



Using the CAS RegistrySM File on STN[®]

Presentation

Content of REGISTRY

Types of substances

- Organics
- Inorganics
- Alloys
- Protein sequences
- Nucleic acid sequences
- Coordination compounds
- Minerals
- Mixtures
- Polymers
- Salts



Sample record

Display fields

- RN - CAS Registry Number[®]
- CN - Chemical and trade names
- MF - Molecular formula
- CI - Class Identifier
- LC - CAS Registry Number Locator
- STR - Structure diagram



LREGISTRYSM

- Training database
- Approximately 125,000 substance records for substances indexed in LCASM



Displaying information for a CAS Registry Number

- Enter REGISTRY
- EXPAND on the CAS Registry Number
- Search the E-number



Locating CASM references

1. Enter REGISTRY
2. Enter your search terms, e.g., a trade name in the Chemical Name (/CN) field
3. Use D SCAN to evaluate your query
4. Enter CA
5. Search the L-number answer set from REGISTRY in CA



Chemical names in REGISTRY

- Names included: CA Index Names, IUPAC names, commonly used names, trade names
- Complete names searched in the Chemical Name (/CN) index



Searching in the /CN index

1. Enter REGISTRY
2. EXPAND in the /CN index
3. Include any spaces or punctuation
4. Follow the name with /CN
5. Enter the number of lines to view
(12 is the default)
6. Search the E-number
7. Enter D to view the substance information
(default format)



Finding references to 1,3-dibromoheptane

1. Enter REGISTRY
2. EXPAND on the name in the /CN index
3. Search the E-number
4. Use D SCAN to verify the structure and name
5. Enter CA
6. Search the L-number from REGISTRY



Using truncation

- EXPAND in the /CN field to determine truncation
- Search the truncated name in the /CN index

S ALATANIN?/CN



Name segments in the Basic Index

Complete name: thiophene, 2,4-dibromo-

Name segments in the Basic Index:

- thiophene
- 2,4
- 2
- 4
- dibromo
- di
- bromo



Searching name segments

- Basic Index is assumed if field code is not specified
- Use the AND operator for broad searches
- Use proximity operators for more precise searches



Using proximity operators with name segments

Operator	Definition
(L)	In the same name, in any order
(A)	Adjacent, in either order
(W)	Adjacent, in the order entered

Find dinitrobromothiophenes

- EXPAND on the significant name segments in the Basic Index
- Use the (L) operator to require the segments to be in the same name
- Use D SCAN to view some answers



Searching molecular formulas

- In the /MF field
- In Hill System Order

C7H8O2

CLNA

H2O4S

- With or without spaces between elements



Combining the molecular formula with name segments

1. EXPAND in the /MF index

E C7H8O2/MF

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

S E3 AND PHENOL

3. Refine by combining with another name segment

S L1 AND 3-METHOXY



Salts in REGISTRY

- Represented as multicomponent substances
- Named and structured by CAS using the acid or base from which they are formed
- Molecular formula displayed in the dot-disconnected format

C2H4O2 . NA



Searching for salts

Content	Field
Name	/CN
Molecular formula	/MF
Component CAS Registry Number	/CRN
Component molecular formula	/BI
Number of components	/NC



Searching for the barium salt of benzoic acid

1. Search the name of the acid in the /CN field
S BENZOIC ACID/CN
2. Display the molecular formula for the acid
3. Combine the molecular formula for each component with AND
S C7H6O2 AND BA
4. Use D SCAN IN MF (CA Index Name and molecular formula)
5. Restrict to two-component substances
S L2 AND 2/NC



Searching for potassium sulfates

- Combine the molecular formula for the acid with the element name in /BI
S H2O4S AND POTASSIUM
- D SCAN IN MF
- Restrict results to two-component salts
S L1 AND 2/NC



Mixtures in REGISTRY

Display code	Content
RN	CAS Registry Number for the mixture
CN	Names
MF	Molecular formula
CM1, CM2	Each component
CRN	Component CAS Registry Number



Searching for mixtures

Content	Field
Names	/CN
Name segments	/BI
Complete molecular formula	/MF
Component molecular formula	/BI
Component CAS Registry Number	/CRN



Using the Component CAS Registry Number

- Find the CAS Registry Numbers for the components
- Search the CAS Registry Numbers in the /CRN field
- Use the AND operator to combine Component CAS Registry Numbers



Find mixtures of azidothymidine

1. EXPAND on the name in the /CN field

E AZIDOTHYIMIDINE/CN

2. Search the name for the component

S E3

3. Display the CAS Registry Number for the component

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

S 30516-87-1/CRN



Searching the number of components

Number of components	Examples
Specific number	S 2/NC S L1 AND 3/NC
Range	S NC>2 S 2-3/NC S NC<=3



Stereoisomers in REGISTRY

- Each stereoisomer assigned its own CAS Registry Number
- Molecular formula is the same
- Stereo designation included in the CA Index Name



Find stereoisomers of ephedrine

1. Search the name in the /CN field
S EPHEDRINE/CN
2. Display the CA Index Name and molecular formula
3. Search the molecular formula in the /MF field
S C10H15NO/MF
4. Search the name or name fragments combined with the (L) operator
S EPHEDRINE/CN OR (BENZENEMETHAN? (L)METHYLAMINO ETHYL)
5. Combine the molecular formula with the name fragment search



Find mixtures containing ephedrine or its stereoisomers

1. Search name segments in the /BI field
2. Search the component molecular formula in the /BI field
3. Search for mixtures in the Class Identifier (/CI) field

S L4 AND MXS/CI

