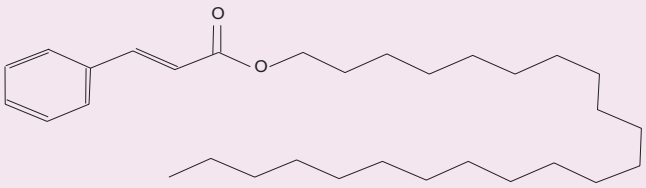
```
L1      STRUCTURE UPLOADED

=> D
L1 HAS NO ANSWERS
L1              STR
```



Draw and upload the structure of cinnamic acid alkyl esters.

```
Structure attributes must be viewed using STN Express
query preparation.


=> S L1 CSS FULL
FULL SEARCH INITIATED 13:13:44 FILE 'BEILSTEIN'
      .
      .
      .
100.0% PROCESSED    34625 ITERATIONS        44 ANSWERS
SEARCH TIME:  00.01.34

L2           44 SEA CSS FUL L1

=> S L2 AND MP/FA
      3992891 MP/FA
L3          11 L2 AND MP/FA

=> D CN STR HIT

L3   ANSWER 1 OF 11 BEILSTEIN COPYRIGHT 2002 BEILSTEIN
     CDS MDL

     Chemical Name (CN):   docosanoic cinnamate
     Autonom Name (AUN):   3-phenyl-acrylic acid docosyl
                            ester
```

Conduct a Closed Substructure Search (CSS) to find cinnamic acid alkyl esters.



Restrict answers to records with available data for Melting Point (MP/FA) .

```
Melting Point:
 Value   |Ref.
 (MP)    |
 (Cel)   |
=========+====
 54 - 56 | 1

Reference(s):
 1. Ruecker, Gerhard; Shenkel, Eloir; Manns, Detlef;
    Falkenberg, Miriam; Marek, Anne, Phytochemistry,
    CODEN: PYTCAS, 41(1), <1996>, 297-300; BABS-6009005
```

Searching Property Hierarchy (/PH)

The Property Hierarchy (/PH) field contains the names and field codes from all chemical and physical property fields as well as all available keywords. Use /PH to search for data without having to know whether the data is in a specific data field or in a keyword field, or which property field contains that data.

Searching property values and conditions

You may use the standard STN numeric operators for searching numeric values. When you search for a numeric value, answers include the exact value plus all ranges that contain the value that you searched. The search for a range retrieves all records in which at least one value of the search range is included in the hit range.

Default units for searching and displaying of physical properties are assumed, unless you change them. To find the default units, refer to the list of search fields on the Beilstein Summary Sheet or enter HELP UNITS at an arrow prompt in the file.

Use the (P) operator to combine a search of property values with corresponding property conditions and to restrict data to the same experiment.

Find substances with quadrupole moment.

```
=> E QUADRUPOLE MOMENT/PH 5
E1       26946     PURIFICATION/PH
E2         401     PVT RELATIONSHIP/PH
E3         196 --> QUADRUPOLE MOMENT/PH
E4         298     RADIAL DISTRIBUTION FUNCTION/PH
E5           3     RADICAL CONTACT SHIFTS/PH

=> S E3
L1         196 "QUADRUPOLE MOMENT"/PH

=> D HIT

L1   ANSWER 1 OF 196 BEILSTEIN COPYRIGHT 2002 BEILSTEIN
     CDS MDL

Dipole Moment:
 Value    | Description       |Ref.
 (DM)     | (.KW)             |
 (D)      |                   |
==========+===================+====
          | Quadrupole moment | 1

Reference(s):
 1. Sham, J.Chem.Phys., CODEN: JCPSA6, 71, <1979>, 3744
```

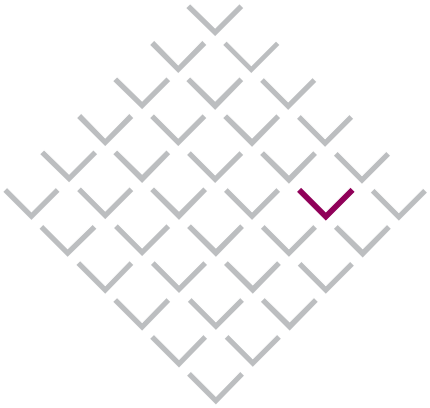
EXPAND on the property of interest in the /PH field.

Quadrupole Moment is a Keyword for the topic Dipole Moment.

Find compounds with a boiling point within the range 99-101 Cel measured at a pressure of 760 Torr.

```
=> S 99-101/BP (P) 760/BP.P
         36402 99 CEL - 101 CEL /BP
         18684 760 TORR /BP.P
L1         436 99 CEL - 101 CEL /BP (P) 760 TORR /BP.P

=> D CN HIT

L1   ANSWER 1 OF 436 BEILSTEIN COPYRIGHT 2002 BEILSTEIN
     CDS MDL

     Chemical Name (CN):       2-bromo-2-chloro-1-
                                difluoromethoxy-
                                1,1-difluoro-ethane
     Autonom Name (AUN):       2-bromo-2-chloro-1-
                                difluoromethoxy-
                                1,1-difluoro-ethane

Boiling Point:
 Value       | Press.      |Ref.
 (BP)        | (.P)        |
 (Cel)       | (Torr)      |
=============+=============+====
 100         | 760         | 1

Reference(s):
 1. Horvath, Ari L., Chemosphere, CODEN: CMSHAF, 44(4),
    <2001>, 897 - 906; BABS-6311562
```

Use the (P) operator to combine property values with property conditions.



Searching keywords

Keywords provide descriptions for the kind of investigation or for the type of data given in the primary literature for a property.

You may now search all keywords for all the properties in the All Keywords (/AKW) field. Because the keywords are present in many data areas, this field offers a simple way to get to the data without knowing which topic contains the wording.

In addition, you may search the keywords for each property by appending .KW to the property search field, e.g., /IR.KW is the field code for keywords associated with IR.

Display enhancements

To make it easier to display information on broad classes of property data, the following formats are available. They contain all the fields associated with the class.

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

Find the keywords associated with /IR.

EXPAND in the field /IR.KW.

```
=> E A/IR.KW 25
**** START OF FIELD ****
E3           0 --> A/IR.KW
E4          89     ANISOTROPY OF IR BANDS/IR.KW
E5     1643784     BANDS/IR.KW
E6          22     FAR IR BANDS/IR.KW
E7          50     FAR IR SPECTRUM/IR.KW
E8         437     FERMI RESONANCE/IR.KW
E9         687     FINE STRUCTURE OF IR BANDS/IR.KW
E10          8     INTENSITY OF FAR IR BANDS/IR.KW
E11       6172     INTENSITY OF IR BANDS/IR.KW
E12          3     INTENSITY OF NEAR IR BANDS/IR.KW
E13     437036     IR/IR.KW
E14         10     IR SECOND MOMENT/IR.KW
E15          1     IR-MICROWAVE DOUBLE RESONANCE/IR.KW
E16         37     LINEWIDTH OF IR BANDS/IR.KW
E17          1     LINEWIDTH OF ROTATIONAL LINES OF IR
                    BANDS/IR.KW
E18         83     NEAR IR BANDS/IR.KW
E19         94     NEAR IR SPECTRUM/IR.KW
E20         28     OVERTONE SPECTRUM/IR.KW
E21        349     POLARIZATION OF IR BANDS/IR.KW
E22        615     REFLECTION SPECTRUM/IR.KW
E23      76608     SPECTRUM/IR.KW
E24         27     VIBRATIONAL ENERGY TRANSFER/IR.KW
E25         12     VIBRATIONAL RELAXATION/IR.KW
**** END OF FIELD ****
```

Cost

Enter HELP COST at an arrow prompt in the Beilstein file for information on the cost of displaying records in the file. There are no connect hour charges in the file. There is a charge for each display.

For more information

For more information on searching and displaying in the reloaded Beilstein file, refer to the revised Beilstein Database Summary Sheet available on the web at:

http://info.cas.org/ONLINE/DBSS/beilstein.html

Enter HELP DIRECTORY at an arrow prompt in the Beilstein file for a complete list of online help messages for the file.

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CAS1782-1202

BEILSTEIN on STN

Workshop Examples

From this document you will learn how to

- ❑ Identify compounds
- ❑ Find reactions
- ❑ Retrieve EcoPharm Information
- ❑ Search for property data

FIZ KARLSRUHE

Workshop Example Questions

1 Search for compounds

1.1 Find the pure compound benzene.
1.2 Find all compositions containing benzene and all compounds including the chemical name segment benzene.
1.3 Search multifragment compounds which contain Au as a single fragment.
1.4 Find C130H172N34O60 hydrochloride.
1.5 Search for all single substances with a molecular weight between 30 and 31.
1.6 How many polymer records are included in the BEILSTEIN file?
1.7 Retrieve all stereoisomers of BRN 8796748.
1.8 Find all organic compounds which contain O and P but no S and N.
1.9 Find organometallic compounds with C, H, and O only, plus an element from group B8, but not Fe.
1.10 Search for a saturated, single halogenated hydrocarbon compound with 10 C.
1.11 Find all available data for the compound with the registry number 6104-58-1.

2 Search for chemical data

2.1 Find compounds purified by recrystallization. (Comment: Consider the spelling of crystallization. Use expand.)
2.2 Find chemical derivatives for ephedrine and the melting point for one of them.
2.3 Where can cytotoxin 5 be isolated form in nature?

3 Search bibliographic data

3.1 Retrieve all citations of Sharpless which contain reaction data.
3.2 Find all publications of Hans Joachim Gais in Tetrahedron Letters.

4 Search reactions

4.1 Find all reactions for prolin-ethyl ester.
4.2 Find all reactions which lead to triphenyl-vinyl-silane.
4.3 Find preparation methods for triphenyl-vinyl-silane.
4.4 Search Diels-Alder reactions in water.
4.5 How reacts acetone to lactic acid?

5 Search EcoPharm data

5.1 Search compounds which have endocrine effects in the environment.

5.2 What are the degradation products of benzo<a>pyrene (BaP) in the environment?

5.3 Find effects of the bioaccumulative substance octachlorostyrene on the food chain.

5.4 Which toxic effects have cytotoxines?

5.5 Is benzene toxic to fish?

5.6 What are the adverse effects of ibuprofen?

5.7 Find information on the effect of malthion, aroclor and DDT on daphnia.

5.8 Find pharmacological data on the effect of cocaine derivatives on macaca species.

6 Search for physical properties

6.1 What is the pK (dissociation exponent) of β-d-glucose (.beta.-d-glucose) in water?

6.2 Does C10H3F8IO4 have a sublimation point?

6.3 Where can you get information on the IR spectrum of 1-Naphtol in KBR?

6.4 Find phthalates with a melting point between 195 and 205 CEL.

6.5 What is the boiling point of nitrofen?

6.6 Find the value for optical rotatory power of (-)-menthol in ethanol. Concentration of the solution should be 1 g/100 ml.

6.7 Find the refractive index of β-citronellol measured at 589 nm and 20 CEL. Find dioxolan derivatives with a density lower than 0.85 g/cm^3.

6.8 Find dioxolan derivatives with a density lower than 0.85 g/cm^3.

Proposed search queries

1 Search for compounds

1.1 => S BENZENE/CN

1.2 => S BENZENE/CNS

1.3 => S AU/FMF

1.4 => S C130H172N34O60.CLH/MF

1.5 => S 30-31/MW AND 1/NF

1.6 => S POLYMER?/CTYPE

1.7 => S 8796748/BRN; D; => S 7444050/CONSID

1.8 => S O/ELS AND P/ELS NOT N/ELS NOT S/ELS

1.9 => S H/ELS AND C/ELS AND O/ELS AND B8/PG NOT FE/ELS AND ELC<=5 AND 1/NF

1.10 => S 10/C (P) 21/H (P) 1/X (P) 3/ELC (P) 32/ATC (Comment: To restrict search terms to the same fragment of multifragment compounds, (P) operator should be employed.)

1.11 => S 6104-58-1/RN; D; D PHARM (Comment: It is advisable to display IDE data first and check for available data in the FA table . " D ALL" can be very expensive depending on the number of data present for a compound.)

2 Search for Chemical Data

2.1 => E RECR/PUR; Search all relevant E-numbers of the expand list.

2.2 => S EPHEDRINE/CN; S L1 AND CDER/FA; D QRD; S 3915113/BRN AND MP/FA (Comment: Chemical derivatives which are used to characterize a compound are indexed as title substances. Search for the BRN of a derivative and restrict to records for which the melting point is given with "MP/FA".)

2.3 => S CYTOTOXIN 5?/CN; S L1 AND INP/FA; D (Comment: For biomolecules, and polymers often the molecular weight is given in the Chemical Name field. That makes the truncation necessary.)

3 Search bibliographic data

3.3 => S SHARPLESS?/AU.RX (Comment: Author Names are indexed as given in the original literature, due to that the spelling may be different. There can be present the whole first name or only the first letter for example. Due to that, truncation is necessary. It is always advisable to look at the expand list.)

3.4 => S GAIS/AU (S) TETRAHEDRON LETT./JT (Comment: Always use the (S)-proximity operator combine different data from one citation.)

4 Search reactions

4.1 => S prolin-ethyl ester/CN; D IDE; D FRX (It is advisable to display IDE data first in order to check that the right compound was retrieved.)

4.2 => S triphenyl-vinyl-silane/CN; D RXPRO

4.3 => S triphenyl-vinyl-silane/CN; SELECT L1 1- RX.PBRN; S E1; S L2 AND PREPARATION/RX.CL.

4.4 => S (DIELS(W)ALDER)/RX.TYP (P) (WATER OR H2O)/RX.SOL (Comment: (P)-proximity operator has to be employed to combine data from one reaction detail.)

4.5

```
=> S ACETONE/CN
L1             2 ACETONE/CN

=> SELECT L1 1- RBN
E1 THROUGH E2 ASSIGNED

=> S E1-2/RX.RBRN
         24083 635680/RX.RBRN
             0 6916792/RX.RBRN
L2       24083 (635680/RX.RBRN OR 6916792/RX.RBRN)

=> S LACTIC ACID/CN
L3             3 LACTIC ACID/CN

=> SELECT L3 1- RBN
E3 THROUGH E5 ASSIGNED

=> S E3-E5/RX.PBRN
           329 1209341/RX.PBRN
           103 1720251/RX.PBRN
             3 5238667/RX.PBRN
L4         428 (1209341/RX.PBRN OR 1720251/RX.PBRN OR 5238667/RX.PBRN)

=> S L2 AND L4
L5             2 L2 AND L4

=> D HIT
```

```
L5   ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2002 BEILSTEIN CDS MDL

Reaction:
RX
     Reaction ID (.ID):              8152705
     Reactant BRN (.RBRN):           635680, 3361712
     Reactant (.RCT):                KMnO4, propan-2-one, 10-bromo-10-(3-bromo-
                                     but-1-enyl)-anthrone
     Product BRN (.PBRN):            3348237, 1209341
     Product (.PRO):                 9-bromo-10-oxo-9,10-dihydro-nthracene- 9- carboxylic
                                     acid, 2-hydroxy-propionic acid
     No. of React. Details (.NVAR):  1
```

5 Search for EcoPharm data

5.1 => S ENDOCRINE/ECTOX.E

5.2 => S BAP/CN

=> D FBIOD, ECDH, ECDP (Hint: Use of the display format “ECO” shows all ecological information including degradation, for one display fee.)

5.3 => S OCTACHLOROSTYRENE/CN AND (BIOACC?)/BIPED; D

5.4 => S CYTOTOXINE?/CN AND PHARM/FA; D

5.5 => S BENZENE/CN AND (TOX?(P)FISH)/ECTOX.E (Comment: If you are not familiar with BEILSTEIN EcoPharm data, use the Basic Index for Pharmacological and Ecological data BIPED. In the example given, you can also search for “(TOX?(P)FISH)” in BIPED. Though searching for it in the “Ecotoxicology Effect” field is more sophisticated.)

5.6 => S IBUPROFEN/CN; S L1 AND PHARM/FA; D 1 2 (Comment: All pharmacological and toxicological information is displayed for one display fee in PHARM.)

5.7 => S malathion/CN or aroclor/CN or DDT/CN AND PHARM/FA; S L2 AND DAPHNIA/ECTOX.SP (Comment: Search for daphnia in BIPED if you are not familiar with the BEILSTEIN field codes.)

5.8 S COCAINE/CNS NOT MIXTURE/CNS AND MACACA/PHARM.SP

6 Search for physical properties

6.1 => S .BETA.-D-GLUCOSE/CN AND DE/FA AND (WATER OR H2O)/DE.SOL

6.2 => S C10H3F8IO4/MF AND SP/FA

6.3 => S 1-NAPHTHOL/CN; S L1 and KBR/IR.SOL AND KBR/IR.COM

6.4 => S PHTHALAT/CNS NOT MIXTURE/CNS AND 1/NF; S L1 AND 195-205/MP

6.5 => S NITROFEN/CN; D BP

6.6 => S “(-)-MENTHOL”/CN; S L1 AND (1 G/100ML/ORP.C (P) ETHANOL/ORP.SOL); D (Comment: ORP.C is no numerical search field. Consider expand list.)

6.7 => S .BETA.-CITRONELLOL/CN AND 589/RI.W (P) 20/RI.T; D (Comment: RI.W and RI.T are numeric search fields. Default unit of RI.W is NM, CEL for RI.T).

6.8 => S DIOXOLAN/CNS AND DEN<0.85. (Comment: g/cm**3 is the default unit for density.)

BEILSTEIN

STN is operated in North America
by Chemical Abstracts Service

STN Database Summary Sheet

BEILSTEIN is a major structure and factual database in organic chemistry. The organic substance records contain the critically reviewed and evaluated documents from the Beilstein Handbook of Organic Chemistry as well as data from 176 leading journals in organic chemistry covering the period from 1779 to the present.

A substance record contains the BEILSTEIN Record Number, the CAS Registry Number®, structure diagram, molecular formula etc., all of which are searchable and displayable. Also searchable and displayable in the BEILSTEIN database is information on physical and chemical data as well as pharmacological and ecological data for a specific substance.

The database is in English, except for some text fields that also contain German terms.

Titles, abstracts, and bibliographic data of the citations in BEILSTEIN, published from 1980 to the present, make the BEILSTEIN Abstracts database (BABS).

Subject Coverage

- Chemical Data
- Electrochemical Behaviour
- Electrical and Magnetic Properties
- Identification of Substance
- Multi-Component Systems
- Optical Properties
- Pharmacological and Ecological Data
- Physical and Mechanical Properties
- Reactions
- Safety Data
- Spectroscopic Data
- State of Aggregation
- Structure and Energy Parameters
- Thermodynamic Properties
- Transport Phenomena

Sources

- Beilstein Handbook of Organic Chemistry
- 176 Organic Chemistry Journals

File Data

- 1779 to the present
- More than 8,128,460 substance records (4/02)
- Updated quarterly
- Automatic current-awareness searches (SDIs) are not available

User Aids

- Building and Searching Structures on STN
- Online Helps (HELP DIRECTORY lists all help messages available)
- STNGUIDE

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April 2002 (Revised)

Search and Display Field Codes

There are no fields that allow left truncation in this file.

Substance Identifying Information

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single words from ADSM.PA **(1)**, ASSM.PA **(1)**, AUN, AZE.PA **(1)**, BSPM.PA **(1)**, CDER **(1)**, CN **(1)**, COMPN **(1)**, CPEM.PA **(1)**, EDM.PA **(1)**, ENEM.PA **(1)**, HHDG.CN **(1)**, INP **(1)**, LLSM.PA **(1)**, LSSM.PA **(1)**, LVSM.PA **(1)**, MECM.PA **(1)**, ODM.PA **(1)**, POT.PRO **(1)**, RSTR.PA **(1)**, SOLM.PA **(1)**, TRAM.PA **(1)**, XREF.CN **(1)** and all Code.KW fields, as well as the Beilstein Record Numbers in ADSM.PABRN, ASSM.PABRN, AZE.PABRN, BRN, BSPM.PABRN, CDER.BRN, COMPBRN, CPEM.PABRN, EDM.PABRN, ENEM.PABRN, FBRN, HHDG.BRN, LLSM.PABRN, LSSM.PABRN, LVSM.PABRN, MECM.PABRN, ODM.PABRN, POT.PBRN, RSTR.PABRN, SOLM.PABRN, TRAM.PABRN, and Beilstein Preferred Registry Number (BPR), and CAS Registry Numbers(RN) and molecular formulas (MF) and fragment molecular formula (FMF))	None (or /BI)	S ETHYL S C106H146O36 S 8086664	ADSM, ASSM, AUN, AZE, BPR, BRN, BSPM, CDER, CN, COMPBRN, COMPN, CPEM, EDM, ENEM, FBRN, FMF, HHDG, INP, LLSM, LSSM, ODM, POT, LVSM, MECM, RSTR.TRAM, RN, STR, SOLM, XREF, CODE **(2)**
Basic Index Pharmacological and Ecological Data (contains single words from all PED fields: BIO, BIOD, COEV, ECDH, ECDP, ECTD, ECTOX, EOD, EXCA, PHARM, and USC)	/BIPED	S (AQUA? TOX?)/BIPED	BIO, BIOD, COEV, ECDH, ECDP, ECTD, ECTOX, EOD, EXCA, PHARM, USC
All Beilstein Record Numbers (BEILSTEIN Record Numbers in ADSM.PABRN, ASSM.PABRN, AZE.PABRN, BIOD.BRN, BRN, BSPM.PABRN, CDER.BRN, COMPBRN, CPEM.PABRN, ECDH.BRN, ECDP.BRN, ECTOX.BRN, EDM.PABRN, ENEM.PABRN, FBRN, HHDG.BRN, LLSM.PABRN, LSSM.PABRN, LVSM.PABRN, MECM.PABRN, ODM.PABRN, PHARM.BRN, POT.PBRN, RSTR.PABRN, SOLM.PABRN, and TRAM.PABRN)	/ABRN	S 1915876/ABRN	ADSM, ASSM, AZE, BIOD, BRN, BSPM, CDER, COMPBRN, CPEM, ECDH, ECDP, ECTOX, EDM, ENEM, FBRN, HHDG, LLSM, LSSM, LVSM, MECM, ODM, PHARM, POT, RSTR, SOLM, TRAM
Beilstein Citation	/BSO	S 3-01-00-00034/BSO	BSO
Beilstein Preferred Registry Number	/BPR	S 106-24-1/BPR	BPR
Beilstein Record Number **(3)**	/BRN	S 1915876/BRN	BRN
CAS Registry Number	/RN	S 100-03-8/RN	RN
Charge **(3)**	/CHA	S -1>CHA	LSF
Chemical Name **(1)**	/CN	S CHOLESTEROL/CN	AUN **(4)**, CN
Chemical Name Segment **(1)**	/CNS	S CHOLESTERYL/CNS	CN
Composition: Component Beilstein Record Number **(3)**	/COMPBRN	S 5811/COMPBRN	COMPBRN
Composition: Component Concentration	/COMPC	S 85?/COMPC	COMPC
Composition: Component Name	/COMPN	S POLYVINYLPYRROLIDONE/COMPN	COMPN
Compound Type	/CTYPE	S ETHYLENE/CNS AND POLYMER?/CTYPE	CTYPE
Constitution ID **(3)**	/CONSID	S 1003/CONSID	CONSID
Data Entry Date	/DED	S 1990?/DED S 2001/07/25/DED	DED

Substance Identifying Information (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Data Update Date	/DUPD	S 2000/10/24/DUPD	DUPD
Element Count (specific) **(3)**	/ELEMENT SYMBOL	S 5/CL	MF
Element Symbol	/ELS	S O/ELS AND SE/ELS	MF
Field Availability **(5)**	/FA	S ISOELECTRIC POINT/FA	FA **(6)**
Field Not Availability	/FNA	S ALCOHOL/CNS AND BP/FNA	Not displayed
File Segment	/FS	S L1 AND STEREO COMPOUND/FS	FS
Fragment Beilstein Record Number **(3)**	/FBRN	S 1073/FBRN	FBRN
Fragment Molecular Formula	/FMF	S C6H12O6/FMF	FMF, MF
Lawson Number **(3)**	/LN	S 22/LN	LN
Linearized Structure Formula	/LSF	S “CH2O(1+)”/LSF	LSF
Molecular Formula	/MF	S C4H9N5.H3O4P/MF	MF
Molecular Weight **(3)** (Formula Weight)	/MW (or /FW)	S 3000<MW	MW
Number of Atoms **(3)**	/ATC	S 34-36/ATC	FMF, MF
Number of Elements **(3)**	/ELC	S 5/C AND 5/ELC	FMF, MF
Number of Fragments **(3)**	/NF	S 3/NF	MF
Periodic Group	/PG	S (A3 AND A6)/PG	Not displayed
Tautomer ID **(3)**	/TAUTID	S 1667788/TAUTID	TAUTID

(1) Contains German text.
(2) Contains all codes with keywords.
(3) Numeric search field that may be searched using numeric operators or ranges.
(4) The CN display field contains, if available, the Chemical Name (CN) and the AUTONOM Name (AUN).
(5) Use to search for all information available for each display field.
(6) DISPLAY FA shows all display field codes available for a record.

Bibliographic information

Search Field Name	Search Code	Search Examples	Display Codes
All Journal Titles (includes titles in JT, and JTW)	/AJT	S IMMUNOCHEMISTRY/AJT	**(1)**
Author **(2)**	/AU	S SHARPLESS?/AU	**(1)**
Country Code	/CC	S GB/CC	Not displayed
Document Type	/DT	S PATENT/DT	Not displayed
International Standard (Document) Number (contains the CODEN) **(2)**	/ISN	S JACSAT/ISN	**(1)**
Journal Review without CODEN	/JTW	S “JOURNAL OF THE SOCIETY OF DYERS AND COLOURISTS”/JTW	**(1)**
Journal Title **(2)**	/JT	S TETRAHEDRON/JT	**(1)**
Language (code and text)	/LA	S JA/LA	Not displayed
Patent Assignee **(2)**	/PA	S BASF/PA	**(1)**
Patent Language (code and text)	/PLA	S EN/PLA	Not displayed
Patent Number **(2)**	/PN	S DE 670683/PN	**(1)**
Patent Year	/PPY	S 1893/PPY	**(1)**
Publication Year	/PY	S JACSAT/CO AND 2000/PY	**(1)**

(1) References are included in the field containing searched term. References may contain a connection to Beilstein Abstracts (BABS) in the form of: BABSNNNNNN. When accessing Beilstein using STN on the Web, this BABS Number is a hyperlink to that reference in BABS. Simply click the number.
(2) To restrict search to bibliographic information in substance documents, append .SUB to the search field code, e.g., /JT.SUB. To restrict search to reaction data, append .RX to the search field code, e.g., /AU.RX.

Chemical Data

Search Field Name	Search Code	Search Examples	Display Codes
Chemical Derivative **(1)**	/CDER	S HYDRAZONE/CDER	CDER
Derivative BRN **(2)**	/CDER.BRN	S 5845535/CDER.BRN	CDER
Derivative Comment **(1)**	/CDER.COM	S BENZIMIDAZOLE/CDER.COM	CDER
Crossfile Reference	/FA	S XREF/FA	XREF
Data Type	/XREF.DTP	S 6279685/BRN AND IR/XREF.DTP	XREF
External Access ID	/XREF.ID	S ALDRICH/XREF.SO AND 250619/XREF.ID	XREF
Name **(1)**	/XREF.CN	S N-BENZOYL-4-PIPERIDONE/XREF.CN	XREF
Other Source	/OS (or XREF.SO)	S MERCK INDEX/OS	XREF
Isolation from Natural Product **(1)**	/INP	S LEAVES/INP	INP
Comment **(1)**	/INP.COM	S DEXTROROTATORY/INP.COM	INP
Purification (method) **(1)**	/PUR	S ALCOHOL/CNS AND ACETYLATION/PUR	PUR
Related Structure **(1)**	/RSTR	S CONSTITUTION/RSTR	RSTR
Comment **(1)**	/RSTR.COM	S HANDBOOK/RSTR.COM	RSTR
Referenced BRN **(2)**	/RSTR.PABRN	S 1581/RSTR.PABRN	RSTR
Referenced Compound **(1)**	/RSTR.PA	S OESTRADIOLDIMETHYLETHER/RSTR.PA	RSTR

(1) Contains German text.
(2) Numeric search field that may be searched using numeric operators or ranges.

Ecological Data

Search Field Name	Search Code	Search Examples	Display Codes
Abiotic Degradation, Hydrolysis	/FA	S ECDH/FA	ECDH
Comment **(1)**	/ECDH.COM	S (FURTHER (W) DEGRADATION(W) PRODUCT?)/ECDH.COM	ECDH
Concentration	/ECDH.C	S 0.21 PPM/ECDH.C	ECDH
Degradation Product **(1)**	/ECDH.DP	S OCTACHLORODIBENZOFURAN/ECDH.DP	ECDH
Degradation Product BRN **(2)**	/ECDH.BRN	S 647116/ECDH.BRN	ECDH
Degradation Rate	/ECDH.D	S 100/ECDH.D	ECDH
Exposure Period	/ECDH.EX	S 24 HOUR?/ECDH.EX	ECDH
Half-life Time	/ECDH.H	S 0.533333 - 16.5/ECDH.H	ECDH
Method, Remarks	/ECDH.MR	S GC/ECDH.MR	ECDH
pH-Value	/ECDH.PH	S 1.01/ECDH.PH	ECDH
Rate Constant	/ECDH.RC	S 1.15 PER HOUR/ECDH.RC	ECDH
Temperature	/ECDH.T	S 10/ECDH.T	ECDH
Type	/ECDH.TYP	S OXIDATION/ECDH.TYP	ECDH
Abiotic Degradation, Photolysis	/FA	S ECDP/FA	ECDP
Comment **(1)**	/ECDP.COM	S (DEGRADATION (W) PRODUCT?)/ECDP.COM	ECDP
Concentration	/ECDP.C	S 5.9 PPM/ECDP.C	ECDP
Degradation Product **(1)**	/ECDP.DP	S HEXACHLOROBENZENE/ECDP.DP	ECDP
Degradation Product BRN **(2)**	/ECDP.BRN	S 1446588/ECDP.BRN	ECDP
Degradation Rate	/ECDP.D	S 80/ECDP.D	ECDP
Exposure Period	/ECDP.EX	S 3 HOUR?/ECDP.EX	ECDP
Half-life Time	/ECDP.H	S 1/ECDP.H	ECDP
Method, Remarks	/ECDP.MR	S H2O2/ECDP.MR	ECDP
pH-Value	/ECDP.PH	S PHOTOOXIDATION/ECDP.TYP AND 2.8/ECDP.PH	ECDP
Rate Constant	/ECDP.RC	S 0.005 - 2.473 min-1/ECDP.RC	ECDP
Temperature	/ECDP.T	S 600/ECDP.T	ECDP
Type	/ECDP.TYP	S PHOTOLYSIS/ECDP.TYP	ECDP
Biodegradation	/FA	S BIOD/FA	BIOD
Comment **(1)**	/BIOD.COM	S (FURTHER (W) DEGRADATION (W) PRODUCT)/BIOD.COM	BIOD
Concentration	/BIOD.C	S 1 G/L/BIOD.C	BIOD
Degradation Product **(1)**	/BIOD.DP	S (CARBOXYLATED (W) ALIPHATIC (W) ALCOHOL)/BIOD.DP	BIOD
Degradation Product BRN **(2)**	/BIOD.BRN	S 8612787/BIOD.BRN	BIOD

Ecological Data (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Degradation Rate	/BIOD.D	S 28 - 36/BIOD.D	BIOD
Exposure Period	/BIOD.EX	S 8 WEEK?/BIOD.EX	BIOD
Half-life Time	/BIOD.H	S 40?/BIOD.H	BIOD
Inoculum	/BIOD.IN	S (ACTIVATED (W) SLUDGE)/BIOD.IN	BIOD
Method, Remarks	/BIOD.MR	S (SEWAGE (W) TREATMENT)/BIOD.MR	BIOD
Temperature	/BIOD.T	S 20/BIOD.T	BIOD
Type	/BIOD.TYP	S AEROBIC/BIOD.TYP	BIOD
Biological Behaviour	/FA	S BIO/FA	BIO
Accumulation Half-Life Time	/BIO.A	S 5 DAY?/BIO.A	BIO
Accumulation Rate Constant	/BIO.AR	S 0.882 PER HOUR/BIO.AR	BIO
Bioconcentration Factor (BCF)	/BIO.BC	S 0.03/BIO.BC	BIO
Biomagnification	/BIO.MAG	S 20/BIO.MAG	BIO
Biomonitoring	/BIO.MON	S LEUKOCYTES/BIO.MON	BIO
Concentration	/BIO.C	S 0.03 - 58 .MY.G/L/BIO.C	BIO
Elimination Rate Constant	/BIO.ER	S 1.1 PER DAY/BIO.ER	BIO
Elimination Half-Life Time	/BIO.H	S 28 DAY?/BIO.H	BIO
Exposure Period	/BIO.EX	S 5 DAY?/BIO.EX	BIO
Log BCF	/BIO.LOG	S CA. 0.5/BIO.LOG	BIO
Media	/BIO.ME	S FOOD/BIO.ME	BIO
Method, Remarks	/BIO.MR	S (FISH (W) BRAIN (W) ACETYLCHOLINESTERASE)/BIO.MR	BIO
Species	/BIO.SP	S (SALMO (W) SOLAR)/BIO.SP	BIO
Temperature **(2,3)**	/BIO.T	S 10-15/BIO.T	BIO
Concentration in Environment	/FA	S COEV/FA	COEV
Background Concentration	/COEV.BC	S (FAT (W) BASIS)/COEV.BC	COEV
Contamination Concentration	/COEV.CC	S 0 - 20.420 MG/KG DRY WT/COEV.CC	COEV
Location	/COEV.LO	S LAKE MICHIGAN/COEV.LO	COEV
Media	/COEV.ME	S TOLUENE/CN AND SOIL/COEV.ME	COEV
Method, Remarks	/COEV.MR	S (FISH? (S) CAPTURE? (S) APRIL (S)1996)/COEV.MR	COEV
Species	/COEV.SP	S FISH/COEV.SP	COEV
Ecological Mobility: Transport and Distribution	/FA	S ECTD/FA	ECTD
Media	/ECTD.ME	S WATER-AL2O3/ECTD.ME	ECTD
Method, Remarks	/ECTD.MR	S (SOLID (W) PHASE (W) EXTRACTION)/ECTD.MR	ECTD
Results	/ECTD.RE	S (SORPTION (W) ISOTHERM)/ECTD.RE	ECTD
Type	/ECTD.TYP	S ADSORPTION/ECTD.TYP	ECTD
Ecotoxicology	/FA	S ECTOX/FA	ECTOX
Comment **(1)**	/ECTOX.COM	S (FURTHER (W) METABOL?)/ECTOX.COM	ECTOX
Concentration	/ECTOX.C	S 3 - 10 .MY.G/L/ECTOX.C	ECTOX
Effect	/ECTOX.E	S ABSORPTION/ECTOX.E	ECTOX
Endpoint of Effect	/ECTOX.EP	S (GROWTH (W) INHIBITION)/ECTOX.EP	ECTOX
Exposure Period	/ECTOX.EX	S 10 DAY?/ECTOX.EX	ECTOX
Further Details	/ECTOX.FD	S TEQ/ECTOX.FD	ECTOX
Kind of Dosing	/ECTOX.KD	S SOIL/ECTOX.KD	ECTOX
Metabolite **(1)**	/ECTOX.META	S TNT/CN AND 4-METHYL-3,5-DINITRO-ANILINE/ECTOX.META	ECTOX
Metabolite BRN **(2)**	/ECTOX.BRN	S 2242347/ECTOX.BRN	ECTOX
Method, Remarks	/ECTOX.MR	S (CHOICE (W) BIOASSAY)/ECTOX.MR	ECTOX
Results	/ECTOX.RE	S (EFFECTS (2W) OVARIES)/ECTOX.RE	ECTOX
Route of Application	/ECTOX.RA	S PERORAL/ECTOX.RA	ECTOX
Sex	/ECTOX.S	S FEMALE/ECTOX.S	ECTOX
Species or Test-System	/ECTOX.SP	S (EISENIA (W) FOETIDA)/ECTOX.SP	ECTOX
Type	/ECTOX.TYP	S LC50/ECTOX.TYP	ECTOX
Value of Type	/ECTOX.V	S CA. 0.2 NKAT/MG PROTEIN/ECTOX.V	
Exposure Assessment	/FA	S EXCA/FA	EXCA
Exposure	/EXCA.HE	S (DISTRIBUTION (S) WATER)/EXCA.HE	EXCA
Sources	/EXCA.SO	S OIL/EXCA.SO	EXCA
Oxygen Demand	/FA	S EOD/FA	EOD
Concentration	/EOD.C	S 1.5 G/EOD.C	EOD
Method, Remarks	/EOD.MR	S (STANDARD(2W)METHOD?)/EOD.MR	EOD
Oxygen Demand	/EOD.D	S 290.7/EOD.D	EOD

Ecological Data (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Ratio BOD5/COD	/EOD.RAT	S 0.98/EOD.RAT	EOD
Related to	/EOD.RE	S DOC/EOD.RE	EOD
Type	/EOD.TYP	S COD/EOD.TYP	EOD
Stability in Soil	/FA	S ECS/FA	ECS
Cation Exchange Rate	/ECS.CE	S “11.45 C MOL (P + T) KG-1"/ECS.CE	ECS
Concentration	/ECS.C	S 50 MG/KG/ECS.C	ECS
Dissipation	/ECS.D	S 33/ECS.D	ECS
Dissipation Time 50	/ECS.5	S 1332/ECS.5	ECS
Dissipation Time 90	/ECS.9	S (25 (W) DAY?)/ECS.9	ECS
Exposure Period	/ECS.EX	S (64 (W) DAY?)/ECS.EX	ECS
Humidity	/ECS.HU	S 0.3 - 2.7 PERCENT/ECS.HU	ECS
Method, Remarks	/ECS.MR	S (SOIL (2W) HOLIDAY (W) BEACH)/ECS.MR	ECS
Microbial Biomass	/ECS.MB	S 9.8E7 CFU/G/ECS.MB	ECS
Organic Carbon	/ECS.OC	S (50 (W) PERCENT)/ECS.OC	ECS
pH-Value **(2)**	/ECS.PH	S 2-5/ECS.PH	ECS
Temperature **(2,3)**	/ECS.T	S 20>ECS.T	ECS
Type	/ECS.TYP	S (SANDY (W) LOAM)/ECS.TYP	ECS

(1) Contains German text.
(2) Numeric search field that may be searched using numeric operators or ranges.
(3) Default unit is Cel.

Laboratory Use and Handling Data

Search Field Name	Search Code	Search Examples	Display Codes
Use of Compound	/FA	S USC/FA	USC
Comment **(1)**	/USC.COM	S LIGHT/USC.COM	USC
Laboratory Use and Handling **(1)**	/USC.LH	S (POLYMERIC (2W) SURFACTANT)/USC.LH	USC
Use Pattern	/USC.PT	S (DETECTION (2W) PENICILLIN (2W)MILK)/USC.PT	USC

(1) Contains German text.

Pharmacological Data

Search Field Name	Search Code	Search Examples	Display Codes
Comment **(1)**	/PHARM.COM	S ANTIFUNGAL/PHARM.COM	PHARM
Concentration	/PHARM.C	S 10 MG/KG/PHARM.C	PHARM
Effect	/PHARM.E	S ACUTE TOXICITY ORAL/PHARM.E	PHARM
Endpoint of Effect	/PHARM.EP	S (CELL (W) DEATH)/PHARM.EP	PHARM
Exposure Period	/PHARM.EX	S YEAR/PHARM.EX	PHARM
Further Details	/PHARM.FD	S ELECTROPHYSIOLOGICAL/PHARM.FD	PHARM
Half-life Time	/PHARM.H	S “2 HOUR(S)”/PHARM.H	PHARM
Kind of Dosing	/PHARM.KD	S DAILY/PHARM.KD	PHARM
Metabolite **(1)**	/PHARM.META	S PYRENE/CN AND PYREN-1-OL/PHARM.META	PHARM
Metabolite BRN **(2)**	/PHARM.BRN	S 8407954/PHARM.BRN	PHARM
Method, Remarks	/PHARM.MR	S (IN (W) VITRO)/PHARM.MR	PHARM
Results	/PHARM.RE	S (DOSE (W) DEPENDEN? AND CYTOTOXICITY)/PHARM.RE	PHARM
Route of Application	/PHARM.RA	S EPICUTANEOUS/PHARM.RA	PHARM
Sex	/PHARM.S	S FEMALE/PHARM.S	PHARM
Species or Test-System	/PHARM.SP	S BACTERIA/PHARM.SP	PHARM
Type	/PHARM.TYP	S BENZENE/CN AND LD50/PHARM.TYP	PHARM
Value of Type	/PHARM.V	S EC50/PHARM.TYP AND 0.1 MG/L/PHARM.V	PHARM

(1) Contains German text.
(2) Numeric search field that may be searched using numeric operators or ranges.

Reaction Data

Search Field Name	Search Code	Search Examples	Display Codes
Reaction Basic Index (contains single words from RX.CAT, RX.CL, RX.COM, RX.PRO, RX.RCT, RX.RGT, RX.SRCT, RX.SUBJ, RX.TYP, as well as reaction BRNs (RX.PBRN, RX.RBRN, and RX.SRBRN)) **(1)**	/BIRX	S CONDENSATION/BIRX	RX
Reaction (includes reactant, reagent, product, subject studied, solvent, catalyst, reaction type, prototype reaction, stage reactant) **(1)**	/RX	S (ACETIC (W) ACID)/RX	RX
All Reaction BRN (includes BRNs from RX.PBRN, RX.RBRN, and RX.SRBRN) **(2)**	/RX.ABRN	S 50000/RX.ABRN	RX
Catalyst **(3)**	/RX.CAT	S SNBR2/RX.CAT	RX
Comment **(1,3)**	/RX.COM	S (CRYSTALLINE (W) SUBSTANCE)/RX.COM	RX
Field Availability Reaction	/FA.RX	S REACTION DOCUMENTS/FA.RX	Not displayed
Number of Reaction Details **(2)**	/RX.NVAR	S 2/RX.NVAR	RX
Number of Stages **(3)**	/RX.SNR	S 2/RX.SNR	RX
Other Conditions **(1,3)**	/RX.COND	S ICEWATER/RX.COND	RX
pH Value **(2,3)**	/RX.PH	S RX.PH<1	RX
Pressure **(2,3,4)**	/RX.P	S 1-25/RX.P	RX
Product **(1)**	/RX.PRO	S “CHLORPROMAZINE N+-GLUCURONIDE CHLORIDE”/RX.PRO	RX
Product BRN **(2)**	/RX.PBRN	S 4885619/RX.PBRN	RX
Prototype Reaction **(3)**	/RX.PRT	S CATALYST?/RX.PRT	RX
Reactant **(1)**	/RX.RCT	S L-PROLINE/RX.RCT	RX
Reactant BRN **(2)**	/RX.RBRN	S 5026/RX.RBRN	RX
Reaction Classification **(3)**	/RX.CL	S (CHEMICAL (W) BEHAVIOUR)/RX.CL	RX
Reaction Details Reaction ID **(3)**	/RX.RID	S 1000.2/RX.RID	RX
Reaction ID **(2)**	/RX.ID	S 5418675/RX.ID	RX
Reaction Type **(3)**	/RX.TYP	S POLYMERIZATION/RX.TYP	RX
Reagent **(1,3)**	/RX.RGT	S ACETONE/RX.RGT	RX
Solvent **(3)**	/RX.SOL	S CH2CL2/RX.SOL	RX
Stage Reactant **(1,3)**	/RX.SRCT	S MALONALDEHYDE/RX.SRCT	RX
Stage Reactant BRN **(2,3)**	/RX.SRBRN	S 742586/RX.SRBRN	RX
Subject Studied **(3)**	/RX.SUBJ	S KINETICS/RX.SUBJ	RX
Temperature **(2,3,5)**	/RX.T	S -100 - -10/RX.T	RX
Time **(3)**	/RX.TIM	S “2.0 HOUR(S)”/RX.TIM	RX
Yield **(2,3,6)**	/RX.YD	S 99.99/RX.YD	RX
Yield Data **(3,6)**	/RX.YDT	S “1 G (BRN=1864069)”/RX.YDT	RX

(1) Contains German text.
(2) Numeric search field that may be searched using numeric operators or ranges.
(3) Reaction Details are included in QRD displays only if a field from the details is a search term.
(4) Default unit is Torr.
(5) Default unit is Cel.
(6) Values given for yield in the /RX.YD and /RX.YDT are identical but the numeric yield field (/RX.YD) does not exist for all reactions.

Property Seach and Display Field Codes

Electrical and Magnetic Properties

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Dielectric Constant **(1)**	none	/DIC	S 2-2.2/DIC	DIC
Comment **(2)**	-	/DIC.COM	S HANDBOOK/DIC.COM	DIC
Frequency **(1)**	Hz	/DIC.F	S 50000/DIC.F	DIC
Temperature **(1)**	Cel	/DIC.T	S 20.5/DIC.T	DIC
Dielectric Static Constant **(1)**	none	/DICS	S 2.3-2.301/DICS	DICS
Comment **(2)**	-	/DICS.COM	S POLARISATION/DICS.COM	DICS
Temperature **(1)**	Cel	/DICS.T	S DICS.T>20	DICS
Electrical Data	-	/FA	S ELE/FA	ELE
Comment **(2)**	-	/ELE.COM	S PHENOL/ELE.COM	ELE
Description	-	/ELE.KW	S PIEZOELECTRICITY/ELE.KW	ELE
Magnetic Data	-	/FA	S MAG/FA	MAG
Comment **(2)**	-	/MAG.COM	S HANDBOOK/MAG.COM	MAG
Description	-	/MAG.KW	S MAGNETIC MOMENT/MAG.KW	MAG
Magnetic Susceptibility **(1)**	cm**3/mol*E6	/MSUS	S 0-410/MSUS	MSUS
Comment **(2)**	-	/MSUS.COM	S RANGE/MSUS.COM	MSUS
Temperature **(1)**	Cel	/MSUS.T	S 20-25/MSUS.T	MSUS

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Contains German text.

Electrochemical Behaviour Properties

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Cross-Section	-	/FA	S XS/FA	XS
Comment **(1)**	-	/XS.COM	S ELEKTRONEN/XS.COM	XS
Description	-	/XS.KW	S COLLISION CROSS-SECTION/XS.KW	XS
Dissociation Exponent (pK) **(2)**	none	/DE	S 1.5-1.55/DE	DE
Comment **(1)**	-	/DE.COM	S HANDBOOK/DE.COM	DE
Method	-	/DE.MET	S CONDUCTOMETRIC/DE.MET	DE
Solvent	-	/DE.SOL	S D2O/DE.SOL	DE
Temperature **(2)**	Cel	/DE.T	S DE.T>180	DE
Type	-	/DE.TYP	S THERMODYNAMIC/DE.TYP	DE
Electrochemical Behaviour	-	/FA	S ELCB/FA	ELCB
Comment **(1)**	-	/ELCB.COM	S GAS/ELCB.COM	ELCB
Description	-	/ELCB.KW	S PROTON AFFINITY/ELCB.KW	ELCB
Electrochemical Characteristics	-	/FA	S POT/FA	POT
Comment **(1)**	-	/POT.COM	S CYCLOVOLTAMMETRY/POT.COM	POT
Description	-	/POT.KW	S OXIDATION POTENTIAL/POT.KW	POT
pH-Value **(2)**	none	/POT.PH	S 1-7/POT.PH	POT
Product	-	/POT.PRO	S PHENYLENEDIAMINE/POT.PRO	POT
Product BRN **(2)**	none	/POT.PBRN	S 2827/POT.PBRN	POT
Solvent	-	/POT.SOL	S METHANOL/POT.SOL	POT
Temperature **(2)**	Cel	/POT.T	S POT.T<-10	POT
Isoelectric Point pH **(2)**	none	/IEP	S IEP>5.5	IEP
Comment **(1)**	-	/IEP.COM	S HANDBOOK/IEP.COM	IEP
Solvent	-	/IEP.SOL	S H2O/IEP.SOL	IEP

(1) Contains German text.
(2) Numeric search field that may be searched using numeric operators or ranges.

Multi-Component Systems (MCS)

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Adsorption (MCS)	-	/FA	S ADSM/FA	ADSM
Comment **(1)**	-	/ADSM.COM	S HANDBOOK/ADSM.COM	ADSM
Description	-	/ADSM.KW	S ENTHALPY OF ADSORPTION/ADSM.KW	ADSM
Partner **(1)**	-	/ADSM.PA	S TRITON X-100/ADSM.PA	ADSM
Partner BRN **(2)**	none	/ADSM.PABRN	S 2343266/ADSM.PABRN	ADSM
Pressure **(2)**	Torr	/ADSM.P	S 0.5-20/ADSM.P	ADSM
Solvent	-	/ADSM.SOL	S H2SO4/ADSM.SOL	
Temperature **(2)**	Cel	/ADSM.T	S 100/ADSM.T	ADSM
Association (MCS)	-	/FA	S ASSM/FA	ASSM
Comment **(1)**	-	/ASSM.COM	S ACIDIC SOLUTION/ASSM.COM	ASSM
Description	-	/ASSM.KW	S ASSOCIATION WITH COMPOUND/ASSM.KW	ASSM
Partner **(1)**	-	/ASSM.PA	S IMIDAZOLE PERCHLORATE/ASSM.PA	ASSM
Partner BRN **(2)**	none	/ASSM.PABRN	S 54438/ASSM.PABRN	ASSM
Pressure **(2)**	Torr	/ASSM.P	S 0.5-1.5/ASSM.P	ASSM
Solvent	-	/ASSM.SOL	S CDCL3/ASSM.SOL	ASSM
Temperature **(2)**	Cel	/ASSM.T	S ASSM.T>100	ASSM
Azeotrope (MCS)	-	/FA	S AZE/FA	AZE
Comment **(1)**	-	/AZE.COM	S HANDBOOK/AZE.COM	AZE
Concentrations	-	/AZE.C	S 60.11 MOL-PERCENT/AZE.C	AZE
Partner **(1)**	-	/AZE.PA	S DODECANE/AZE.PA	AZE
Partner BRN **(2)**	none	/AZE.PABRN	S 1697175/AZE.PABRN	AZE
Pressure **(2)**	Torr	/AZE.P	S 199.8/AZE.P	AZE
Temperature **(2)**	Cel	/AZE.T	S 20-25/AZE.T	AZE
Boundary Surface Phenomena	-	/FA	S BSPM/FA	BSPM
Comment **(1)**	-	/BSPM.COM	S HANDBOOK/BSPM.COM	BSPM
Description	-	/BSPM.KW	S SURFACE TENSION/BSPM.KW	BSPM
Partner **(1)**	-	/BSPM.PA	S METHANOL/BSOM.PA	BSPM
Partner BRN **(2)**	none	/BSPM.PABRN	S 1098229/BSPM.PABRN	BSPM
Pressure **(2)**	Torr	/BSPM.P	S 0-750060/BSPM.P	BSPM
Solvent	-	/BSPM.SOL	S H2O/BSPM.SOL	BSPM
Temperature **(2)**	Cel	/BSPM.T	S 100/BSPM.T	BSPM
Complex Phase Equilibria	-	/FA	S CPEM/FA	CPEN
Comment **(1)**	-	/CPEM.COM	S DEPENDENCE/CPEM.COM	CPEM
Description	-	/CPEM.KW	S PHASE EQUILIBRIUM/CPEM.KW	CPEM
Partner **(1)**	-	/CPEM.PA	S (NAPHTHALENE AND WATER)/CPEM.PA	CPEM
Partner BRN **(2)**	none	/CPEM.PABRN	S 1421310/CPEM.PABRN	CPEM
Pressure **(2)**	Torr	/CPEM.P	S 30000-40000/CPEM.P	CPEM
Solvent	-	/CPEM.SOL	S H2O/CPEM.SOL	CPEM
Temperature **(2)**	Cel	/CPEM.T	S 20/CPEM.T	CPEM
Critical Micelle Concentration **(2)**	g/L	/CMC	S 0.025/CMC	CMC
Comment **(1)**	-	/CMC.COM	S HANDBOOK/CMC.COM	CMC
Solvent	-	/CMC.SOL	S H2O/CMC.SOL	CMC
Temperature **(2)**	Cel	/CMC.T	S 0.025/CMC AND 40/CMC.T	CMC
Electrical Data	-	/FA	S EDM/FA	EDM
Comment **(1)**	-	/EDM.COM	S CONCENTRATION/EDM.COM	EDM
Description	-	/EDM.KW	S DIELECTRIC CONSTANT/EDM.KW	EDM
Partner **(1)**	-	/EDM.PA	S TETRATRIACONTAN-1-OL/EDM.PA	EDM
Partner BRN **(2)**	none	/EDM.PABRN	S 1798829/EDM.PABRN	EDM
Temperature **(2)**	Cel	/EDM.T	S 20-30/EDM.T	EDM
Energy Data (MCS)	-	/FA	S ENEM/FA	ENEM
Comment **(1)**	-	/ENEM.COM	S CYCLOHEXANON/ENEM.COM	ENEM
Description	-	/ENEM.KW	S ENTHALPY OF SOLUTION/ENEM.KW	ENEM
Partner **(1)**	-	/ENEM.PA	S 1,4-DIOXANE/ENEM.PA	ENEM
Partner BRN **(2)**	none	/ENEM.PABRN	S 969148/ENEM.PABRN	ENEM
Pressure **(2)**	Torr	/ENEM.P	S 2-20/ENEM.P	ENEM
Solvent	-	/ENEM.SOL	S TOLUENE/ENEM.SOL	ENEM
Temperature **(2)**	Cel	/ENEM.T	S 25-30/ENEM.T	ENEM

Multi-Component Systems (MCS) (cont'd)

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Henry Constant (MCS) **(2)**	PA*M**3 /MOL	/HNC	S 20-30/HNC	HNC
Comment **(1)**	-	/HNC.COM	S CONSTANT/HNC.COM	HNC
log Henry Constant **(2)**	none	/HNC.LOG	S -5.72/HNC.LOG	HNC
Solvent	-	/HNC.SOL	S H2O/HNC.SOL	HNC
Temperature **(2)**	Cel	/HNC.T	S 25/HNC.T	HNC
Liquid/Liquid System (MCS)	-	/FA	S LLSM/FA	LLSM
Comment **(1)**	-	/LLSM.COM	S HANDBOOK/LLSM.COM	LLSM
Description	-	/LLSM.KW	S LIQUID/LIQUID PHASE DIAGRAM/LLSM.KW	LLSM
Partner	-	/LLSM.PA	S TETRACHLOROMETHANE/LLSM.PA	LLSM
Partner BRN **(2)**	none	/LLSM.PABRN	S 1098295/LLSM.PABRN	LLSM
Pressure **(2)**	Torr	/LLSM.P	S 0-10000/LLSM.P	LLSM
Solvent	-	/LLSM.SOL	S DIMETHYLSULFOXIDE/LLSM.SOL	LLSM
Temperature **(2)**	Cel	/LLSM.T	S 5-10/LLSM.T	LLSM
Liquid/Solid System (MCS)	-	/FA	S LSSM/FA	LSSM
Comment **(1)**	-	/LSSM.COM	S HANDBOOK/LSSM.COM	LSSM
Description	-	/LSSM.KW	S PHASE TRANSITION TEMPERATURE?/LSSM.KW	LSSM
Partner **(1)**	-	/LSSM.PA	S STRYCHNIDIN-10-ONE/LSSM.PA	LSSM
Partner BRN **(2)**	none	/LSSM.PABRN	S 52979/LSSM.PABRN	LSSM
Pressure **(2)**	Torr	/LSSM.P	S 0-20000/LSSM.P	LSSM
Solvent	-	/LSSM.SOL	S NAPHTHALENE/LSSM.SOL	LSSM
Temperature **(2)**	Cel	/LSSM.T	S LSSM.T>200	LSSM
Liquid/Vapour System (MCS)	-	/FA	S LVSM/FA	LVSM
Comment **(1)**	-	/LVSM.COM	S HANDBOOK/LVSM.COM	LVSM
Description	-	/LVSM.KW	S CRITICAL VOLUME/LVSM.KW	LVSM
Partner **(1)**	-	/LVSM.PA	S ACETALDEHYDE/LVSM.PA	LVSM
Partner BRN **(2)**	none	/LVSM.PABRN	S 506007/LVSM.PABRN	LVSM
Pressure **(2)**	Torr	/LVSM.P	S 19000-90000/LVSM.P	LVSM
Solvent	-	/LVSM.SOL	S PROPAN-1-OL/LVSM.SOL	LVSM
Temperature **(2)**	Cel	/LVSM.T	S 120/LVSM.T	LVSM
Mechanical & Physical Property (MCS)	-	/FA	S MECM/FA	MECM
Comment **(1)**	-	/MECM.COM	S DIAGRAM/MECM.COM	MECM
Description	-	/MECM.KW	S ISOTHERMAL COMPRESS?/MECM.KW	MECM
Partner **(1)**	-	/MECM.PA	S OCTAN-1-OL/MECM.PA	MECM
Partner BRN **(2)**	none	/MECM.PABRN	S 1697461/MECM.PABRN	MECM
Pressure **(2)**	Torr	/MECM.P	S 1-10/MECM.P	MECM
Solvent	-	/MECM.SOL	S HCL/MECM.SOL	MECM
Temperature **(2)**	Cel	/MECM.T	S 25-65/MECM.T	MECM
Optical Data (MCS)	-	/FA	S ODM/FA	ODM
Description	-	/ODM.KW	S KERR CONSTANT/ODM.KW	ODM
Partner **(1)**	-	/ODM.PA	S PHENOL/ODM.PA	ODM
Partner BRN **(2)**	none	/ODM.PABRN	S 969616/ODM.PABRN	ODM
Partition octan-1-ol /water (MCS) **(2)**	none	/POW	S 1.5-2/POW	POW
log POW **(2)**	none	/POW.LOG	S -0.9- -0.7/POW.LOG	POW
Temperature **(2)**	Cel	/POW.T	S 20/POW.T	POW
Solubility (MCS) **(2)**	g/L	/SLB	S SLB<0.0001	SLB
Comment **(1)**	-	/SLB.COM	S PH/SLB.COM	SLB
Ratio of Solvents	-	/SLB.RAT	S (6 AND 1)/SLB.RAT	SLB
Saturation	-	/SLB.SAT	S (PURE AND SOLVENT)/SLB.SAT	SLB
Solvent	-	/SLB.SOL	S DIETHYL ETHER/SLB.SOL	SLB
Temperature **(2)**	Cel	/SLB.T	S 10/SLB.T	SLB
Solubility Product (MCS) **(2)**	none	/SLBP	S SLBP<0.00002	SLBP
Comment **(1)**	-	/SLBP.COM	S HANDBOOK/SLBP.COM	SLBP
Ratio of Solvents	-	/SLBP.RAT	S (30 (P) PERCENT)/SLBP.RAT	SLBP
Solvent	-	/SLBP.SOL	S H2O/SLBP.SOL	SLBP

Multi-Component Systems (MCS) (cont'd)

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Temperature **(2)**	Cel	/SLBP.T	S 25/SLBP.T	SLBP
Solution	-	/FA	S SOLM/FA	SOLM
Behaviour (MCS)				
Comment **(1)**	-	/SOLM.COM	S PRESSURE/SOLM.COM	SOLM
Description	-	/SOLM.KW	S MISCIBILITY/SOLM.KW	SOLM
Partner **(1)**	-	/SOLM.PA	S XYLITOL/SOLM.PA	SOLM
Partner BRN **(2)**	none	/SOLM.PABRN	S 2049713/SOLM.PABRN	SOLM
Pressure **(2)**	Torr	/SOLM.P	S 780-850/SOLM.P	SOLM
Solvent	-	/SOLM.SOL	S TETRAHYDROFURAN/SOLM.SOL	SOLM
Temperature **(2)**	Cel	/SOLM.T	S 20/SOLM.T	SOLM
Transport	-	/FA	S TRAM/FA	TRAM
Phenomena (MCS)				
Comment **(1)**	-	/TRAM.COM	S HANDBOOK/TRAM.COM	TRAM
Description	-	/TRAM.KW	S DYNAMIC VISCOSITY/TRAM.KW	TRAM
Partner **(1)**	-	/TRAM.PA	S ETHANOL/TRAM.PA	TRAM
Partner BRN **(2)**	none	/TRAM.PABRN	S 1718733/TRAM.PABRN	TRAM
Pressure **(2)**	Torr	/TRAM.P	S 0-800000/TRAM.P	TRAM
Solvent	-	/TRAM.SOL	S PYRIDINE/TRAM.SOL	TRAM
Temperature **(2)**	Cel	/TRAM.T	S 9.9/TRAM.T	TRAM

(1) Contains German text.
(2) Numeric search field that may be searched using numeric operators or ranges.

Optical Properties

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Circular Dichroism	-	/FA	S CDIC/FA	CDIC
Comment **(1)**	-	/CDIC.COM	S HANDBOOK/CDIC.COM	CDIC
Solvent	-	/CDIC.SOL	S CHCL3/CDIC.SOL	CDIC
Mutarotation **(2)**	deg	/MUT	S 10-20/MUT	MUT
Comment **(1)**	-	/MUT.COM	S HANDBOOK/MUT.COM	MUT
Concentration	-	/MUT.C	S 0.7 G/100ML/MUT.C	MUT
Length of Path **(2)**	cm	/MUT.LEN	S MUT.LEN>10	MUT
Solvent	-	/MUT.SOL	S H2O/MUT.SOL	MUT
Temperature **(2)**	Cel	/MUT.T	S 21/MUT.T	MUT
Time	-	/MUT.TIM	S 1 DAY?/MUT.TIM	MUT
Type	-	/MUT.TYP	S M/MUT.TYP	MUT
Wavelength **(2)**	nm	/MUT.W	S 589/MUT.W	MUT
Optical Rotatory Dispersion	-	/FA	S ORD/FA	ORD
Comment **(1)**	-	/ORD.COM	S CYCLOHEXANOL/ORD.COM	ORD
Solvent	-	/ORD.SOL	S ETHANOL/ORD.SOL	ORD
Optical Rotatory Power **(2)**	deg	/ORP	S 39.65-40/ORP	ORP
Comment **(1)**	-	/ORP.COM	S ACETAMIDE/ORP.COM	ORP
Concentration	-	/ORP.C	S 1 MOL/L/ORP.C	ORP
Length of Path **(2)**	cm	/ORP.LEN	S 10/ORP.LEN	ORP
Solvent	-	/ORP.SOL	S BENZENE/ORP.SOL	ORP
Temperature **(2)**	Cel	/ORP.T	S 20/ORP.T	ORP
Type	-	/ORP.TYP	S ALPHA/ORP.TYP	ORP
Wavelength **(2)**	nm	/ORP.W	S 578/ORP.W	ORP
Optics	-	/FA	S OPT/FA	OPT
Comment **(1)**	-	/OPT.COM	S ACETON/OPT.COM	OPT
Description	-	/OPT.KW	S LINEAR DICHROISM/OPT.KW	OPT
Refractive Index **(2)**	none	/RI	S 1.00056/RI	RI
Comment **(1)**	-	/RI.COM	S HANDBOOK/RI.COM	RI
Temperature **(2)**	Cel	/RI.T	S 0/RI.T	RI
Wavelength **(2)**	nm	/RI.W	S 586/RI.W	RI

(1) Contains German text.
(2) Numeric search field that may be searched using numeric operators or ranges.

Physical and Mechanical Properties

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Acoustic Property	-	/FA	S SOUND/FA	SOUND
Comment **(1)**	-	/SOUND.COM	S HANDBOOK/SOUND.COM	SOUND
Description	-	/SOUND.KW	S VELOCITY OF SOUND/SOUND.KW	SOUND
Compressibility	-	/FA	S CMP/FA	CMP
Comment **(1)**	-	/CMP.COM	S HANDBOOK/CMP.COM	CMP
Description	-	/CMP.KW	S ADIABATIC COMPRESSIBILITY/CMP.KW	CMP
Further Information **(2)** (Physical and Chemical Properties)	-	/FA	S FINFO/FA	FINFO
Liquid Density **(3)**	g*cm**3	/DEN	S 1/DEN	DEN
Comment **(1)**	-	/DEN.COM	S ALCOHOL/DEN.COM	DEN
Measurement Temperature **(3)**	Cel	/DEN.T	S 20/DEN.T	DEN
Reference Temperature **(3)**	Cel	/DEN.RT	S 10/DEN.RT	DEN
Mechanical Property	-	/FA	S MEC/FA	MEC
Comment **(1)**	-	/MEC.COM	S HANDBOOK/MEC.COM	MEC
Description	-	/MEC.KW	S VISCOSITY/MEC.KW	MEC
Surface Tension **(3)**	g/s**2	/ST	S 1.9-2/ST	ST
Comment **(1)**	-	/ST.COM	S HANDBOOK/ST.COM	ST
Temperature **(3)**	Cel	/ST.T	S 20-22/ST.T	ST

(1) Contains German text.
(2) Field contains citations concerning physical and chemical properties not covered in detail in BEILSTEIN.
(3) Numeric search field that may be searched using numeric operators or ranges.

Safety Data

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Autoignition Temperature	-	/FA	S AIT/FA	AIT
Temperature **(1)**	Cel	/AIT.T	S 430 CEL/AIT.T	AIT
Flash Point	-	/FA	S FP/FA	FP
Temperature **(1)**	Cel	/FP.T	S 105/FP.T	FP
Type of Test	-	/FP.TYP	S DIN/FP.TYP	FP

1) Numeric search field that may be searched using numeric operators or ranges.

Spectroscopic Data

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
ESR Data	-	/FA	S ESR/FA	ESR
Comment **(1)**	-	/ESR.COM	S (INORGANIC AND COMPOUNDS/ESR.COM	ESR
Coupling Nuclei	-	/ESR.NUI	S 2D/ESR.NUI	ESR
Description	-	/ESR.KW	S SPECTRUM/ESR.KW	ESR
Solvents	-	/ESR.SOL	S CH2CL2/ESR.SOL	ESR
Temperature **(2)**	Cel	/ESR.T	S 19-20/ESR.T	ESR
Fluoroscence	-	/FA	S FLU/FA	FLU
Comment **(1)**	-	/FLU.COM	S HANDBOOK/FLU.COM	FLU
Description	-	/FLU.KW	S MAXIMA/FLU.KW	FLU
Solvent	-	/FLU.SOL	S ACETONITRILE/FLU.SOL	FLU
Temperature **(2)**	Cel	/FLU.T	S 25/FLU.T	FLU

Spectroscopic Data (cont'd)

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Infrared Spectrum	-	/FA	S IR/FA	IR
Comment **(1)**	-	/IR.COM	S PH/IR.COM	IR
Description	-	/IR.KW	S FINE STRUCTURE OF IR BANDS/IR.K	IR
Solvent	-	/IR.SOL	S CHCL3/IR.SOL	IR
Temperature **(2)**	Cel	/IR.T	S IR.T>50	IR
Luminescence	-	/FA	S LUM/FA	LUM
Comment **(1)**	-	/LUM.COM	S (TEMPERATURE AND DEPENDE?)/LUM.COM	LUM
Description	-	/LUM.KW	S LUMINESCENCE QUENCHING/LUM.KW	LUM
Mass Spectrum	-	/FA	S MS/FA	MS
Comment **(1)**	-	/MS.COM	S METASTABLE/MS.COM	MS
Description	-	/MS.KW	S FRAGMENTATION PATTERN/MS.KW	MS
Nuclear Magnetic Resonance	-	/FA	S NMR/FA	NMR
Comment **(1)**	-	/NMR.COM	S (AMBIENT AND TEMPERATURE)/NMR.COM	NMR
Coupling Nuclei	-	/NMR.NUI	S (1H and 13C)/NMR.NUI	NMR
Description	-	/NMR.KW	S 2D-NMR/NMR.KW	NMR
Frequency **(2)**	MHz	/NMR.F	S 50/NMR.F	NMR
Nucleus	-	/NMR.NUC	S 31P/NMR.NUC	NMR
Solvents	-	/NMR.SOL	S CDCL3/NMR.SOL	NMR
Temperature **(2)**	Cel	/NMR.T	S 20-22/NMR.T	NMR
Nuclear Quadrupole Resonance	-	/FA	S NQR/FA	NQR
Comment **(1)**	-	/NQR.COM	S (NQR AND ABSORPTION)/NQR.COM	NQR
Description	-	/NQR.KW	S NUCLEAR QUADRUPOLE RESONANCE/NQR.KW	NQR
Nucleus	-	/NQR.NUC	S 35CL/NQR.NUC	NQR
Other Spectroscopic Methods	-	/FA	S OSM/FA	OSM
Comment **(1)**	-	/OSM.COM	S SHIFTS/OSM.COM	OSM
Description	-	/OSM.KW	S PHOTOELECTRON SPECTRUM/OSM.KW	OSM
Phosphorescence	-	/FA	S PHO/FA	PHO
Comment **(1)**	-	/PHO.COM	S HANDBOOK/PHO.COM	PHO
Description	-	/PHO.KW	S TRIPLET STATE LIFETIME/PHO.KW	PHO
Solvent	-	/PHO.SOL	S ETHANOL/PHO.SOL	PHO
Temperature **(2)**	Cel	/PHO.T	S 25/PHO.T	PHO
Raman Spectrum	-	/FA	S RAS/FA	RAS
Comment **(1)**	-	/RAS.COM	S (GASEOUS AND MATRIX)/RAS.COM	RAS
Description	-	/RAS.KW	S RAMAN INTENSITIES/RAS.KW	RAS
Solvent	-	/RAS.SOL	S KBR/RAS.SOL	RAS
Rotational Spectrum	-	/FA	S ROT/FA	ROT
Comment **(1)**	-	/ROT.COM	S ROTATIONSDISPERSION/ROT.COM	ROT
Description	-	/ROT.KW	S ROTATIONAL SPECTRUM/ROT.KW	ROT
UV and Visible Spectrum	-	/FA	S UVS/FA	UVS
Absorption Maxima **(2)**	nm	/UVS.AM	S 139-139.1/UVS.AM	UVS
Comment **(1)**	-	/UVS.COM	S (ACIDIC AND SOLUTION)/UVS.COM	UVS
Description	-	/UVS.KW	S ABSORPTION MAXIMA/UVS.KW	UVS
Ext./Abs. Coef. **(2)**	1/MOL*CM	/UVS.EAC	S 4.4/UVS.EAC	UVS
Solvent	-	/UVS.SOL	S CYCLOHEXANE/UVS.SOL	UVS

(1) Contains German text.
(2) Numeric search field that may be searched using numeric operators or ranges.

BEILSTEIN

State of Aggragation - Crystals

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Crystal Density **(1)**	g/cm**3	/CDEN	S 5-5.1/CDEN	CDEN
Comment **(2)**	-	/CDEN.COM	S ORTHORHOMBISCH?/CDEN.COM	CDEN
Temperature **(1)**	Cel	/CDEN.T	S 293 K/CDEN.T	CDEN
Crystal Phase	-	/FA	S CRYPH/FA	CRYPH
Comment **(2)**	-	/CRYPH.COM	S ANISOTROPIC/CRYPH.COM	CRYPH
Description	-	/CRYPH.KW	S CRYSTAL STRUCTURE?/CRYPH.KW	CRYPH
Temperature **(1)**	Cel	/CRYPH.T	S 14.85/CRYPH.T	CRYPH
Crystal Property Description: Colour + Other Properties **(2)**	-	/CPD	S GLAS?/CPD	CPD
Comment **(2)**	-	/CPD.COM	S HANDBOOK/CPD.COM	CPD
Crystal Space Group	-	/CSG	S P212121/CSG	CSG
Comment **(2)**	-	/CSG.COM	S HANDBOOK/CSG.COM	CSG
Crystal System	-	/CSYS	S MONOCLINIC/CSYS	CSYS
Comment **(2)**	-	/CSYS.COM	S (LABILE AND FORM)/CSYS.COM	CSYS
Crystal Transition Point **(1)**	Cel	/CTP	S 100.05-100.1/CTP	CTP
Change of Modification	-	/CTP.CM	S GLASS/CTP.CM	CTP
Comment **(2)**	-	/CTP.COM	S HANDBOOK/CTP.COM	CTP
Decomposition Point **(1)**	Cel	/DP	S 0-10/DP	DP
Comment **(2)**	-	/DP.COM	S CRYSTALLIZATION/DP.COM	DP
Solvent	-	/DP.SOL	S PROPAN-2-OL/DP.SOL	DP
Melting Point **(1)**	Cel	/MP	S 250-260/MP	MP
Comment **(2)**	-	/MP.COM	S DECOMPOSITION/MP.COM	MP
Solvent	-	/MP.SOL	S XYLENE/MP.SOL	MP
Sublimation Point **(1)**	Cel	/SP	S SP>=500	SP
Comment **(2)**	-	/SP.COM	S (MELTING AND FORM)/SP.COM	SP
Pressure **(1)**	Torr	/SP.P	S 1/SP.P	SP
Triple Point **(1)**	Cel	/TP	S 218.85/TP	TP
Comment **(2)**	-	/TP.COM	S BAR/TP.COM	TP

State of Aggragation - Liquids

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Boiling Point **(1)**	Cel	/BP	S BP> 200	BP
Comment **(2)**	-	/BP.COM	S BADTEMPERATUR/BP.COM	BP
Pressure **(2)**	Torr	/BP.P	S 1/BP.P	BP
Liquid Phase	-	/FA	S LIQPH/FA	LIQPH
Comment **(2)**	-	/LIQPH.COM	S AETHANOL/LIQPH.COM	LIQPH
Description	-	/LIQPH.KW	S SELF-ASSOCIATION IN SOLUTION/LIQPH.KW	LIQPH
Transition Point of Liquid Modification **(1)**	Cel	/LPTP	S 20/LPTP	LPTP
Change of Modification	-	/LPTP.CM	S (NEMATIC AND ISOTROPIC)/LPTP.CM	LPTP
Comment **(2)**	-	/LPTP.COM	S HANDBOOK/LPTP.COM	LPTP

State of Aggragation - Gases

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Critical Density **(1)**	g/cm**3	/CRD	S 0.2-0.2022/CRD	CRD
Comment **(2)**	-	/CRD.COM	S HANDBOOK/CRD.COM	CRD
Critical Pressure **(1)**	Torr	/CRP	S CRP >760 MBAR	CRP
Comment **(2)**	-	/CRP.COM	S HANDBOOK/CRP.COM	CRP
Critical Temperature **(1)**	Cel	/CRT	S 500-600/CRT	CRT
Comment **(2)**	-	/CRT.COM	S HANDBOOK/CRT.COM	CRT

State of Aggragation - Gases (cont'd)

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Critical Volume **(1)**	cm**3/mol	/CRV	S 210/CRV	CRV
Comment **(2)**	-	/CRV.COM	S HANDBOOK/CRV.COM	CRV
Gas Phase	-	/FA	S GP/FA	GP
Comment **(2)**	-	/GP.COM	S (SATURATED AND LIQ?)/GP.COM	GP
Description		/GP.KW	S FUGACITY/GP.KW	GP
Vapour Pressure **(1)**	Torr	/VP	S 4-5/VP	VP
Comment **(2)**	-	/VP.COM	S EQUATION/VP.COM	VP
Temperature **(1)**	Cel	/VP.T	S VP>80 and VP.T<5	VP

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Contains German text.

Structure and Energy Parameters

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Conformation	-	/FA	S CNF/FA	CNF
Object of Investigation	-	/CNF.OBJ	S CONFORMER EQUILIBRIUM/CNF.OBJ	CNF
Dipole Moment **(1)**	D	/DM	S 1-1.22/DM	DM
Comment **(2)**	-	/DM.COM	S CONCENTRATION/DM.COM	DM
Description	-	/DM.KW	S QUADRUPOLE MOMENT/DM.KW	DM
Method	-	/DM.MET	S DIELECTRIC/DM.MET	DM
Solvent	-	/DM.SOL	S CCL4/DM.SOL	DM
Temperature **(1)**	Cel	/DM.T	S 20>DM.T	DM
Electrical Polarizability	-	/FA	S POL/FA	POL
Comment **(2)**	-	/POL.COM	S (TIME AND DEPENDENCE)/POL.COM	POL
Description	-	/POL.KW	S ELECTRON POLARIZATION/POL.KW	POL
Electron Binding	-	/FA	S CIP/FA	CIP
Comment **(2)**	-	/CIP.COM	S (EXCITED AND STATE)/CIP.COM	CIP
Description	-	/CIP.KW	S ELECTRON AFFINITY/CIP.KW	CIP
Energy Barrier of Conformation **(1)**	J/mol	/EBC	S 1000<=EBC	EBC
Barrier Type	-	/EBC.TYP	S CF3/EBC.TYP	EBC
Comment **(2)**	-	/EBC.COM	S ROTATION/EBC.COM	EBC
Solvent	-	/EBC.SOL	S TOLUENE/EBC.SOL	EBC
Energy of Dissociation **(1)**	J/mol	/EDIS	S 12000-14000/EDIS	EDIS
Bond Type	-	/EDIS.TYP	S (P AND H)/EDIS.TYP	EDIS
Comment **(2)**	-	/EDIS.COM	S DISSOZIATIONSENERGIE/EDIS.COM	EDIS
Interatomic Distance and Angle	-	/FA	S GEO/FA	GEO
Comment **(2)**	-	/GEO.COM	S METHOD/GEO.COM	GEO
Description	-	/GEO.KW	S “INTERATOMIC DISTANCES AND ANGLES”/GEO.KW	GEO
Ionization Potential **(1)**	eV	/IP	S 7-8/IP	IP
Comment **(2)**	-	/IP.COM	S VERTICAL/IP.COM	IP
Method	-	/IP.MET	S PHOTOIONIZATION/IP.MET	IP
Molecular Deformation	-	/FA	S DFM/FA	DFM
Comment **(2)**	-	/DFM.COM	S ACETONITRIL?/DFM.COM	DFM
Description	-	/DFM.KW	S FORCE CONSTANTS/DFM.KW	DFM

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Contains German text.

Thermodynamic Properties

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Enthalpy of Combustion **(1)**	J/mol	/HCOM	S HCOM>-100000	HCOM
Comment **(2)**	-	/HCOM.COM	S HANDBOOK/HCOM.COM	HCOM
Pressure **(1)**	Torr	/HCOM.P	S 760/HCOM.P	HCOM
Temperature **(1)**	Cel	/HCOM.T	S 25/HCOM.T	HCOM
Enthalpy of Formation **(1)**	J/mol	/HFOR	S 808052/HFOR	HFOR
Comment **(2)**	-	/HFOR.COM	S HANDBOOK/HFOR.COM	HFOR
Pressure **(1)**	Torr	/HFOR.P	S 759-761/HFOR.P	HFOR
Temperature **(1)**	Cel	/HFOR.T	S HFOR.T<10	HFOR
Enthalpy of Fusion **(1)**	J/mol	/HFUS	S 1000-2000/HFUS	HFUS
Comment **(2)**	-	/HFUS.COM	S HANDBOOK/HFUS.COM	HFUS
Enthalpy of Hydrogenation **(1)**	J/mol	/HHDG	S 153362/HHDG	HHDG
Comment **(2)**	-	/HHDG.COM	S HANDBOOK/HHDG.COM	HHDG
Product BRN **(1)**	none	/HHDG.BRN	S 1862856/HHDG.BRN	HHDG
Product Name **(2)**	-	/HHDG.CN	S PHENYL-CYCLOOCTANE/HHDG.CN	HHDG
Temperature **(1)**	Cel	/HHDG.T	S 24.9/HHDG.T	HHDG
Enthalpy of Phase Transitions **(1)**	J/mol	/HPT	S 650-700/HPT	HPT
Comment **(2)**	-	/HPT.COM	S (HEXAGONAL AND CUBIC)/HPT.COM	HPT
Enthalpy of Sublimation **(1)**	J/mol	/HSUB	S HSUB<40000	HSUB
Comment **(2)**	-	/HSUB.COM	S HANDBOOK/HSUB.COM	HSUB
Temperature **(1)**	Cel	/HSUB.T	S 25/HSUB.T	HSUB
Enthalpy of Vaporization **(1)**	J/mol	/HVAP	S 90000>HVAP	HVAP
Comment **(2)**	-	/HVAP.COM	S HANDBOOK/HVAP.COM	HVAP
Pressure **(1)**	Torr	/HVAP.P	S 250>HVAP.P	HVAP
Temperature **(1)**	Cel	/HVAP.T	S 20-25/HVAP.T	HVAP
Heat Capacity (CP) **(1)**	J/mol*K	/CP	S 500-501/CP	CP
Comment **(2)**	-	/CP.COM	S HANDBOOK/CP.COM	CP
Temperature **(1)**	F	/CP.T	S CP.T>500	CP
Heat Capacity (CP0) **(1)**	J/mol*K	/CP0	S 200>CP0	CP0
Comment **(2)**	-	/CP0.COM	S DETERMIN?/CP0.COM	CP0
Temperature **(1)**	Cel	/CP0.T	S 200-220/CP0.T	CP0
Heat Capacity (CV) **(1)**	J/mol*K	/CV	S 113/CV	CV
Comment **(2)**	-	/CV.COM	S HANDBOOK/CV.COM	CV
Temperature **(1)**	Cel	/CV.T	S 113/CV.T AND 25/CP	CV
Other Thermochemical Data	-	/FA	S OTHE/FA	OTHE
Comment **(2)**	-	/OTHE.COM	S HANDBOOK/OTHE.COM	OTHE
Description	-	/OTHE.KW	S HEAT OF COMBUSTION AT CONSTANT VOLUME/OTHE.KW	OTHE

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Contains German text.

Transport Phenomena

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Bulk Viscosity **(1)**	g/cm*s	/BV	S 52-54/BV	BV
Comment **(2)**	-	/BV.COM	S CONCENTRATION/BV.COM	BV
Temperature **(1)**	Cel	/BV.T	S 40-60/BV.T	BV
Dynamic Viscosity **(1)**	g/cm*s	/DV	S 1.58-1.59/DV	DV
Comment **(2)**	-	/DV.COM	S RANGE/DV.COM	DV
Temperature **(1)**	Cel	/DV.T	S 20/DV.T	DV
Kinematic Viscosity **(1)**	cm**2/s	/KV	S 1.9988-1.9999/KV	KV
Comment **(2)**	-	/KV.COM	S HANDBOOK/KV.COM	KV
Temperature **(1)**	Cel	/KV.T	S 10/KV.T	KV

Transport Phenomena (cont'd)

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Self-Diffusion Coefficient **(1)**	cm**2/s	/SDIF	S SDIF>=25	SDIF
Comment **(2)**	-	/SDIF.COM	S HANDBOOK/SDIF.COM	SDIF
Temperature **(1)**	Cel	/SDIF.T	S 100/SDIF.T	SDIF
Transport Data	-	/FA	S TRAN/FA	TRAN
Comment **(2)**	-	/TRAN.COM	S PRESSURE/TRAN.COM	TRAN
Description	-	/TRAN.KW	S THERMAL CONDUCTIVITY/TRAN.KW	TRAN

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Contains German text.

Structure Search

Structure Search Terms

Terms	Search Examples
L-number of a structure built using the STRUCTURE command or uploaded from STN Express (Boolean logic allowed between the L-numbers) **(1)**	SEARCH L1 CSS FUL S L1 NOT L2
L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers) **(1)**	S L3 OR L4
L-numbers of structures built using the STRUCTURE command or uploaded from STN Express combined with L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers) **(1)**	S L1 NOT L3

(1) The L-number answer set from a structure search may be combined with dictionary or factual terms, e.g., S L1 AND AMINO or S L3 AND IR?/FA.

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Substructure (default)	Search for substances that match the query. Substitution is allowed at all open positions.	SSS	SEARCH L1 SSS FUL S L2 OR L3 SSS SAM S L7 SSS RAN
Closed	Search for substances that match the query	CSS	SEARCH L1 CSS FUL
Substructure	exactly. Substitution is allowed at positions opened by CONNECT.		S L2 OR L3 CSS S L4 NOT L5 CSS RAN
Family	Search for substances that match the query exactly. Additional components may be retrieved.	FAM	S L6 FAM FUL
Exact	Search for substances that match the query exactly.	EXA	SEA L5 EXA FUL

Scopes of Structure Searches

Type	Definition	Search Code	Search Examples
Sample (default)	Search a fixed 5% of the file.	SAM	SEARCH L3 EXA SAM S L6 NOT L7 SSS SAM
Full	Search 100% of the file.	FUL	S L5 OR L8 SSS FUL
Range	Search a user-specified portion of the file.	RAN	S L4 RAN=(5471081,) S L3 FAM RAN=(77542,80001)
Subset Sample	Search a fixed sample of an answer set created by a search in BEILSTEIN.	SUB SAM	S L7 CSS SUB=L5 SAM
Subset Range	Search a user-specified portion of an answer set created by a search in BEILSTEIN.	SUB RAN	S L3 SUB=L2 RAN=(,72810)
Subset Full	Search 100% of an answer set created by a search in BEILSTEIN.	SUB FUL	S L8 SUB=L6 FAM FUL

DISPLAY and PRINT Formats

Any combination of formats may be used to display or print answers. Multiple codes must be separated by commas or spaces. The fields are displayed or printed in the order requested.

Hit-term highlighting is available for BRN, BSO, CN, COMPBRN, COMPC, COMPN, CONSID, CTYPE, DED, DUPD, FBRN, FMF, FS, FW, LN, LSF, MF, RN, and TAUTID. Highlighting must be ON during SEARCH in order to use the HIT format.

Substance data and reactions are located in different file segments. After searching for a substance or for substance data, two options are available for displaying the reaction information directly related to the substance searched. RX is used to the display all reactions, regardless of search terms.

1. RXPRO - to display the reactions with the substance as the reaction product
2. RXREA - to display the reactions with the substance as a reactant

For cost information, see HELP COST.

Format	Content	Examples
ADSM	Adsorption (MCS) (Description, Partner Beilstein Record Number, Partner, Solvent, Temperature, Pressure, Notes, References)	D ADSM
AIT	Autoignition Temperature (table containing Temperature, References)	D L3 AIT
ASSM	Association (MCS) (Description, Partner Beilstein Record Number, Partner, Solvent, Temperature, Pressure, Notes, References)	D ASSM
AUN	Autonom Name	D AUN
AZE	Azeotropes (MCS) (table containing Value, Temperature, Pressure, Concentration, and Azeotrope BRN, References, Notes)	D AZE
BIO	Biological Behaviour (Species, Media, Concentration, Exposure Period, Temperature, Log BCF, Bioconcentration Factor (BCF), Accumulation Half-Life Time, Accumulation Rate Constant, Elimination Half-Life Time, Elimination Rate Constant, Method, Remarks, Biomagnification, Notes, References)	D BIO
BIOD	Biodegradation (Type, Inoculum, Concentration, Degradation Product BRN, Degradation Rate, Exposure Period, Temperature, Half-Life Time Method, Remarks, Notes, References)	D 3 BIOD
BP	Boiling Point (table containing Value, Pressure, References, Notes)	D L3 BP
BPR	Beilstein Preferred Record Number	D BPR
BRN	Beilstein Record Number	D BRN
BSO	Beilstein Citation	D BSO
BSPM	Boundary Surface Phenomena (MCS) (Description, Partner Beilstein Record Number, Partner, Solvent, Temperature, Pressure, Notes, References)	D BSPM

DISPLAY and PRINT Formats (cont'd)

Format	Content	Examples
BV	Bulk Viscosity (table containing Value, Temperature, References, Notes)	D BV
CDEN	Density of the Crystal (table containing Value, Temperature, References, Notes)	D CDEN
CDER	Chemical Derivative (Derivative BRN, Derivative, Notes, References)	D CDER
CDIC	Circular Dichroism (Solvent, Notes, References)	D L1 CDIC
CIP	Electron Binding (Description, Notes, References)	D CIP
CMC	Critical Micelle Concentration (MCS) (table containing Value, Solvent, Temperature, References, Notes)	D CMC
CMP	Compressibility (Description, Notes, References)	D CMP
CN	Chemical Name	D CN
CNF	Conformation (Object of Investigation, References)	D CNF
COEV	Concentration in Environment (Species, Location, Contamination Concentration, Background Concentration, Method, Remarks, Notes, References)	D COEV
COMPBRN	Composition: Component Beilstein Record Number	D COMPBRN
COMPN	Composition: Component Name	D COMPN
CONSID	Constitution ID	D CONSID
CP	Heat Capacity CP (table containing Value, Temperature, References, Notes)	D L2 CP
CP0	Heat Capacity CP0 (table containing Value, Temperature, References, Notes)	D CP0
CPD	Crystal Property Description (Colour + Other Properties, Notes, References)	D CPD
CPEM	Complex Phase Equilibria (MCS) (Description, Partner Beilstein Record Number, Partner, Solvent, Temperature, Pressure, Notes, References)	D CPEM L7 2
CRD	Critical Density (table containing Value, References, Notes)	D CRD
CRP	Critical Pressure (table containing Value, References, Notes)	D CRP
CRT	Critical Temperature (table containing Value, References, Notes)	D CRT
CRV	Critical Volume (table containing Value, References, Notes)	D CRV
CRYPH	Crystal Phase Description (Description, Temperature, Notes, References)	D CRYPH
CSG	Crystal Space Group (CSG, Notes, References)	D CSG
CSYS	Crystal System (CSYS, Notes, References)	D CSYS
CTP	Crystal Transition Point (table containing Value, Change of Modification, References, Notes)	D L8 CTP
CTYPE	Compound Type	D CTYPE
CV	Heat Capacity CV (table containing Value, Temperature, References, Notes)	D CV
DE	Dissociation Exponent (table containing Value, Dissociation Group, Temperature, Solvent, Method, Type, References, Notes)	D DE
DED	Data Entry Date	D DED
DEN	Liquid Density (table containing Value, Temperature, Reference Temperature, References, Notes)	D DEN
DFM	Molecular Deformation (Description, Notes, References)	D DFM
DIC	Dielectric Constant (table containing Value, Temperature Frequency, References, Notes)	D DIC
DICS	Dielectric Static Constant (table containing Value, Temperature, References, Notes)	D DICS
DM	Dipole Moment (table containing Value, Temperature, Method, Solvent, Description, References, Notes)	D DM L5
DP	Decomposition Point (table containing Value, Solvent, References, Notes)	D DP
DUPD	Data Update Date	D DUPD
DV	Dynamic Viscosity (table containing Value, Temperature, References, Notes)	D DV
EBC	Energy Barrier of Conformation (table containing Value, Barrier Type, Solvent, References, Notes)	D EBC
ECDH	Abiotic Degradation, Hydrolysis (Type, Concentration Degradation Rate, Exposure Period, Temperature, pH-Value, Degradation Product BRN, Degradation Product, Rate Constant, Half-Life Time, Method, Remarks, Notes, References)	D ECDH
ECDP	Abiotic Degradation, Photolysis (Type, Concentration, Degradation Rate, Exposure Period, Temperature, Rate Constant, Half-Life Time, pH-Value, Degradation Product BRN, Degradation Product, Method, Remarks, Notes, References)	D ECDP
ECS	Stability in Soil (Type, Concentration, Dissipation, Dissipation Time 50, Dissipation Time 90, Exposure Period, Temperature, pH-Value, Humidity, Organic Carbon, Cation Exchange Rate, Microbial Biomass, Method, Remarks, Notes, References)	D ECS
ECTD	Ecological Mobility: Transport and Distribution (Type, Media, Results, Method, Remarks, References)	D ECTD
ECTOX	Ecotoxicology (Effect, Endpoint of Effect, Species or Test-System, Sex, Route of Application, Concentration, Kind of Dosing, Exposure Period, Method, Remarks, Further Details, Type, Value of Type, Results, Metabolite BRN, Metabolite, Notes, References)	D ECTOX
EDIS	Energy of Dissoziation (table containing Value, Bond Type, References, Notes)	D EDIS

DISPLAY and PRINT Formats (cont'd)

Format	Content	Examples
EDM	Electrical Data (MCS) (Description, Partner Beilstein Record Number, Partner, Temperature, Notes, References)	D EDM
ELCB	Electrochemical Behaviour Description (Description, Notes, References)	D ELCB 5
ELE	Electrical Data (Description, Notes, References)	D ELE
ENEM	Energy Data (MCS) (Description, Partner Beilstein Record Number, Partner, Solvent, Temperature, Pressure, Notes, References)	D ENEM
EOD	Oxygen Demand (Type, Related to, Oxygen Demand, Ratio BOD5/COD, Concentration, Method, Remarks, References)	D EOD
ESR	ESR Data (Description, Coupling Nuclei, Solvents, Temperature, Notes, References)	D ESR
EXCA	Exposure Assessment (Exposure BRN, Sources, References)	D EXCA
FA	Fields Available in the record	D FA
FBRN	Component Beilstein Record Number	D FBRN
FINFO	Further Information (References)	D FINFO
FLU	Fluorescence (table containing Description, Solvent, Temperature, References, Notes)	D FLU
FMF **(1)**	Fragment Molecular Formula	D FMF
FP	Flash Point (table containing Temperature, Type of Test References)	D FP
FS	File Segment	D FS
GEO	Interatomic Distance and Angle (Description, Notes, References)	D GEO
GP	Gas Phase (Description, Notes, References)	DISPLAY L5 GP
HCOM	Enthalpy of Combustion (table containing Value, Temperature, Pressure, References, Notes)	D HCOM
HFOR	Enthalpy of Formation (table containing Value, Temperature, Pressure, References, Notes)	D HFOR
HFUS	Enthalpy of Fusion (table containing Value, References, Notes)	D HFUS
HHDG	Enthalpy of Hydrogenation (table containing Value, Product BRN, Product Name, Temperature, References, Notes)	D HHDG
HNC	Henry Constant (MCS) (table containing Value, Log, Temperature, Solvent, References, Notes)	D HNC
HPT	Enthalpy of Phase Transition (table containing Value, References, Notes)	D L8 HPT
HSUB	Enthalpy of Sublimation (table containing Value, Temperature, References, Notes)	D HSUB
HVAP	Enthalpy of Vaporization (table containing Value, Temperature, Pressure, References, Notes)	D HVAP
IEP	Isoelectric Point (table containing Value, Solvent, References, Notes)	D IEP
INP	Isolation from Natural Product (INP, Notes, References)	D INP
IP	Ionization Potential (table containing Value, Method, References, Notes)	D IP
IR	Infrared Spectrum (table containing Description, Solvent, Temperature, References, Notes)	D IR
KV	Kinematic Viscosity (table containing Value, Temperature, References, Notes)	D KV 17
LIQPH	Liquid Phase Description (Description, Notes, References)	D LIQPH
LLSM	Liquid/Liquid System (MCS) (Description, Partner Beilstein Record Number, Partner, Solvent, Temperature, Pressure, Notes, References)	D LLSM
LN	Lawson Number	D LN
LPTP	Transition Point of Liquid Modification (table containing Value, Change of Modification, References, Notes)	D LPTP
LSF	Linearized Structure Formula	D LSF
LSSM	Liquid/Solid System (MCS) (Description, Partner Beilstein Record Number, Partner, Solvent, Temperature, Pressure, Notes, References)	D 2 LSSM
LUM	Luminescence (Description, Notes, References)	D LUM
LVSM	Liquid/Vapour System (MCS) (Description, Partner Beilstein Record Number, Partner, Solvent, Temperature, Pressure, Notes, References)	D 5 LVSM
MAG	Magnetic Data (Description, Notes, References)	D MAG
MEC	Mechanical Property (Description, Notes, References)	D MEC
MECM	Mechanical & Physical Property (MCS) (Description, Partner Beilstein Record Number, Partner, Solvent, Temperature, Pressure, Notes, References)	D MECM L3
MF	Molecular Formula	D MF CN
MP	Melting Point (table containing Value, Solvent, References, Notes)	D MP
MS	Mass Spectrum (Description, Notes, References)	D MS
MSUS	Magnetic Susceptibility (table containing Value, Temperature, References, Notes)	D MSUS
MUT	Mutarotation (table containing Value, Type, Concentration, Length of Path, Solvent, Wavelength, Temperature, Time, References, Notes)	D MUT
MW (FW)	Molecular Weight	D MW

DISPLAY and PRINT Formats (cont'd)

Format	Content	Examples
NMR	Nuclear Magnetic Resonance (Description, Nucleus, Coupling Nuclei, Solvents, Temperature, Frequency, Notes, References)	D NMR L1 1
NQR	Nuclear Quadrupole Resonance (Description, Nucleus, Notes, References)	D NQR
ODM	Optical Data (MCS) (Description, Partner BRN, Partner, Notes, References)	D ODM
OPT	Optics (Description, Notes, References)	D OPT
ORD	Optical Rotatory Dispersion (Solvent, Notes, References)	D ORD
ORP	Optical Rotatory Power (table containing Value, Type, Concentration, Length, Solvent, Rotary Wavelength, Temperature, References, Notes)	D ORP
OSM	Other Spectroscopic Methods (Description, Notes, References)	D OSM
OTHE	Other Thermodynamic Data (Description, Notes, References)	D OTHE
PHARM	Pharmacological Data (Effect, Endpoint of Effect, Species or Test-System, Sex, Type, Value of Type, Route of Application, Concentration, Kind of Dosing, Exposure Period, Method, Remarks, Further Details, Results, Metabolite BRN, Metabolite, Notes, References)	D L3 PHARM
PHO	Phosphorescence (table containing Description, Solvent, Temperature, References, Notes)	D PHO
POL	Electrical Polarizability (Description, Notes, References)	D POL
POT	Electrochemical Characteristics (Description, Solvent, pH-Value, Temperature, Product BRN, Product, Notes, References)	D POT
POW	Partition octan-1-ol/water) (MCS) (table containing Value, Log, Temperature, References)	D POW
PUR	Purification (PUR, References)	D L4 PUR
RAS	Raman Spectrum (Description, Solvent, Notes, References)	D RAS
RI	Refractive Index (table containing Value, Temperature, Wavelength, References, Notes)	D RI
RN	CAS Registry Number	D RN
ROT	Rotational Spectrum (Description, Notes, References)	D ROT
RSTR	Related Structure (Related Structure, Referenced BRN, Referenced Compound, Notes, References)	D L2 RSTR
RXPRO **(2)**	Reactions with the searched substance as a product	D L4 RXPRO
RXREA **(2)**	Reactions with the searched substance as a reactant	D RXREA 1-2
SDIF	Self-Diffusion (table containing Value, Temperature, References, Notes)	D SDIF L17
SLB	Solubility (MCS) (table containing Value, Saturation, Temperature, Solvent, Ratio of Solvents, References, Notes)	D SLB
SLBP	Solubility Product (MCS) (table containing Value, Temperature, Solvent, Ratio of Solvents, References, Notes)	D SLBP
SOLM	Solution Behaviour (MCS) (Description, Partner BRN, Partner, Solvent, Temperature, Notes, Pressure, References)	D SOLM
SOUND	Acoustic Property (Description, Notes, References)	D SOUND
SP	Sublimation Point (table containing Value, Pressure References, Notes)	D SP
ST	Surface Tension (table containing Value, Temperature, References, Notes)	D ST
STR	Structure	D STR
TAUTID	Tautomer ID	D TAUTID
TP	Triple Point (table containing Value, References, Notes)	D TP
TRAM	Transport Phenomena (MCS) (Description, Partner BRN, Partner, Solvent, Temperature, Pressure, Notes, References)	D TRAM
TRAN	Transport Data (Description, Notes, References)	D L1 TRAN
USC	Use of Compound (Laboratory Use and Handling, Use Pattern, Notes, References)	D USC
UVS	UV and Visible Spectrum (table containing Description, Solvent, Absorption Maxima, Ext./Abs. Coeff., References, Notes)	DISPLAY 1 UVS
VP	Vapour Pressure (table containing Value, Temperature, References, Notes)	D VP
XREF	Crossfile Reference (Data Type, Crossfile Source, Name, External Access ID, References)	D XREF
XS	Cross Section (Description, Notes, References)	D XS

DISPLAY and PRINT Formats (cont'd)

Format	Content	Examples
ALL **(3)**	All display fields (CHE, IDE, MCS, PED, PHY, RX)	DISPLAY ALL
CHE **(4)**	Chemical Data (RSTR, INP, CDER, PUR, XREF)	D CHE
IDE	Identification of Substance (BRN, BPR, RN, CN, AUN, LSF, FMF **(1)**, MF, MW, FBRN, LN, FS, CTYPE, CONSID, TAUTID, BSO, COMPBRN, COMPN, DED, DUPD, FBRN, FMF, STR, FA	DISPLAY L1 IDE
RX	Reaction (Reaction ID, Reactant BRN, Reactant, Product BRN, Product, Number of Reaction Details, Reaction Details (Reaction RID, Reaction Classification, Yield, Number of Stages, Reagent, Stage reactant, Catalyst, Solvent, Time, Temperature, Pressure, pH Value, Subject Studied, Prototype Reaction, Other Conditions, Notes, References)	D RX 1-3
MCS **(3)**	Multi-Component Systems (SOL, LLSM, LSSM, LVS, MECM, TRAM, ENEM, EDM, ODM, BSPM, ADSM, ASSM)	D MCSO
LVS	Liquid/Vapour System Data (MCS) (LVSM, AZE, CPEM)	D LVS
SOL	Solution Behaviour (MCS) (SLB, SLBP, SOLM, CMC, HNC, POW)	D SOL
PED **(4)**	Pharmacological and Ecological Data (PHARM, ECO)	D PED
ECO **(4)**	Ecological Data (ECTOX, EXCA, COEV, ECTD, BIO, BIOD, ECDH, ECDP, ECS, EOD, USC)	D ECO
PHY **(3)**	Physical Properties (ECB, ELEP, FINFO, MAGP, MECP, OPTP, SAG, SEP, SF, SPE, THE, TRA)	D PHY L6
ECB **(4)**	Electrochemical Behaviour (ELCB, DE, IEP, POT, XS)	D ECB
ELEP **(4)**	Electrical Properties (DICS, DIC, ELE)	D ELEP
MAGP **(4)**	Magnetic Properties (MSUS, MAG)	D L3 MAGP
MECP **(4)**	Physical and Mechanical Properties (DEN, MEC, CMP, SOUND, ST)	D L9 1-3 MECP
OPTP **(4)**	Optical Properties (RI, OPT, ORP, MUT, ORD, CDIC)	D OPTP
SAG **(3)**	State of Aggregation (CRY, GAS, LIQ)	D SAG L3
CRY **(4)**	Crystals (CPD, MP, CRYPH, DP, SP, TP, CTP, CSYS, CSG, CDEN)	D CRY
GAS **(4)**	Gases (CRT, CRP, CRD, CRV, VP, GP)	D GAS
LIQ **(4)**	Liquids (BP, LIQPH, LPTP)	D LIQ
SEP **(4)**	Structure and Energy Parameters (CNF, GEO, DM, POL, DFM, EBC, EDIS, IP, CIP)	D SEP
SF **(4)**	Safety Data (AIT, FP)	D SF L8
SPE **(3)**	Spectroscopic Data (NMR, ESR, NQR, ROT, IR, RAS, UVS, LUM, FLU, PHO, OSM, MS)	D SPE
THE **(4)**	Thermodynamic Properties (HCOM, HFOR, HHDG, HFUS, HVAP, HSUB, HPT, CP, CP0, CV, OTHE)	D THE
TRA **(4)**	Transport Phenomena (DV, KV, BV, SDIF, TRAN)	D TRA
HIT	All fields containing hit terms	D HIT 1-3
QRD	IDE, HIT (QRD is the default)	D L7 1 5

(1) For compounds consisting of one fragment, FMF is identical with MF and only MF is displayed.
(2) Used when a substance or substance information is searched. RX is used to display all the reaction information, regardless of search terms.
(3) This format may contain data from multiple fee units.
(4) All separate fields included in this format are charged together as one fee unit.

SELECT, ANALYZE and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphanumeric (A) or numeric (N) order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Abiotic Degradation, Hydrolysis; Degradation Product BRN	ECDH.BRN	Y **(2)**	N
Abiotic Degradation, Photolysis; Degradation Product BRN	ECDP.BRN	Y **(2)**	N
Adsorption (MCS), Partner BRN	ADSM.PABRN	Y **(2)**	N
Association (MCS), Partner BRN	ASSM.PABRN	Y **(2)**	N
Azeotropes BRN	AZE.PABRN	Y **(2)**	N
Beilstein Preferred Registry Number	BPR	Y	N
Beilstein Record Number	BRN	Y	N
Beilstein Source	BSO	Y	N
Biodegradation, Degradation Product BRN	BIOD.BRN	Y **(2)**	N
Boundary Surface Phenomena (MCS), Partner BRN	BSPM.PABRN	Y **(2)**	N
CAS Registry Number	RN	Y	N
Chemical Derivative BRN	CDER.BRN	Y **(2)**	N
Chemical Name	CN	Y	N
Complex Phase Equilibria Partner BRN	CPEM.PABRN	Y **(2)**	N
Composition: Compound BRN	COMPBRN	Y	N
Data Update Date	UP	Y **(2,5)**	N
Ecotoxicology, Metabolite BRN	ECTOX.BRN	Y **(2)**	N
Electrical Data, Partner BRN	EDM.PABRN	Y **(2)**	N
Electrochemical Characteristics, Product BRN	POT.PBRN	Y **(2)**	N
Energy Data (MCS), Partner BRN	ENEM.PABRN	Y **(2)**	N
Enthalpy of Hydrogenation Product BRN	HHDG.BRN	Y **(2)**	N
Formula Weight	FW	Y **(3)**	Y
Fragment BRN	FBRN	y	N
Fragment Molecular Formula	FMF	Y	N
Lawson Number	LN	Y	N
Linearized Structure Formula	LSF	Y	N
Liquid/Liquid System, Partner BRN	LLSM.PABRN	Y **(2)**	N
Liquid/Solid System, Partner BRN	LSSM.PABRN	Y **(2)**	N
Liquid Vapour System, Partner BRN	LVSM.PABRN	Y **(2)**	N
Mechanical and Physical Property (MCS), Partner BRN	MECM.PABRN	Y **(2)**	N
Molecular Formula	MF	Y (default)	N
Molecular Weight	MW	Y	N
Optical Data (MCS), Partner BRN	ODM.PABRN	Y **(2)**	N
Other Source	XREF	Y **(4)**	N
Pharmacological Data, Metabolite BRN	PHARM.BRN	Y **(2)**	N
Product BRN	RX.PBRN	Y **(2)**	N
Reactant BRN	RX.RBRN	Y **(2)**	N
Reaction Solvent	RX.SOL	Y **(2)**	N
Related Structure Referenced BRN	RSTR.PABRN	Y **(2)**	N
Stage Reactant BRN	RX.SRBRN	Y **(2)**	N
Solution Behaviour, Partner BRN	SOLM.PABRN	Y **(2)**	N
Transport Phenomena (MCS), Partner BRN	TRAM.PABRN	Y **(2)**	N

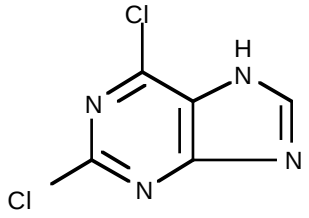
(1) Hit may be used to restrict extracted terms to terms that match the search expression used to create the answer set, e.g., SEL HIT RN.
(2) SELECT HIT and ANALYZE HIT are not valid with ths field.
(3) Appends /MW to the terms created by SELECT.
(4) Appends /FXREF to the terms created by SELECT.
(5) Appends /DUPD to the terms created by SELECT.

BEILSTEIN

Sample Record

DISPLAY QRD (=> S UVS/FA AND 610966/BRN)

```
Beilstein Records (BRN):      610966
Beilstein Pref. RN (BPR):     5451-40-1
CAS Reg. No. (RN):            5451-40-1
Chemical Name (CN):           2,6-dichloro-7(9)H-purine,
                              2,6-dichloro-1H-purine, 2,6-dichloropurine
Autonom Name (AUN):           2,6-dichloro-9H-purine
Molec. Formula (MF):          C5 H2 Cl2 N4
Molecular Weight (MW):        189.00
Lawson Number (LN):           30405
Compound Type (CTYPE):        heterocyclic
Constitution ID (CONSID):     571617
Tautomer ID (TAUTID):         17483
Beilstein Citation (BSO):     5-26, 6-26
Entry Date (DED):             1988/11/28
Update Date (DUPD):           2001/07/25
```



UV and Visible Spectrum:

Description (.KW)	Ref.
Absorption maxima	1, 2
UV/VIS	3

Reference(s):

1. Barlin; Chapman, J.Chem.Soc., CODEN: JCSOA9, <1965>, 3017,3020
2. Ballweg, Justus Liebigs Ann. Chem., CODEN: JLACBF, 649, <1961>, 114,120
3. Hosono et al., Bull.Chem.Soc.Jpn., CODEN: BCSJA8, 46, <1973>, 2814,2819

BABS

STN is operated in North America
by Chemical Abstracts Service

STN Database Summary Sheet

BABS (Beilstein Abstracts database) provides access to titles, abstracts, and bibliographic data from the top journals in organic and related chemistry, published from 1980 to the present.

The records in this file contain bibliographic and indexing information, and abstracts.

Subject Coverage

Organic and related chemistry

Sources

More than 180 journals

File Data

- 1980 to the present
- More than 618,155 records (04/00)
- Updated quarterly
- Automatic current-awareness searches (SDIs) are not available

User Aids

- Online Helps (HELP DIRECTORY lists all help messages available)
- STNGUIDE

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May 2000

Search and Display Field Codes

There are no fields that allow left truncation in this file.

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single words from the abstract (AB), controlled term (CT), and title (TI) fields)	None (or /BI)	S MOPAC S MOLECULAR (L) ORBITAL? S SOLVENT PROTON	AB, CT, TI
Accession Number	/AN	S 6140634/AN	AN
Author	/AU	S MANCINI M/AU	AU
Controlled Term	/CT	S MANNICH REACTIONS/CT	CT
Controlled Word	/CW	S ABIES/CW	CT
Document Type (code and text)	/DT (or /TC)	S JOURNAL/DT S L1 AND J/DT	DT
Entry Date **(1)**	/ED (or /UP)	S ED>APR 2000	ED
Field Availability	/FA	S L5 AND AB/FA	Not displayed
Issue **(1)**	/IS	S 10/IS AND 102/VL AND JPCBFK/ISN	SO
International Standard (Document) Number (CODEN)	/ISN	S ASBSDK/ISN	ISN, SO
Journal Title	/JT	S J ORG CHEM/JT	JT, SO
Language (ISO code and text)	/LA	S DE/LA S GERMAN/LA	LA
Publication Year **(1)**	/PY	S 1999/PY	PY, SO
Source (contains journal title, CODEN, collation information (volume, issue, pagination), and publication year)	/SO	S (SYNLES AND 4)/SO S CHEM EUROP J/SO	SO
Summary Language (ISO code and text)	/SL	S FR/SL S FRENCH/SL	SL
Title	/TI	S ASYMMETRIC SYNTHES!S/TI	TI
Volume **(1)**	/VL	S 10-12/VL	SO
Word Count, Title **(1)**	/WC.T	S WC.T<10	WC.T

(1) Numeric search field that may be searched with numeric operators or ranges.

DISPLAY and PRINT Formats

Any combination of display fields and formats may be used to display or print answers. Multiple codes must be separated by commas or spaces, e.g., D L1 1-10 TI AU. The fields are displayed or printed in the order requested.

Hit-term highlighting is available for all display fields. Highlighting must be ON during SEARCH in order to use the HIT, KWIC, and OCC formats.

Format	Content	Examples
AB	Abstract	D AB 1-5
AN **(1)**	Accession Number	D AN
AU	Author	D AU 2 4
CT **(1)**	Controlled Term	D CT L1 2-5
DT (TC) **(1)**	Document Type	D DT
ED (UP) **(1,2)**	Entry Date	D ED
ISN **(2)**	International Standard (Document) Number	D ISN
JT **(2)**	Journal Title	D JT
LA **(1)**	Language	D LA, SL
PY **(1,2)**	Publication Year	D PY
SL **(1)**	Summary Language	D SL
SO	Source	D SO TI
TI **(1)**	Title	D TI
WC.T **(1,2)**	Word Count, Title	D WC.T
ABS	AN, AB	D ABS
ALL	AN, TI, AU, SO, DT, LA, SL, AB, CT	D ALL
BIB	AN, TI, AU, SO, DT, LA, SL (BIB is the default)	D BIB
DALL	ALL, with delimiter for post processing	D DALL
IALL	ALL, indented with text labels	D IALL
IBIB	BIB, indented with text labels	D IBIB
SCAN **(1,3)**	TI, CT (random display without answer numbers)	D SCAN
TRIAL **(1)** (TRI, SAMPLE, SAM, FREE)	AN, TI, CT	D TRIAL TOTAL
HIT	Fields containing hit terms	D HIT
KWIC	Hit terms with 20 words on either side (KeyWord-In-Context)	D KIWC NOH
OCC **(1)**	Number of occurrences of hit terms and fields in which they occur	D OCC

(1) No online display fee for this format.
(2) Custom display only.
(3) SCAN must be specified on the command line, i.e., D SCAN or DISPLAY SCAN.

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Abstract	AB	Y **(2)**	N
Accession Number	AN	Y	N
Author	AU	Y	Y
CODEN	CODEN	Y	Y
Controlled Term	CT	Y	N
Document Type	DT	Y	N
Entry Date	ED	Y	Y
International Standard (Document) Number (CODEN)	ISN	Y	Y
Journal Title	JT	Y	Y
Language	LA	Y	Y
Occurrence Count of Hit Terms	OCC	N	Y
Publication Year	PY	Y	Y
Source	SO	Y **(3)**	Y
Summary Language	SL	Y	Y
Title	TI	Y (default)	Y
Treatment Code	TC	Y **(4)**	N
Update Date	UP	Y **(5)**	Y
Word Count, Title	WC.T	Y	Y

(1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answers set, e.g., SEL HIT CT.
(2) Appends /BI to the terms created by SELECT.
(3) Selects or analyzes the CODEN with /SO appended to the terms created by SELECT.
(4) Appends /DT to the terms created by SELECT.
(5) Appends /ED to the terms created by SELECT.

Sample Records

DISPLAY IALL

ACCESSION NUMBER: 6138470 BABS
TITLE: Nonlinear Effects in Asymmetric Synthesis and Stereoselective Reactions: Ten Years of Investigation
AUTHOR(S): Girard, Christian; Kagan, Henri B.
SOURCE: Angew.Chem.Int.Ed.Engl. (1998), 37(21), 2922-2959
CODEN: ACIEAY
SOURCE: Angew.Chem. (1998), 110, 3088-3127
CODEN: ANCEAD
DOCUMENT TYPE: Journal
LANGUAGE: English; German
SUMMARY LANGUAGE: English
ABSTRACT: The first preoccupation of organic chemists was to develop their ability to reproduce the organization of atoms in natural products.This incursion in nature’s laboratory gave rise to numerous techniques to transform matter but led to the discovery of her subtle way of produucing substances with chirality and the preference of one enantiomer over the other in the living matter gave a lesson in perfection.The development of asymmetric synthesis gave the opportunity to elaborate methods, reagents, and reactions in order to prepare enantiomerically pure compounds.But this jorney is far from being over, and there is a lot of surprises left.No chemist would have thought that an enantiomerically impure chiral auxiliary or ligand could give a stereoselection higher than its own and even equivalent to the pure one.Molecules can behave in numerous ways in solution; aggregation or organization can occur depending on the nature of the molecule or its environment.These phenomena give rise to modification of the anticipated enantiomeric excess (ee) of the reaction product.The relation between the ee value of the auxiliary or ligand and the ee value of the product deviates from linearity to give what we now call nonlinear effects (NLEs).The nonlinear effects in asymmetric synthesis and stereoselective reaction reflect molecular interactions and complexity in reaction mechanisms.They can be used to generate products with high ee’s from an enantiomerically impure, and more economical to prepare, chiral auxiliary or ligand.Furthermore, the NLEs can also act as a probe to obtain information on the subtle mechanisms by which the enantioselectivity is generated.
CONTROLLED TERM(S): asymmetric amplication; asymmetric catalysis; asymmetric synthesis; autocatalysis; chiral auxiliaries

BABS

DISPLAY BIB

AN 6140733 BABS
TI Reaction of tetramethylammonium fluoride with trifluoromethyltrimethylsilane
AU Adams, Dave J.; Clark, James H.; Hansen, Liv B.; Sanders, Victoria C.; Tavener, Stewart J.
SO J.Fluorine Chem. (1998), 92(2), 123-126
CODEN: JFLCAR
DT Journal
LA English
SL English

DISPLAY FREE

AN 5723848 BABS
TI Resin Glycosides. V. Identification and Characterization of the Component Organic and Glycosidic Acids of the Ether-Soluble Crude Resin Glycosides (“Jalapin”) from Rhizoma Jalapae Braziliensis (Roots of Ipomoea operculata)
CT resin glycoside; Rhizoma Jalapae Braziliensis; Ipomoea operculata; jalapin; organic acid; n-decanoic acid; n-dodecanoic acid; glycosidic acid; operculinic acid; S-jalapinolic acid glycoside.

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