

Using the CAS RegistrySM File on STN[®]

Student Manual

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Preface

These materials were designed to serve as teaching aids for experienced STN searchers who are also involved in training others. It is assumed that students have had prior experience searching online on STN. Students without previous training may refer to the following training materials:

- *STN Basics Training Modules* at:

www.cas.org/support/stngen/acad/basics/page1.html

- *Using CAS Databases on STN* at:

www.cas.org/support/stngen/acad/casdb.html

The objective of these lessons is to teach basic techniques for searching the REGISTRY database on STN. Search examples illustrate some approaches to finding substance information in REGISTRY. Structure searching is not discussed.

For additional information on searching in REGISTRY, refer to:

- The *REGISTRY Database Summary Sheet* available at:

www.cas.org/support/stngen/dbss/index.html

- *How to Search for CAS Registry Numbers in the CAS REGISTRY File Quick Reference Card* available at:

www.cas.org/support/stngen/qrc/index.html

Additional resources for STN searchers are available at:

www.cas.org/support/stngen/index.html

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Lesson 1 Overview of the REGISTRY Database

- Objectives:** At the end of this lesson, the student will:
- Know the content of REGISTRY and LREGISTRYSM and the records in these databases
 - Be able to EXPAND and SEARCH on a CAS Registry Number[®] in REGISTRY, and DISPLAY information for a record or records
 - Know how to search for references to a CAS Registry Number in CASM or LCASM

- Topics:** Content of REGISTRY
The LREGISTRY Database
Displaying Information for a CAS Registry Number
Locating CA References to a CAS Registry Number

Content of REGISTRY

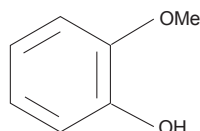
REGISTRY contains all types of organic and inorganic substances, including biochemical compounds, alloys, protein and nucleic acid sequences, coordination compounds, minerals, mixtures, polymers, and salts. Each specific substance is identified by a CAS Registry Number.

Sample Record from REGISTRY

```

RN  90-05-1  REGISTRY
CN  Phenol, 2-methoxy- (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN  Phenol, o-methoxy- (8CI)
OTHER NAMES:
CN  1-Hydroxy-2-methoxybenzene
CN  2-Hydroxyanisole
CN  2-Methoxyphenol
CN  Anastil
CN  Guaiacol
CN  Guaiastil
CN  Methylcatechol
CN  NSC 3815
CN  o-Guaiacol
CN  o-Hydroxyanisole
CN  o-Methoxyphenol
CN  O-Methyl catechol
CN  Pyrocatechol monomethyl ether
CN  Pyroguaiac acid
FS  3D CONCORD
MF  C7 H8 O2
CI  COM
LC  STN Files:  ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*,
      BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS,
      CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHM,
      CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, GMELIN*,
      HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS,
      NAPRALERT, NIOSHTIC, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE,
      TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL, VTB
      (*File contains numerically searchable property data)
      Other Sources:  DSL**, EINECS**, TSCA**
      (**Enter CHEMLIST File for up-to-date regulatory information)
      .
      .

```



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```

6670 REFERENCES IN FILE CA (1907 TO DATE)
 221 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
6684 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 19 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```

Display Fields

RN
CN
FS
MF
CI
LC

Definition

CAS Registry Number
Chemical Names
File Segment
Molecular Formula
Substance Class Identifier
CAS Registry Number Locator
(STN databases with information or references
on this CAS Registry Number)

The LREGISTRY Database

LREGISTRY (Learning REGISTRY) is a companion training database for REGISTRY. LREGISTRY contains approximately 125,000 substance records for the substances indexed in LCA (Learning CA). The number of records in LREGISTRY is static, but the record content is updated as REGISTRY records are updated.

LREGISTRY records contain the same substance information as the corresponding REGISTRY records. However, the number of references in CAS databases is not included.

Displaying Information for a CAS Registry Number

CAS Registry Numbers are widely used in non-CAS materials, for example, catalogs, inventories, and other references, to identify or keep track of substances. Use REGISTRY as the most complete and authoritative database of CAS Registry Numbers with the corresponding substance information.

If you have a CAS Registry Number, you can easily find or verify substance information such as its structure or names. Simply search the CAS Registry Number in REGISTRY. You can also use the EXPAND command first. Notice that you can EXPAND or SEARCH a CAS Registry Number directly, without having to use a field code. The system automatically looks up or searches CAS Registry Numbers in the CAS Registry Number (/RN) index.

To display substance information in REGISTRY for a record or a group of records, you can use any combination of display field codes. Separate multiple codes by commas or spaces, e.g., D L1 1-5 RN CN MF. In addition, you can use display formats. The main ones are:

IDE (default) substance identifying information
HIT fields containing hit terms

Find information on the CAS Registry Number 90-05-1.

```

=> FILE REGISTRY

=> E 90-05-1
E1          1      90-03-9/RN
E2          1      90-04-0/RN
E3          1  --> 90-05-1/RN
E4          1      90-06-2/RN
E5          1      90-07-3/RN
E6          1      90-08-4/RN
E7          1      90-09-5/RN
E8          1      90-10-8/RN
E9          1      90-11-9/RN
E10         1      90-12-0/RN
E11         1      90-13-1/RN
E12         1      90-14-2/RN

=> S E3
L1          1 90-05-1/RN

```

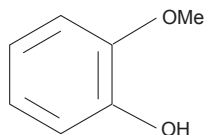
Enter REGISTRY.

EXPAND on the CAS Registry Number.

Search the E-number.

=> D CN STR

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
 CN Phenol, 2-methoxy- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Phenol, o-methoxy- (8CI)
 OTHER NAMES:
 CN 1-Hydroxy-2-methoxybenzene
 CN 2-Hydroxyanisole
 CN 2-Methoxyphenol
 CN Anastil
 CN Guaiacol
 CN Guaiastil
 CN Methylcatechol
 CN NSC 3815
 CN o-Guaiacol
 CN o-Hydroxyanisole
 CN o-Methoxyphenol
 CN O-Methyl catechol
 CN Pyrocatechol monomethyl ether
 CN Pyroguaiac acid



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Display substance information.
 Display CN to view the chemical names and STR to view the structure.

Locating CA References to a CAS Registry Number

The key to finding references on a specific substance in CA is the CAS Registry Number for that substance. This is because CA and LCA records contain CAS Registry Numbers for the specific substances that have been indexed by CAS from a particular document.

In general, the most effective (most comprehensive and most precise) strategy for finding information on a particular substance in CA is to search the CAS Registry Number for that substance.

If you find the CAS Registry Numbers in REGISTRY, you can automatically transfer them to CA. This is known as an L-number crossover, since you simply search in CA the L-number answer set resulting from a REGISTRY search.

The following example shows the crossover of an L-number from REGISTRY to CA using one of the chemical names for the substance. Complete chemical names are searched in the Chemical Name (/CN) index of REGISTRY.

Using D SCAN

If you want to evaluate answers and do not need the CAS Registry Numbers for the records, take advantage of the DISPLAY SCAN option, for which there is no display charge. In DISPLAY SCAN, answer numbers are not displayed and answers are displayed in random order. The full SCAN format includes the CA Index name (IN), Molecular Formula (MF), Class Identifier (CI), and structure diagram (STR). You can use DISPLAY SCAN with any combination of these fields, for example, DISPLAY SCAN IN STR.

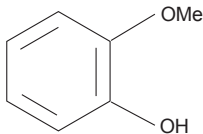
```

=> FILE REGISTRY

=> S ANASTIL/CN
L1          1 ANASTIL/CN

=> D SCAN

L1  1 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN  Phenol, 2-methoxy- (9CI)
MF  C7 H8 O2
CI  COM



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

ALL ANSWERS HAVE BEEN SCANNED

=> FILE CA

=> S L1
L2          6672 L1

```

Enter REGISTRY.
Enter your search terms.

Use D SCAN in REGISTRY to evaluate your query.

Enter CA.

Search the L-number answer set from REGISTRY in CA.

There are many techniques for refining substance searches and using subject or bibliographic terms in CA. Please refer to the manual *Using CAS Databases on STN* as well as other reference materials on CA.

The rest of the lessons in this manual focus on the techniques for searching substance information in REGISTRY to find CAS Registry Numbers. Using CAS Registry Numbers in other databases is not illustrated.

For information about the cost of searching in REGISTRY, please refer to Section 9.

Lesson 2



Searching Chemical Names

2

Objectives: At the end of this lesson, the student will be able to:

- Search complete chemical names in the /CN index

Topics: Chemical Name (/CN) Index

Chemical Names in REGISTRY

In REGISTRY you can search millions of names for chemical substances. Various types of names are included:

- *Chemical Abstracts* index names
- IUPAC names
- other systematic or semisystematic names
- commonly used names
- trade names

Chemical Name (/CN) Index

Complete names are searched in the Chemical Name (/CN) index. Use the EXPAND (or E) command to verify that the name you have is present in the index. Include any spaces or punctuation, such as hyphens, parentheses, or commas, in the name. Follow the name with /CN to indicate that you want to check the name in the Chemical Name index.

You can search the E-number or a range of E-numbers obtained with EXPAND.

Searching complete names is easy and convenient when you have a trade name or another commonly used name and you want to:

- Verify substance information such as the structure and molecular formula
- Obtain the CAS Registry Number for use as search term in CA

What is the chemical composition of a drug with the trade name RO 31-8959?

=> **FILE REGISTRY**

=> **E RO 31-8959/CN 6**

E1 1 RO 31-8830/CN
 E2 1 RO 31-8875/CN
 E3 1 --> RO 31-8959/CN
 E4 1 RO 31-8959/000/CN
 E5 1 RO 31-8959/003/CN
 E6 1 RO 31-9790/CN

=> **S E3**

L1 1 "RO 31-8959"/CN

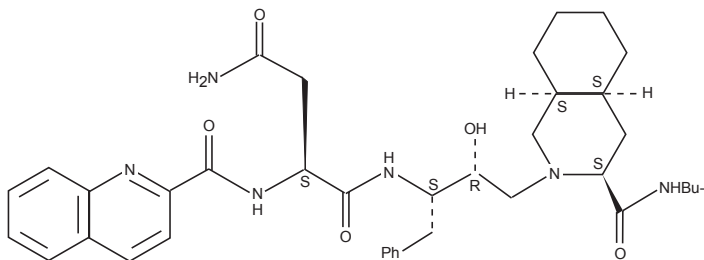
=> **D**

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 127779-20-8 REGISTRY
 CN Butanediamide, N1-[(1S,2R)-3-[(3S,4aS,8aS)-3-[[[(1,1-dimethylethyl)amino]carbonyl]octahydro-2(1H)-isoquinolinyl]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI)
 (CA INDEX NAME)

OTHER NAMES:

CN (S)-N-[(αS)-α-[(1R)-2-[(3S,4aS,8aS)-3-(tert-Butylcarbamoyl)octahydro-2(1H)-isoquinolyl]-1-hydroxyethyl]phenethyl]-2-quinaldamidossuccinamide
 CN Fortovase
 CN **Ro 31-8959**
 CN Ro 31-8959/000
 CN Saquinavir
 CN Sch 52852
 FS STEREOSEARCH
 DR 131176-13-1
 MF C38 H50 N6 O5
 CI COM
 SR CA
 LC STN Files: ADISINSIGHT, ADISNEWS, ANABSTR,
 .
 .
 .

Absolute stereochemistry.



1454 REFERENCES IN FILE CA (1907 TO DATE)
 27 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1461 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Enter REGISTRY.

EXPAND on the name. Follow the name with /CN. Enter the number (6) of lines to view.

Search the E-number.

Enter D to take the default display option in REGISTRY.

All substance information is displayed.

Find references to 1,3-dibromoheptane.

=> FILE REGISTRY

=> E 1,3-DIBROMOHEPTANE/CN

E1 1 1,3-DIBROMODITHIENO(3,4-B:3',2'-D)
PYRIDINE/CN

E2 1 1,3-DIBROMOETHYL BENZOATE-2,5-
DIDECYLOXYPHENYL-1,3-BISBORONIC ACID
COPOLYMER, SRU/CN

E3 1 --> 1,3-DIBROMOHEPTANE/CN

E4 1 1,3-DIBROMOHEXAFLUOROBICYCLO(1.1.1)
PENTANE/CN

E5 1 1,3-DIBROMOHEXAFLUOROPROPANE/CN

E6 1 1,3-DIBROMOHEXANE/CN

E7 1 1,3-DIBROMOHYDANTOIN/CN

E8 1 1,3-DIBROMOHYDRIN/CN

E9 1 1,3-DIBROMOISOINDENONE/CN

E10 1 1,3-DIBROMOISOQUINOLINE/CN

E11 1 1,3-DIBROMONAPHTHALENE/CN

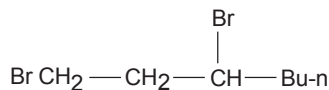
E12 1 1,3-DIBROMONEOPENTANE/CN

=> S E3

L1 1 "1,3-DIBROMOHEPTANE"/CN

=> D SCAN

L1 1 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Heptane, 1,3-dibromo- (9CI)
MF C7 H14 Br2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> FILE CA

=> S L1

L2 4 L1

Enter REGISTRY.

EXPAND on the
name followed by
/CN.

Search the E-number.

Use D SCAN to verify
the structure and
name.Search the L-number
from REGISTRY in
CA to obtain
references.

You can also use right truncation in the /CN field. This is especially useful in searching for a series of trade names. Always use EXPAND first to verify what terms will be searched when you use truncation.

```

=> E ALATANIN/CN
E1          1      ALATAMINE/CN
E2          1      ALATAMINE ACETATE/CN
E3          0 --> ALATANIN/CN
E4          1      ALATANIN 1/CN
E5          1      ALATANIN 2/CN
E6          1      ALATANIN A/CN
E7          1      ALATANIN B/CN
E8          1      ALATANIN C/CN
E9          1      ALATERNIFOLINE/CN
E10         2      ALATERNIN/CN
E11         1      ALATERNIN (GLYCOSIDE)/CN
E12         1      ALATERNIN (QUINONE)/CN

=> S ALATANIN?/CN
L3          5      ALATANIN?/CN
    
```

Lesson 3 Searching Name Segments

Objectives: At the end of this lesson, the student will be able to:

- Search name segments in the Basic Index

Topics: Searching Name Segments in the Basic Index

Name Segments in the Basic Index

If you do not know a complete name, you can search a variety of name segments in the Basic Index of REGISTRY.

Each complete name appearing in the CN field of REGISTRY is broken down into segments created by removing parentheses, brackets, and hyphens. In addition, smaller, chemically significant name segments are also created. Locants may be searched together or separately as individual segments. This is illustrated in the following example.

Complete chemical name	Name segments in the Basic Index
Thiophene, 2,4-dibromo-3,5-dinitro-	thiophene
	2,4
	2
	4
	dibromo
	di
	bromo
	3,5
	3
	5
	dinitro
	di
	nitro

Searching Name Segments

When you enter a search term in REGISTRY without following it by a specific field code, the Basic Index is assumed. You can also use right truncation to allow for variation in name segment endings. For example, searching on CHOLEST? retrieves CHOLEST, CHOLESTANE, or CHOLESTEROL.

Generally you need more than one name segment to search for a compound or a class of compounds. You can use the AND operator to combine name segments. For a more precise search, use the (L) or other proximity operators. The (L) operator requires the segments to be in the same name. You can also enter a phrase in the Basic Index instead of using the (W) operator. For example, searching BENZOIC ACID is equivalent to BENZOIC (W) ACID.

Operator	Definition	Example	Retrievals
(L)	In the same name, in any order	=> S CIS(L)MENTH(L)ENE L1 37 CIS(L)MENTH(L)ENE	CIS-P-MENTH-2-ENE
(W)	Adjacent, in the order entered	=> S BENZOIC ACID L2 260428 BENZOIC ACID => S BENZOIC(W)ACID L3 260428 BENZOIC(W)ACID	BENZOIC ACID
(A)	Adjacent, in either order	=> S CHLORO(A)BROMO L4 2308 CHLORO(A)BROMO	CHLOROBROMO BROMOCHLORO

Searching name segments in the Basic Index is especially useful in the following cases:

- When you know chemically distinct segments of the possible names for a class of compounds
- When you want to refine a molecular formula search

Using name segments to refine molecular formula searches is illustrated in Lesson 4.

The following example illustrates a search for a class of compounds.

Find dinitrodibromothiophenes.

=> E THIOPHENE		
E1	1	THIOPHENDIOXIDE/BI
E2	1	THIOPHENDIOXIDES/BI
E3	263465	--> THIOPHENE/BI
E4	5489	THIOPHENEACET/BI
E5	110	THIOPHENEACETALDEHYDE/BI
E6	2	THIOPHENEACETAMID/BI
E7	4055	THIOPHENEACETAMIDE/BI
E8	9	THIOPHENEACETAMIDINE/BI
E9	12	THIOPHENEACETAMIDO/BI
E10	2	THIOPHENEACETAMIDOX/BI
E11	2	THIOPHENEACETAMIDOXIME/BI
E12	205	THIOPHENEACETATE/BI
=> E DIBROMO		
E1	1	DIBROMIUMOSMIUM/BI
E2	2	DIBROMMERCURY/BI
E3	164916	--> DIBROMO/BI
E4	2	DIBROMOACENAPHTH/BI
E5	4	DIBROMOACENAPHTHENE/BI
E6	2	DIBROMOACENAPHTHO/BI
E7	4	DIBROMOACENAPHTHYLENE/BI
E8	205	DIBROMOACET/BI
E9	2	DIBROMOACETALDEHYDE/BI
E10	3	DIBROMOACETAMID/BI
E11	3	DIBROMOACETAMIDATO/BI
E12	6	DIBROMOACETAMIDE/BI

EXPAND on the significant name segments in the Basic Index to verify that they are present.

=> **E DINITRO**

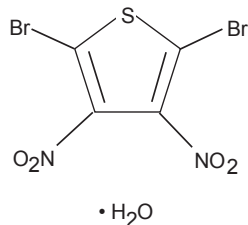
E1 2 DINITRITOTRIS/BI
 E2 1 DINITRITTOZINC/BI
 E3 138848 --> DINITRO/BI
 E4 2 DINITROACE/BI
 E5 1 DINITROACENAPHTH/BI
 E6 7 DINITROACENAPHTHENE/BI
 E7 1 DINITROACENAPHTHENEQUIN/BI
 E8 1 DINITROACENAPHTHENEQUINONE/BI
 E9 1 DINITROACENAPHTHO/BI
 E10 1 DINITROACENAPHTHOPHENAZINE/BI
 E11 6 DINITROACENAPHTHYLENE/BI
 E12 2 DINITROACEPERIMIDINE/BI

=> **S THIOPHENE(L)DIBROMO(L)DINITRO**

263465 THIOPHENE
 164916 DIBROMO
 138848 DINITRO
 138960 DINITRO
 L1 28 THIOPHENE(L)DIBROMO(L)DINITRO

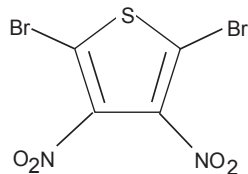
=> **D SCAN**

L1 28 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN **Thiophene, 2,5-dibromo-3,4-dinitro-, monohydrate (9CI)**
 MF C4 Br2 N2 O4 S . H2 O



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L1 28 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN **Thiophene, 2,5-dibromo-3,4-dinitro- (6CI, 7CI, 9CI)**
 MF C4 Br2 N2 O4 S
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Search the name segments. Use the (L) operator to require the name segments to be in the same name.

Use DISPLAY SCAN to view the index name and the structures of some answers.

Lesson 4 Searching Molecular Formulas

- Objectives:** At the end of this lesson, the student will be able to:
- Search the complete molecular formula
 - Combine a molecular formula search with name segments

Topics: Molecular Formula (/MF) Index
Combining the Molecular Formula with Name Segments

The Molecular Formula (/MF) Index

The complete molecular formula for specific substances in REGISTRY is searched in the Molecular Formula (/MF) index. Molecular formulas are present and searched in the /MF index in Hill System Order.

For carbon-containing compounds, Hill System Order means that carbons are listed first, hydrogens are listed second (if present), and all other elements are then listed in alphabetical order.

For compounds that do not contain carbon, the elements are simply listed in alphabetical order with the number of each element indicated.

Compound	Molecular formula in Hill System Order
2-Methoxyphenol	C7H8O2
Sodium chloride	CLNA
Sulfuric acid	H2O4S

For substances containing deuterium or tritium, two formulas may be searched. One formula contains the deuterium or tritium isotope, and the second formula replaces the deuterium or tritium with hydrogen. Abnormal mass of elements other than hydrogen is not shown in the MF field but is reflected in the CA Index name.

You can SEARCH and EXPAND on any molecular formula without spaces between elements, e.g., ASCL6/MF or with spaces, e.g., AS CL6/MF.

Always EXPAND on the molecular formula first in the /MF index. With EXPAND you can find if the term is present and how many compounds in REGISTRY have that molecular formula.

Find the CAS Registry Number for sulfuric acid by using its molecular formula.

```

=> FILE REGISTRY

=> E H2SO4/MF 6
E1          1      H2SNYB3/MF
E2          4      H2SNZN/MF
E3          0 --> H2SO4/MF
E4          2      H2SR/MF
E5          2      H2SSC/MF
E6          3      H2SSE/MF

=> E H2O4S/MF
E1          1      H2O4RH/MF
E2          1      H2O4RU/MF
E3          17 --> H2O4S/MF
E4          1      H2O4S.1/10H2O/MF
E5          1      H2O4S.1/10K.LI.9/10RB/MF
E6          1      H2O4S.1/10MG.9/5NA/MF
E7          1      H2O4S.1/10SB/MF
E8          1      H2O4S.1/11IR.9/10K.5/11SN/MF
E9          1      H2O4S.1/25K.LI.24/25RB/MF
E10         1      H2O4S.1/2H2O.1/2HF/MF
E11         1      H2O4S.1/2H2O.1/2HO.1/2K/MF
E12         1      H2O4S.1/2H2O.1/2HO.1/2NA/MF

=> S E3
L1          17 H2O4S/MF

=> D CN 1-17
L1 ANSWER 1 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN
CN Sulfuric-32S acid (8CI) (CA INDEX NAME)

L1 ANSWER 2 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN
CN Sulfuric-34S acid (9CI) (CA INDEX NAME)

L1 ANSWER 3 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN
CN Sulfuric acid, labeled with oxygen-17 (9CI)
(CA INDEX NAME)

L1 ANSWER 4 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN
CN Sulfuric-180 acid (9CI) (CA INDEX NAME)

L1 ANSWER 5 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN
CN Sulfuric-1804 acid (9CI) (CA INDEX NAME)
.
.
.
L1 ANSWER 16 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN
CN Sulfuric-35S acid (6CI, 7CI, 8CI, 9CI)
(CA INDEX NAME)
OTHER NAMES:
CN Sulfuric acid (H235S04)
CN Sulfuric acid-35S
    
```

Enter REGISTRY and EXPAND on the molecular formula in the /MF index.

Answers are missed if Hill System Order is not used for the molecular formula.

EXPAND on the molecular formula using Hill System Order.

Search the E-number.

Display names (CN) to check what compounds are retrieved.

Labeled compounds are included.

```

L1 ANSWER 17 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN
CN Sulfuric acid (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN BOV
CN Brimstone acid
CN Contact acid
CN Dihydrogen sulfate
CN Dipping acid
CN NSC 248648
CN NSC 38965
CN Oil of vitriol
CN Sulphuric acid
CN Vitriol brown oil

=> D RN 17
L1 ANSWER 17 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN
RN 7664-93-9 REGISTRY

```

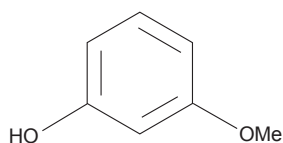
Display the CAS Registry Number for the compound of interest.

Combining the Molecular Formula with Name Segments

Because the molecular formula is generally not unique, you can expect to have to refine your molecular formula search by combining it with other terms, for example, name fragments.

Combining the molecular formula with name segments is most effective if you can identify a few chemically distinct name segments. With this approach you can produce a small set of answers to browse.

Find the CAS Registry Number for the compound with the following structure:



```

=> E C7H8O2/MF
E1          1      C7H8O13S4/MF
E2          1      C7H8O13S4.4NA/MF
E3          686 --> C7H8O2/MF
E4          1      C7H8O2.(C6H10O2)X/MF
E5          3      C7H8O2.1/2BA/MF
E6          1      C7H8O2.1/2BR6SN.H/MF
E7          4      C7H8O2.1/2C4H10N2/MF
E8          1      C7H8O2.1/2C4H8O2/MF
E9          1      C7H8O2.1/2C6H15N/MF
E10         1      C7H8O2.1/2C6H3N3O6.K/MF
E11         1      C7H8O2.1/2C6H6O2/MF
E12         3      C7H8O2.1/2CA/MF

```

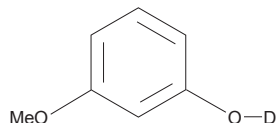
EXPAND on the molecular formula in the /MF index.

```

=> S E3 AND PHENOL
      686 C7H8O2/MF
      337238 PHENOL
      32 PHENOLS
      337238 PHENOL
          (PHENOL OR PHENOLS)
L1      40 C7H8O2/MF AND PHENOL

=> S L1 AND 3-METHOXY
      14358935 3
      3880633 METHOXY
      400207 3-METHOXY
          (3(W)METHOXY)
L2      7 L1 AND 3-METHOXY

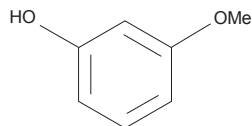
=> D SCAN
L2 7 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN Phenol-d, 3-methoxy- (9CI)
MF C7 H7 D O2
    
```



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

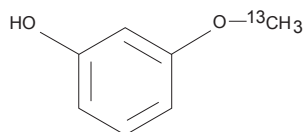
```

L2 7 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN Phenol, 3-methoxy-, labeled with deuterium (9CI)
MF C7 H8 O2
    
```



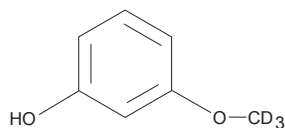
```

L2 7 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN Phenol, 3-(methoxy-13C)- (9CI)
MF C7 H8 O2
    
```



```

L2 7 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN Phenol, 3-(methoxy-d3)- (9CI)
MF C7 H5 D3 O2
    
```



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Combine a search of the molecular formula with a name segment.

Refine the answer set by combining it with another name fragment.

Use DISPLAY SCAN to browse structures and CA Index names.

Labeled compounds are also retrieved.

Lesson 5 Searching for Salts

Objectives: At the end of this lesson, the student will know how:

- Salts are represented in REGISTRY
- To search for salts in REGISTRY

Topics: Salts in REGISTRY
Searching for Salts
Searching for Inorganic Salts

Salts in Registry

Salts are represented in REGISTRY as multicomponent substances. They are named and structured by CAS using the acid or base from which they are derived. Their molecular formula appears in the “dot-disconnected” format, i.e., two or more constituent formulas separated by periods.

This is most easily illustrated by some examples of common salts and how they are represented in REGISTRY.

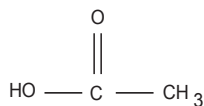
Example: Sodium acetate

```

RN  127-09-3  REGISTRY
CN  Acetic acid, sodium salt (7CI, 8CI, 9CI)
    (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN  Sodium acetate (6CI)
OTHER NAMES:
CN  Anhydrous sodium acetate
CN  Cryotech NAAC
DR  325477-99-4
MF  C2 H4 O2 . Na
CI  COM

CRN (64-19-7)

```



• Na

Each salt has its own CAS Registry Number displayed in the RN field.

Systematic and common names are included in the CN field.

The molecular formula is displayed in dot-disconnected format.

The CRN field displays the Component Registry Number for acetic acid. A CRN for the metal is NOT included.

Example: Trimethylammonium chloride

```

RN  593-81-7  REGISTRY
CN  Methanamine, N,N-dimethyl-, hydrochloride (9CI)
    (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN  Trimethylamine, hydrochloride (8CI)
OTHER NAMES:
CN  Trimethylamine monohydrochloride
CN  Trimethylammonium chloride
MF  C3 H9 N . Cl H
CI  COM
CRN (75-50-3)

      CH3
      |
H3C — N — CH3
      • HCl

704 REFERENCES IN FILE CA (1907 TO DATE)
109 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
706 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
    
```

Each salt has its own CAS Registry Number.

Systematic and common names are included in the CN field.

The molecular formula is displayed in dot-disconnected format.

The CRN field displays the Component Registry Number for the trimethylamine. A CRN for HCl is NOT included.

Searching for Salts

You can use various techniques to search for salts. They are illustrated by using sodium acetate as an example.

Chemical Names in the /CN Index

```

=> S SODIUM ACETATE/CN
L1          1 SODIUM ACETATE/CN
    
```

Search any of the names in the /CN field.

Name Segments in the Basic Index

Name segments from any of the systematic or common names in the CN field may also be searched in the Basic Index. Use the (L) operator to restrict the terms to the same name. You can also use phrases if you want to search adjacent fragments.

Name segment searches typically retrieve many substances that contain those segments.

```

=> S ACETATE(L)SODIUM
    479889 ACETATE
    288160 SODIUM
L1          3095 ACETATE(L)SODIUM

=> S SODIUM ACETATE
    288160 SODIUM
    479889 ACETATE
L2          104 SODIUM ACETATE
              (SODIUM(W)ACETATE)
    
```

Many substances containing these name segments are retrieved.

Component CAS Registry Number in the /CRN Index

Many salts contain a multiatom component, e.g., acetic acid, and a single atom fragment, e.g., Na. Single atom fragments are components consisting solely of any number of hydrogens and/or one or zero non-hydrogen atoms, e.g., NH₃, HCl, BH₃, Ag, F, H.

In these salts, only the multiatom component has its own Component Registry Number. You can search the Component Registry Number in the /CRN field to obtain any salts, mixtures, and other multicomponent substances with that component.

```
=> S ACETIC ACID/CN
L3          1 ACETIC ACID/CN

=> D RN
L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN  64-19-7 REGISTRY

=> S 64-19-7/CRN
L4          27991 64-19-7/CRN
```

Search the name of the acid.

Display the CAS Registry Number.

Search the Component Registry Number in the /CRN field.

Complete Molecular Formula in the /MF Index

The complete molecular formula is searched in the dot-disconnected format. The elements in each component are arranged in Hill System Order (see Lesson 4). In addition, special rules are applied by CAS to keep the order of components consistent. For example, carbon-containing component is listed first if there is also a non-carbon-containing component. See the supplementary information in Section 8 for a complete list of these rules.

```
=> E C2H4O2.NA/MF
E1          6 C2H4O2.LI/MF
E2          1 C2H4O2.N2O4/MF
E3         32 --> C2H4O2.NA/MF
E4          1 C2H4O2.O2S/MF
E5          1 C2H4O2.OPB.1/2PB/MF
E6          1 C2H4O2.OZN.1/2ZN/MF
            .
            .
            .

=> S C2H4O2.NA/MF
L5          32 C2H4O2.NA/MF
```

Use the EXPAND command first to verify how the molecular formula is indexed in /MF.

Component Molecular Formula in the Basic Index

Instead of searching the complete formula in the /MF field, it may be easier to search the molecular formula for each component of a salt. The Basic Index of REGISTRY includes all components of dot-disconnected formulas as separate searchable segments. To search in the Basic Index, simply enter the component molecular formula without any field code. Use the AND operator to combine the component molecular formulas.

```
=> S C2H4O2 AND NA
      25876 C2H4O2
      280156 NA
L1      262 C2H4O2 AND NA
```

Search the molecular formula of each component without any field code. Combine with AND.

Number of Components

The Number of Components (/NC) index contains a count of the number of fragment formulas that make up the molecular formula. You can restrict the number of components in your search results by searching for an exact number or a range of components in the Number of Components (/NC) index. For example, you can restrict results to two-component substances by combining other search terms with 2/NC.

```
=> S C2H4O2 AND NA AND 2/NC
      25876 C2H4O2
      280156 NA
      2907770 2/NC
L2      48 C2H4O2 AND NA AND 2/NC
```

These techniques are generally used in combination, as illustrated in the following example.

Find the CAS Registry Number for the barium salt of benzoic acid.

```
=> FILE REGISTRY

=> S BENZOIC ACID/CN
L1      1 BENZOIC ACID/CN

=> D MF

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
MF C7 H6 O2

=> S C7H6O2 AND BA
      4403 C7H6O2
      78367 BA
L2      6 C7H6O2 AND BA

=> D SCAN IN MF

L2 6 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Benzaldehyde, 2-hydroxy-, barium salt (9CI)
MF C7 H6 O2 . 1/2 Ba
```

Enter REGISTRY.

Search the name of the acid in /CN.

Display the molecular formula for the acid.

Search the molecular formula for each component in the Basic Index. Combine with AND.

Use DISPLAY SCAN IN MF to view the CA Index name and the molecular formulas for some answers.

```

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 6 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN Benzoic acid, barium salt, dihydrate (8CI, 9CI)
MF C7 H6 O2 . 1/2 Ba . H2 O

L2 6 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN Benzoic acid, barium salt (7:2), monohydrate (9CI)
MF C7 H6 O2 . 2/7 Ba . 1/7 H2 O

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L2 AND 2/NC
    2907770 2/NC
L3          3 L2 AND 2/NC

=> D RN IN 1-3

L3 ANSWER 1 OF 3  REGISTRY  COPYRIGHT 2005 ACS on STN
RN 106448-28-6  REGISTRY
IN Benzaldehyde, 2-hydroxy-, barium salt (9CI)

L3 ANSWER 2 OF 3  REGISTRY  COPYRIGHT 2005 ACS on STN
RN 31990-35-9  REGISTRY
IN 2,4,6-Cycloheptatrien-1-one, 2-hydroxy-, barium
salt (9CI)

L3 ANSWER 3 OF 3  REGISTRY  COPYRIGHT 2005 ACS on STN
RN 533-00-6  REGISTRY
IN Benzoic acid, barium salt (8CI, 9CI)

```

Other compounds with the same molecular formula are retrieved as well as hydrates consisting of more than two components.

Restrict to two-component compounds to eliminate hydrates.

Display some substance information, e.g., CA Index name (IN) to identify the desired CAS Registry Number.

Searching for Inorganic Salts

The same techniques can be used to search for inorganic salts.

Search for potassium sulfates.

```

=> FILE REGISTRY

=> S H2O4S AND POTASSIUM
    22370 H2O4S
    112069 POTASSIUM
L1          807 H2O4S AND POTASSIUM

=> D SCAN IN MF

L1 807 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN Sulfuric acid, aluminum potassium thallium(1+)
salt (10:5:1:4), hexacontahydrate (9CI)
MF Al . 2 H2 O4 S . 12 H2 O . 1/5 K . 4/5 Tl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L1 807 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN Sulfuric acid, lithium potassium salt (5:7:3) (9CI)
MF H2 O4 S . 3/5 K . 7/5 Li

```

Enter REGISTRY.

Search the molecular formula for sulfuric acid in the Basic Index. Combine with the element name in the Basic Index.

Review the CA Index name and molecular formula for some answers. Salts with additional components are also retrieved.

```

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L1 AND 2/NC
    2907770 2/NC
L2      12 L1 AND 2/NC

=> D SCAN IN
L2  12 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN  Sulfuric acid, potassium salt (3:4) (9CI)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2  12 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN  Sulfuric acid, potassium salt (4:5) (8CI, 9CI)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2  12 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN  Sulfuric-34S acid, dipotassium salt (9CI)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> D RN IN MF 1-12
L2  ANSWER 1 OF 12  REGISTRY  COPYRIGHT 2005 ACS on STN
RN  121734-20-1  REGISTRY
IN  Sulfuric acid, potassium salt (9CI)
MF  H2 O4 S . x K

L2  ANSWER 2 OF 12  REGISTRY  COPYRIGHT 2005 ACS on STN
RN  110905-06-1  REGISTRY
IN  Sulfuric-34S acid, dipotassium salt (9CI)
MF  H2 O4 S . 2 K

L2  ANSWER 3 OF 12  REGISTRY  COPYRIGHT 2005 ACS on STN
RN  73655-07-9  REGISTRY
IN  Sulfuric acid-d2, potassium salt (2:3) (9CI)
MF  D2 O4 S . 3/2 K

L2  ANSWER 4 OF 12  REGISTRY  COPYRIGHT 2005 ACS on STN
RN  73034-02-3  REGISTRY
IN  Sulfuric acid, potassium salt (3:4) (9CI)
MF  H2 O4 S . 4/3 K

L2  ANSWER 5 OF 12  REGISTRY  COPYRIGHT 2005 ACS on STN
RN  23725-97-5  REGISTRY
IN  Sulfuric-35S acid, dipotassium salt (8CI, 9CI)
MF  H2 O4 S . 2 K

L2  ANSWER 6 OF 12  REGISTRY  COPYRIGHT 2005 ACS on STN
RN  14337-15-6  REGISTRY
IN  Sulfuric acid-d, monopotassium salt (8CI, 9CI)
MF  D H O4 S . K

L2  ANSWER 7 OF 12  REGISTRY  COPYRIGHT 2005 ACS on STN
RN  13778-48-8  REGISTRY
IN  Sulfuric acid, potassium salt (2:1) (9CI)
MF  H2 O4 S . 1/2 K

L2  ANSWER 8 OF 12  REGISTRY  COPYRIGHT 2005 ACS on STN
RN  13778-46-6  REGISTRY
IN  Sulfuric acid, potassium salt (2:3) (8CI, 9CI)
MF  H2 O4 S . 3/2 K
    .
    .
    .

```

Restrict results to two-component salts.

Scan the CA Index names for some answers.

Answers include labeled salts and salts with various ratios of the components.

Lesson 6 Searching for Mixtures

Objectives: At the end of this lesson, the student will know how:

- Mixtures are represented in REGISTRY
- To search for mixtures in REGISTRY

Topics: Mixtures in Registry
Searching for Mixtures
Using the Component Registry Number
Restricting the Number of Components

Mixtures in Registry

There are many pharmaceutical or agrochemical mixtures in REGISTRY. Mixtures are represented in REGISTRY in terms of their distinct active ingredients. When you display a record for a mixture, each component is identified as CM 1, CM 2, etc. Each component has its own CAS Registry Number displayed in the CRN field, the molecular formula in the CMF field, and the structure. In addition, the entire substance has its own CAS Registry Number displayed in the RN field, the CA index name and any other common or trade names in the CN field, and the complete molecular formula in the MF field. Mixtures are identified in the Class Identifier (CI) field as MXS.

```

RN      8003-03-0  REGISTRY
CN      Benzoic acid, 2-(acetyloxy)-, mixt. with 3,7-
        dihydro-1,3,7-trimethyl-1H-purine-2,6-dione and N-
        (4-ethoxyphenyl)acetamide (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN      1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-,
        mixt. contg. (9CI)
CN      Acetamide, N-(4-ethoxyphenyl)-, mixt. contg. (9CI)
OTHER NAMES:
CN      Acetylsalicylic acid-caffeine-phenacetin mixt.
CN      APC
CN      APC (pharmaceutical)
CN      Ascophen
CN      Askophen
CN      Aspirin, phenacetin and caffeine
CN      Aspirin-caffeine-phenacetin mixt.
CN      Citramon
CN      Empirin compound
        .
        .
        .
MF      C10 H13 N O2 . C9 H8 O4 . C8 H10 N4 O2
CI      MXS
        .
        .
        .

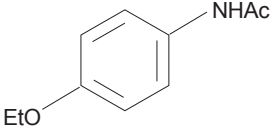
```

The CAS Registry Number for the mixture displays in the RN field.

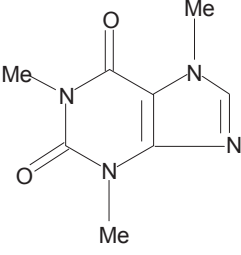
The CA Index name and other common or trade names display in the CN field.

The molecular formula displays in the MF field.

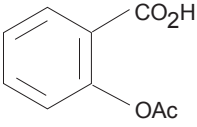
CM 1
 CRN 62-44-2
 CMF C10 H13 N O2



CM 2
 CRN 58-08-2
 CMF C8 H10 N4 O2



CM 3
 CRN 50-78-2
 CMF C9 H8 O4



54 REFERENCES IN FILE CA (1907 TO DATE)
 54 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Each component is identified as CM 1, CM 2, etc.

Each component has its own CAS Registry Number displayed in the CRN field, the molecular formula in the CMF field, and the structure.

Searching for Mixtures

Mixtures may be searched by using a variety of techniques:

- Chemical or trade names for the mixture in the /CN field (see Lesson 2)
- Name segments in the Basic Index (see Lesson 3)
- Complete molecular formula in the /MF index (see Lesson 4 and supplementary information in Section 8)
- Component molecular formula in the Basic Index (see Lessons 5 and 7)
- Component Registry Numbers

Using the Component Registry Number

The easiest way to search for mixtures is to search the CAS Registry Numbers for one or more of the active ingredients using the following steps:

- Find the CAS Registry Numbers for the components of interest
- Search the CAS Registry Number in the Component Registry Number (/CRN) index
- Use the AND operator to combine more than one Component Registry Number

This strategy may also retrieve other multicomponent substances such as salts or molecular addition compounds. If you want to eliminate them, use MXS/CI to restrict results only to mixtures.

Find mixtures of azidothymidine.

```
=> FILE REGISTRY

=> E AZIDOTHYIMIDINE/CN
E1          1      AZIDOTHIOCARBONIC ACID/CN
E2          1      AZIDOTHIOCYANATOBIS(ETHYLENEDIAMINE)
                COBALT CHLORIDE/CN
E3          1  --> AZIDOTHYIMIDINE/CN
E4          1      AZIDOTHYIMIDINE MONOPHOSPHATE/CN
E5          1      AZIDOTHYIMIDINE PHOSPHONATE/CN
E6          1      AZIDOTHYIMIDINE TRIPHOSPHATE/CN
E7          1      AZIDOTRIBUTYLSTANNANE/CN
E8          1      AZIDOTRIBUTYLTIN/CN
E9          1      AZIDOTRICHORO-P-BENZOQUINONE/CN
E10         1      AZIDOTRICHLOROSILANE/CN
E11         1      AZIDOTRICYCLOPENTADIENYLCERIUM/CN
E12         1      AZIDOTRIETHYLSILANE/CN
```

Enter REGISTRY and EXPAND on the name in the CN field.

```

=> S E3
L1 1 AZIDOTHYIMIDINE/CN

=> D RN
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 30516-87-1 REGISTRY

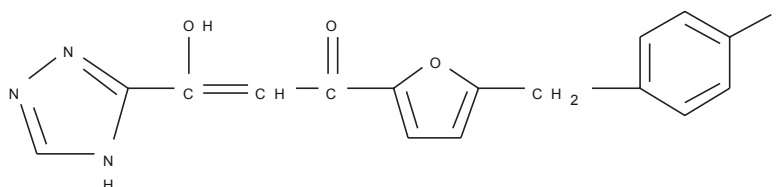
=> S 30516-87-1/CRN
L2 48 30516-87-1/CRN

=> D 3
L2 ANSWER 3 OF 48 REGISTRY COPYRIGHT 2005 ACS on STN
RN 381223-99-0 REGISTRY
CN Thymidine, 3'-azido-3'-deoxy-, compd. with 1-[5-[(4-
fluorophenyl)methyl]-2-furanyl]-3-hydroxy-3-(1H-1,2,
4-triazol-3-yl)-2-propen-1-one (1:1) (9CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C16 H12 F N3 O3 . C10 H13 N5 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

```

CM 1

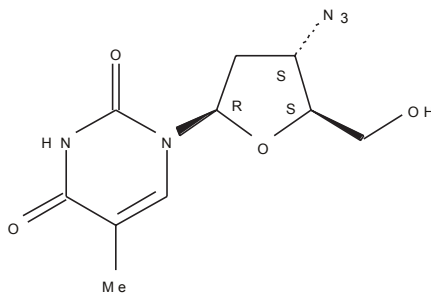
CRN 280571-30-4
 CMF C16 H12 F N3 O3



CM 2

CRN 30516-87-1
 CMF C10 H13 N5 O4

Absolute stereochemistry. Rotation (+).



1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Search the name for the component.

Display the CAS Registry Number for the component (RN).

Search the CAS Registry Number for the component in the /CRN field.

Mixtures such as this example are retrieved. The mixture has its own CAS Registry Number.

Each component (CM 1, CM 2, etc.) has its own CAS Registry Number (CRN), molecular formula (CMF), and structure.

Restricting the Number of Components

You can easily refine searches for mixtures by restricting the number of components. The number of components is a count of the number of the molecular formula fragments in MF, and is searched in the Number of Components (/NC) index. You can search for an exact number or a range of components.

Number of Components	Examples
A specific number	S 2/NC S L1 AND 3/NC
A range	S NC>2 S 2-3/NC S NC<=3

Find mixtures of Captan with one other ingredient.

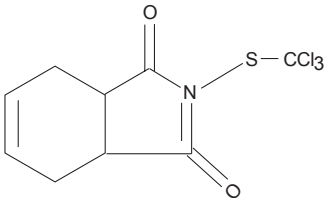
```

=> FILE REGISTRY

=> S CAPTAN/CN
L1          1 CAPTAN/CN

=> D RN STR
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN  133-06-2 REGISTRY

```



```

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

```

Enter REGISTRY.

Search the trade name in the /CN index.

Display the CAS Registry Number (RN) for Captan. Display some substance information, e.g., structure (STR) to verify the chemical composition.

```

=> S 133-06-2/CRN
L2      245 133-06-2/CRN

=> S L2 AND 2/NC
      2907770 2/NC
L3      176 L2 AND 2/NC

=> D 3
L3 ANSWER 3 OF 176 REGISTRY COPYRIGHT 2005 ACS on STN
RN 642463-25-0 REGISTRY
CN Phosphonic acid, (2-chloroethyl)-, mixt. with 3a,4,
   7,7a-tetrahydro-2-[(trichloromethyl)thio]-1H-
   isoindole-1,3(2H)-dione (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Ethrel-captan mixt.
MF C9 H8 Cl3 N O2 S . C2 H6 Cl O3 P
CI MXS
SR CA
LC STN Files:  CA, CAPLUS

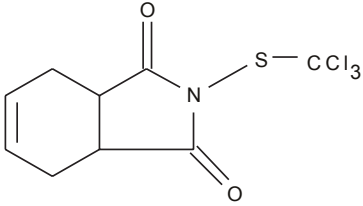
      CM 1

      CRN 16672-87-0
      CMF C2 H6 Cl O3 P

      ClCH2 - CH2 - PO3H2

      CM 2

      CRN 133-06-2
      CMF C9 H8 Cl3 N O2 S
  
```



```

      1 REFERENCES IN FILE CA (1907 TO DATE)
      1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
  
```

Search the CAS Registry Number for Captan in the /CRN field.

Restrict to two components.

Display substance information for one of the mixtures.

Substance information for the Captan component is displayed as CM 2. The CAS Registry Number for Captan displays in the CRN field.

Searching Component Registry Numbers is very fast, economical, and effective when you are searching for very specific components. However, sometimes you may be looking for mixtures containing an optically active component. In such cases, you need to be aware that unique CAS Registry Numbers are used for each distinct stereoisomer or a racemate. Searching the CAS Registry Number for one of the stereoisomers in the /CRN field would not retrieve mixtures containing other stereoisomers. To retrieve mixtures regardless of stereochemistry, search the molecular formulas of the components. This technique is described in Lesson 7.

Lesson 7 Searching for Stereoisomers

Objectives: At the end of this lesson, the student will know how:

- Stereoisomers are represented in REGISTRY
- To search for a class of stereoisomers in REGISTRY

Topics: Stereoisomers in REGISTRY
 Searching for Stereoisomers
 Searching for Compositions Containing Stereoisomers

Stereoisomers in REGISTRY

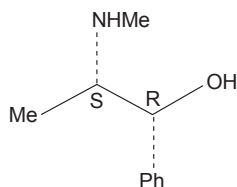
CAS registers substances as specifically as possible. Therefore, specific stereoisomers and racemates are assigned their own unique CAS Registry Numbers. Their molecular formula is the same, and the CA index name is the same except for the stereo designation.

Stereoisomer 1

```

RN  299-42-3  REGISTRY
CN  Benzenemethanol,  $\alpha$ -[(1S)-1-(methylamino)ethyl]-,
    ( $\alpha$ R)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN  Benzenemethanol,  $\alpha$ -[1-(methylamino)ethyl]-, [R-
    (R*,S*)]-
CN  Ephedrine, (-)- (8CI)
OTHER NAMES:
CN  (-)-(1R,2S)-Ephedrin
CN  (-)-(1R,2S)-Ephedrine
CN  (-)-Ephedrin
CN  (-)-Ephedrine
CN  (-)-erythro-Ephedrine
CN  (_R)-_-[(1S)-1-(Methylamino)ethyl]benzenemethanol
CN  (1R,2S)-(-)-Ephedrine
CN  (1R,2S)-1-Hydroxy-2-(methylamino)-1-phenylpropane
CN  (1R,2S)-Ephedrine
CN  1(R),2(S)-erythro-(-)-Ephedrine
CN  L-Ephedrine
MF  C10 H15 N O
CI  COM
  
```

Absolute stereochemistry.

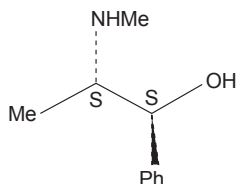


Stereoisomer 2

```

RN  4125-58-0  REGISTRY
CN  Benzenemethanol,  $\alpha$ -[(1R)-1-(methylamino)ethyl]-, ( $\alpha$ R)-
    rel- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN  Benzenemethanol,  $\alpha$ -[1-(methylamino)ethyl]-, (R*,R*)-
    ( $\pm$ )-
CN  Pseudoephedrine, ( $\pm$ )- (8CI)
OTHER NAMES:
CN  ( $\pm$ )- $\alpha$ -Ephedrine
CN  ( $\pm$ )-Isoephedrine
CN  ( $\pm$ )-Pseudoephedrine
MF  C10 H15 N O
CI  COM
    
```

Relative stereochemistry.



Searching for Stereoisomers

To find all stereoisomers of a given flat structure, search:

- Their molecular formula
- Name fragments from their CA Index name and common names

Find stereoisomers of ephedrine.

```

=> FILE REGISTRY
=> S EPHEDRINE/CN
L1          1 EPHEDRINE/CN

=> D IN MF
L1 ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2005 ACS on STN
IN  Benzenemethanol,  $\alpha$ -[(1S)-1-(methylamino)ethyl]-, ( $\alpha$ R)-
    (9CI)
MF  C10 H15 N O

=> S C10H15NO/MF
L2          2238 C10H15NO/MF
    
```

Enter REGISTRY.

Search the common name in the /CN index.

Display the CA index name (IN) and the molecular formula (MF).

Search the molecular formula in the /MF index.

```

=> S EPHEDRINE OR (BENZENEMETHAN?(L)METHYLAMINO ETHYL)
      764 EPHEDRINE
      143517 BENZENEMETHAN?
      667623 METHYLAMINO
      6521955 ETHYL
      89324 METHYLAMINO ETHYL
            (METHYLAMINO(W)ETHYL)
            2184 BENZENEMETHAN?(L)METHYLAMINO ETHYL
L3      2782 EPHEDRINE OR (BENZENEMETHAN?(L)METHYLAMINO
            ETHYL)

=> S L2 AND L3
L4      28 L2 AND L3

=> D SCAN IN

L4      28 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN      Benzenemethanol,  $\alpha$ -[1-(methylamino)ethyl]- (9CI)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L4      28 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN      Benzenemethan-t-ol,  $\alpha$ -[1-(methylamino)ethyl]-,
      [R-(R*,S*)]- (9CI)

L4      28 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN      Benzenemethanol-14C,  $\alpha$ -[1-(methylamino)ethyl]-,
      [S-(R*,S*)]- (9CI)

L4      28 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN      Ephedrine-14C, ( $\pm$ )- (8CI)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

```

Search the common name or fragments of the CA Index name. Combine the name segments with the (L) operator to restrict terms to the same name.

Combine the molecular formula search with the name segments search.

SCAN the CA Index names or structures to verify answers.

Labeled stereoisomers are also retrieved.

Searching for Compositions Containing Stereoisomers

Stereoisomers may also be constituents of multicomponent compounds such as salts, mixtures, or molecular addition compounds. To retrieve these multicomponent substances regardless of stereochemistry, use the same basic strategy of combining the molecular formula and name segments, but now search the component molecular formula in the Basic Index. The Basic Index of REGISTRY includes all components of dot-disconnected formulas as separate searchable segments. To search in the Basic Index, simply enter the component molecular formula without any field code. Use the AND operator to combine the component molecular formulas. Refine the molecular formula search using name segments to ensure precise results.

Find mixtures containing ephedrine or its stereoisomers.

```

=> FILE REGISTRY

=> S EPHEDRINE/CN
L1          1 EPHEDRINE/CN

=> D IN MF

L1  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2005 ACS on STN
IN  Benzenemethanol,  $\alpha$ -[(1S)-1-(methylamino)ethyl]-,
    ( $\alpha$ R)- (9CI)
MF  C10 H15 N O

=> S C10H15NO
L2          3834 C10H15NO

=> S EPHEDRINE OR (BENZENEMETHAN?(L)METHYLAMINO ETHYL)
L3          2782 EPHEDRINE OR (BENZENEMETHAN?(L)METHYLAMINO
    ETHYL)

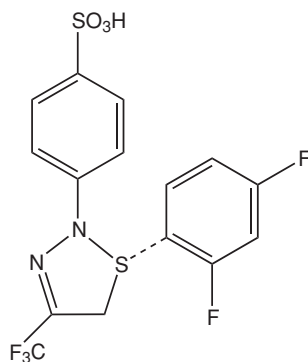
=> S L2 AND L3
L4          1009 L2 AND L3

=> D SCAN

L4  1009 ANSWERS  REGISTRY  COPYRIGHT 2005 ACS on STN
IN  Benzenesulfonic acid, 4-[(5S)-5-(2,4-difluorophenyl)-
    4,5-dihydro-3-(trifluoromethyl)-1H-pyrazol-1-yl]-,
    compd. with ( $\alpha$ S)- $\alpha$ -[(1R)-1-(methylamino)ethyl]
    benzenemethanol (1:1) (9CI)
MF  C16 H11 F5 N2 O3 S . C10 H15 N O

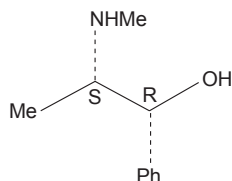
    CM  1
  
```

Absolute stereochemistry.



CM 2

Absolute stereochemistry.



Enter REGISTRY.

Search the common name in the /CN field.

Display the molecular formula (MF) and CA index name (IN).

Search the molecular formula of ephedrine and its stereoisomers in the Basic Index.

Search the common name and name segments from the CA Index name in the Basic Index. Use the (L) operator to restrict terms to the same name.

Combine the molecular formula and name segment searches.

Use DISPLAY SCAN to verify some of the answers.

Molecular addition compounds are also retrieved.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> **S L4 AND MXS/CI**

73860 MXS/CI

L5 124 L4 AND MXS/CI

=> **D SCAN**

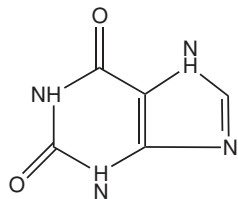
L5 124 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN **1H-Purine-2,6-dione, 3,7-dihydromethyl-, mixt. with
 [R-(R*,S*)]- α -[1-(methylamino)ethyl]benzenemethanol
 (9CI)**

MF **C10 H15 N O . C6 H6 N4 O2**

CI **MXS**

CM 1

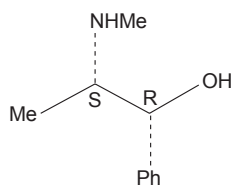
Double bond geometry as shown.



D1—Me

CM 2

Absolute stereochemistry. Rotation (+).



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

To restrict answers to mixtures only, combine the L-number with MXS/CI.

SCAN some answers.

Mixtures containing ephedrine or its isomers are retrieved.

Section 8 Supplementary Information

This section is a collection of supplementary information on topics related to the content of the lessons in this manual. While the lessons focus on the basic strategies, this section provides some additional information that you might find useful in more advanced searches.

Searching Chemical Names with Special Symbols

Complete chemical names in the Chemical Name (/CN) index may contain symbols or characters that require special treatment to find them with the EXPAND command or to search them.

Symbol	Action	Example
Greek letter	put periods before and after the spelled-out name	S .ALPHA.-TOCOPHEROL/CN
Apostrophe (prime)	enclose the entire name in quotes	E "N,N'-DIMETHYLCARBANILIDE"/CN
Parentheses	enclose the entire name in quotes when searching; quotes are not needed when you EXPAND and search E#	S "(2-HYDROXYETHOXY)ACETIC ACID"/CN E (2-HYDROXYETHOXY)ACETIC ACID/CN
Brackets	replace brackets with parentheses and enclose the entire name in quotes when searching; replace brackets with parentheses when you EXPAND and search E#	S "BICYCLO(2.2.1)HEPTANE"/CN E BICYCLO(2.2.1)HEPTANE/CN

Superscripts, subscripts, and italicized letters or numbers are typed on the line with no special notations.

Proximity Operators in the Basic Index

The following proximity operators are available for searching name segments in the Basic Index.

Operator/Definition	Example	Retrievals
(W) Adjacent, in the order entered	BENZOIC(W)ACID	BENZOIC ACID
(nW) In the order entered, with n or fewer intervening segments	IRON(1W)PHOSPHATE	IRON PHOSPHATE IRON HYDROXIDE PHOSPHATE
(XW) In the order entered, with any number of intervening segments	BROMO(XW)BROMO	2-BROMO-2-(BROMOETHYL)-
(A) Adjacent, in either order	CHLORO(A)BROMO	CHLOROBROMO BROMOCHLORO
(nA) Adjacent, in either order, with n or fewer intervening segments	LEAD(1A)OXIDE	LEAD STRONTIUM OXIDE
(XA) In any order, with any number of intervening segments	CHLOROPROPYL(XA)CHLORO	CHLOROPROPYL BIS(2-CHLOROETHYL) CHLORO-1-(3-CHLOROPROPYL)
(L) In the same name	ENE(L)CIS	CIS-P-MENTH-2-ENE

Molecular Formulas for Salts, Mixtures, and Other Multicomponent Substances

For the following classes of compounds, the molecular formulas in REGISTRY appear and are searched in the "dot-disconnected" format:

- Salts and addition compounds
- Mixtures
- Copolymers
- Hydrates
- Alloys and tabular inorganic compounds

These types of substances are represented in REGISTRY as consisting of more than one component. Their complete molecular formula is made up of two or more constituent formulas separated by periods.

Examples:

Organic salts and addition compounds

```
RN 127-09-3 REGISTRY
CN Acetic acid, sodium salt (7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Sodium acetate (6CI)
MF C2 H4 O2 . Na
```

Metal salts of inorganic acids

Metal salts of acids containing O, S, Se, or Te are represented as salts of the acid. The metal is disconnected by a dot from the acid. A "line formula" may appear with the name to identify the salt. However, the line formula is not used for searching in the /MF index.

```
RN 13598-37-3 REGISTRY
CN Phosphoric acid, zinc salt (2:1) (8CI, 9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Zinc phosphate (Zn(H2PO4)2) (6CI, 7CI)
MF H3 O4 P . 1/2 Zn
```

Mixtures

Pharmaceutical, agrochemical, and other mixtures are multicomponent substances in REGISTRY.

```
RN 8003-20-1 REGISTRY
CN 1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-
[(trichloromethyl)thio]-, mixt. with pentachloronitrobenzene
(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzene, pentachloronitro-, mixt. contg. (9CI)
CN Orthocide soil treater X (8CI)
OTHER NAMES:
CN Captan-PCNB mixt.
CN Captan-PCNB mixture
CN PCNB-captan mixt.
MF C9 H8 Cl3 N O2 S . C6 Cl5 N O2
```

Copolymers

Dot-disconnected formulas are used for copolymers. Molecular formulas for each monomer are listed, and the entire expression is enclosed in parentheses. An "x" is used to indicate its polymeric nature.

```
RN 25085-34-1 REGISTRY
CN 2-Propenoic acid, polymer with ethenylbenzene (9CI) (CA INDEX
NAME)
OTHER CA INDEX NAMES:
CN Acrylic acid, polymer with styrene (8CI)
CN Benzene, ethenyl-, polymer with 2-propenoic acid (9CI)
MF (C8 H8 . C3 H4 O2)x
```

Hydrates

```
RN 6192-52-5 REGISTRY
CN Benzenesulfonic acid, 4-methyl-, monohydrate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN p-Toluenesulfonic acid, monohydrate (8CI)
OTHER NAMES:
CN 4-Toluenesulfonic acid monohydrate
MF C7 H8 O3 S . H2 O
```

Alloys and tabular inorganic compounds

The molecular formulas for these compounds are also represented as alphabetic lists of dot-disconnected metals or other components. Information on the composition, for example, relative percentage of each metal, a ratio, or a fractional composition, may be included and displayed as part of the name for each compound.

```
RN 138413-28-2 REGISTRY
CN Aluminum alloy, base, Al 94,Mg 4.9,Mn 1,Ti 0.2,Fe 0.1 (9CI)
(CA INDEX NAME)
MF Al . Fe . Mg . Mn . Ti
```

```
RN 138701-56-1 REGISTRY
CN Gallium, compd. with germanium and manganese (10.5:2.5:20) (9CI)
(CA INDEX NAME)
MF Ga . Ge . Mn
```

```
RN 166092-66-6 REGISTRY
CN Aluminum gallium arsenide (Al0-0.95Ga0.05-1As) (9CI) (CA INDEX
NAME)
MF Al . As . Ga
```

The easiest way to search the molecular formula of multicomponent substances is to EXPAND on the molecular formula of the first component and select the E-numbers from the EXPAND list. However, you still need to know the order in which the molecular formulas for the components are listed. The Hill System Order is applied to arrange elements within each component. CAS also applies the following rules to keep the order of components consistent.

Substance Content	Order and Example
No carbon-containing components	Alphabetical, using the first element of each component H6 O6 Te. Li. Nb
There is a carbon-containing component and a non-carbon-containing component	Carbon component comes first C37 H31 N. Cl O4
All components contain carbon	Component with the highest number of carbons first, with others arranged in descending order C17 H20 Cl N3 O. C13 H29 N3. C2 H4 O2
Two or more components have the same number of carbon atoms	Order determined by the number of hydrogen atoms, the component with the highest number of hydrogens coming first C6 H10 O7. C6 H8 O6. H2 O4 S. Zn
Two or more components have the same number of carbons and hydrogens	Alphabetical, using the remaining elements

Complete molecular formulas may contain special characters that need to be masked before searching. To mask a special character, simply enclose the entire molecular formula in quotes.

Special character	Example
Parentheses and "x" for polymers	=> S "(C8H8.C3H4O2)X"/MF
A slash in fractions	=> S "H3O4P.1/2ZN"/MF

Section 9 Cost of Searching in REGISTRY

- Objectives:**
- To understand the variety of charges associated with searching
 - To know how to find the costs incurred in a session
 - To know how to find information about the costs of using a certain file

- Topics:**
- Types of Charges
 - Cost of Using REGISTRY and LREGISTRY
 - DISPLAY COST to view charges incurred

There are many advantages to searching for information online rather than in the library stacks. However, online searching does have certain costs associated with it. The purpose of this section is to present background information on the full costs of online searching. Discounts are not discussed or shown in the specific examples.

Types of Charges

There are four types of charges on STN:

- Connect-hour charges in each database
You are charged a certain fee per minute while you are in the database.
- Display charges
In each database, there are charges for records displayed. This fee varies depending on how much data you display.
- Search-term charges
In some databases, there is a charge for each term you search.
- Telecommunication charges
If you use a telecommunications service, each service has its own charges. The costs of an internal network or Internet may be transparent to you.

Cost of Using REGISTRY and LREGISTRY

Costs vary by database. To see the current charges for a database, enter HELP COST in the database. HELP COST shows the full cost for an online session. Discounts are not shown.

Use LREGISTRY for training and displaying online help messages. Except for the HELP COST message, LREGISTRY has the same help messages as REGISTRY.

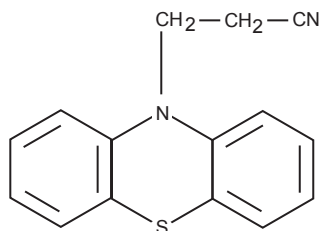
DISPLAY COST

Enter D COST at any time to see the charges that have been incurred so far in the session. Enter D COST FULL to see more detailed information on the cost.

Section 10 Practice Problems in REGISTRY and LREGISTRY

You can use these practice problems in both REGISTRY and LREGISTRY.

1. What is the chemical composition of Alachlor?
2. Find the CAS Registry Numbers for all Lexans.
3. Find the CAS Registry Number for arsenic trichloride.
4. Search for cobaltocene or cobaltocenium compounds.
5. Find the CAS Registry Numbers for dibromobenzenes.
6. Find the CAS Registry Number for the compound with the following structure:



7. What is the CAS Registry Number for the mixture of Captan and PCNB?
8. Find any mixtures or salts of ibuprofen.
9. Find any mixtures or salts of naproxen or any of its stereoisomers.

