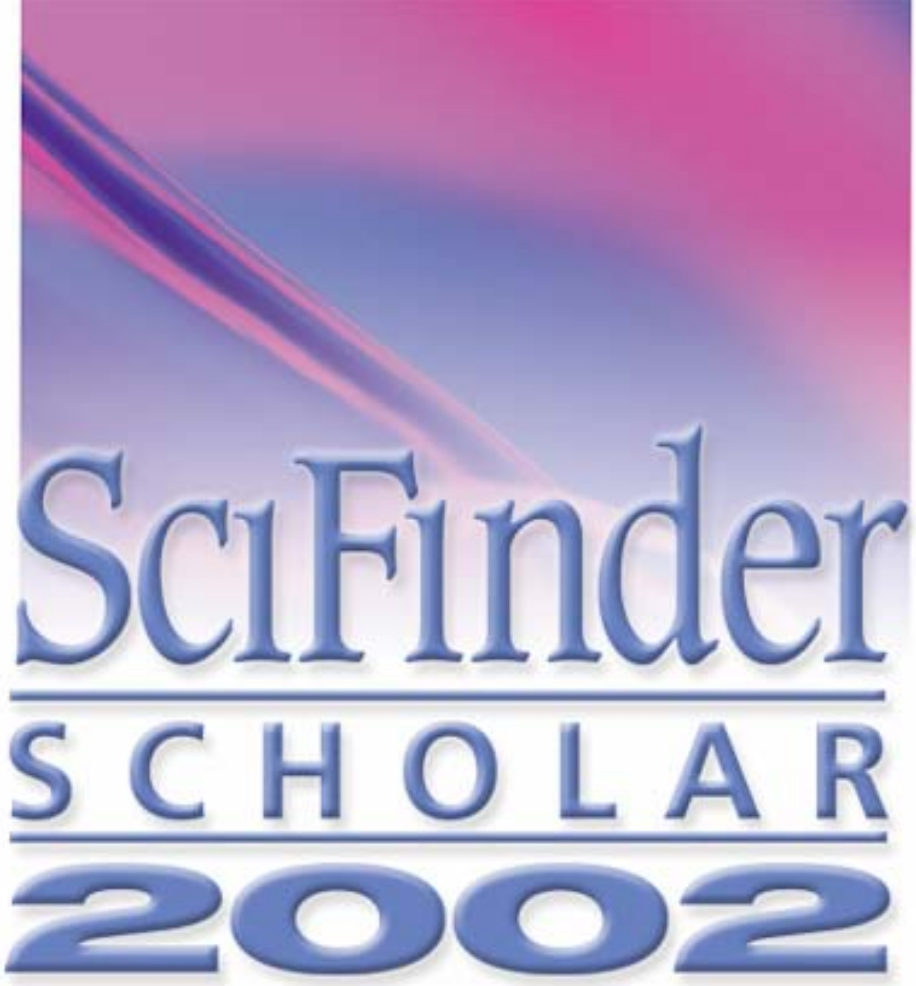


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# Substances with no references in CAS Registry

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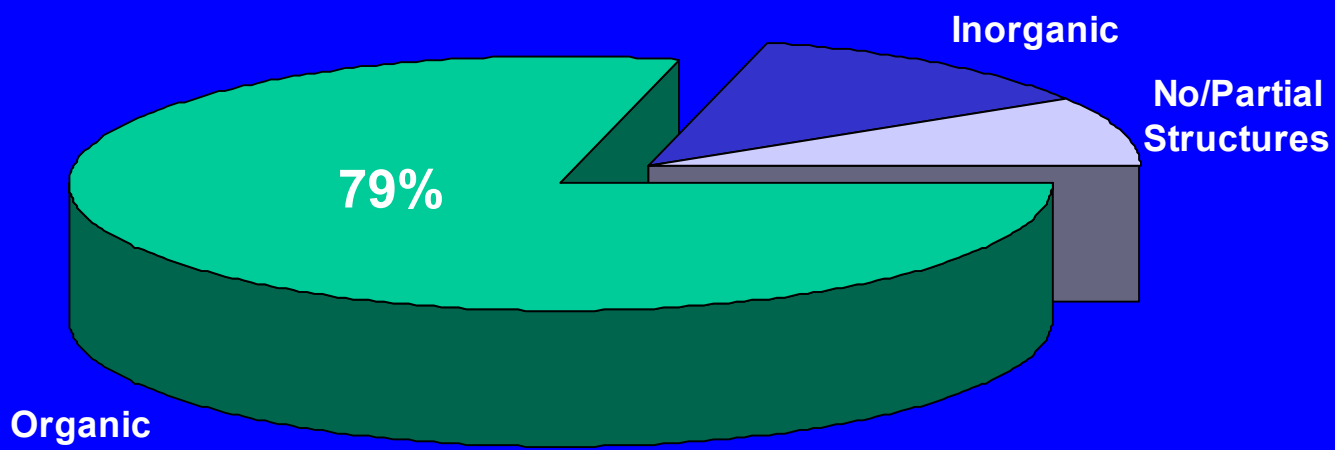
*bdunne@cas.org*

# CAS REGISTRY

- The CAS Registry file contains mainly substances that were encountered in the literature and patents
  - ~8,000 scientific and technical journals
  - patents from 37 patent-issuing authorities
- There are situations where a substance is not associated with any literature information

# Chemical substances in Registry

**21,126,771** non-sequence substances (March 2003)




SciFinder SCHOLAR 2002

# CAS is adding substance information to CAS databases at a record pace

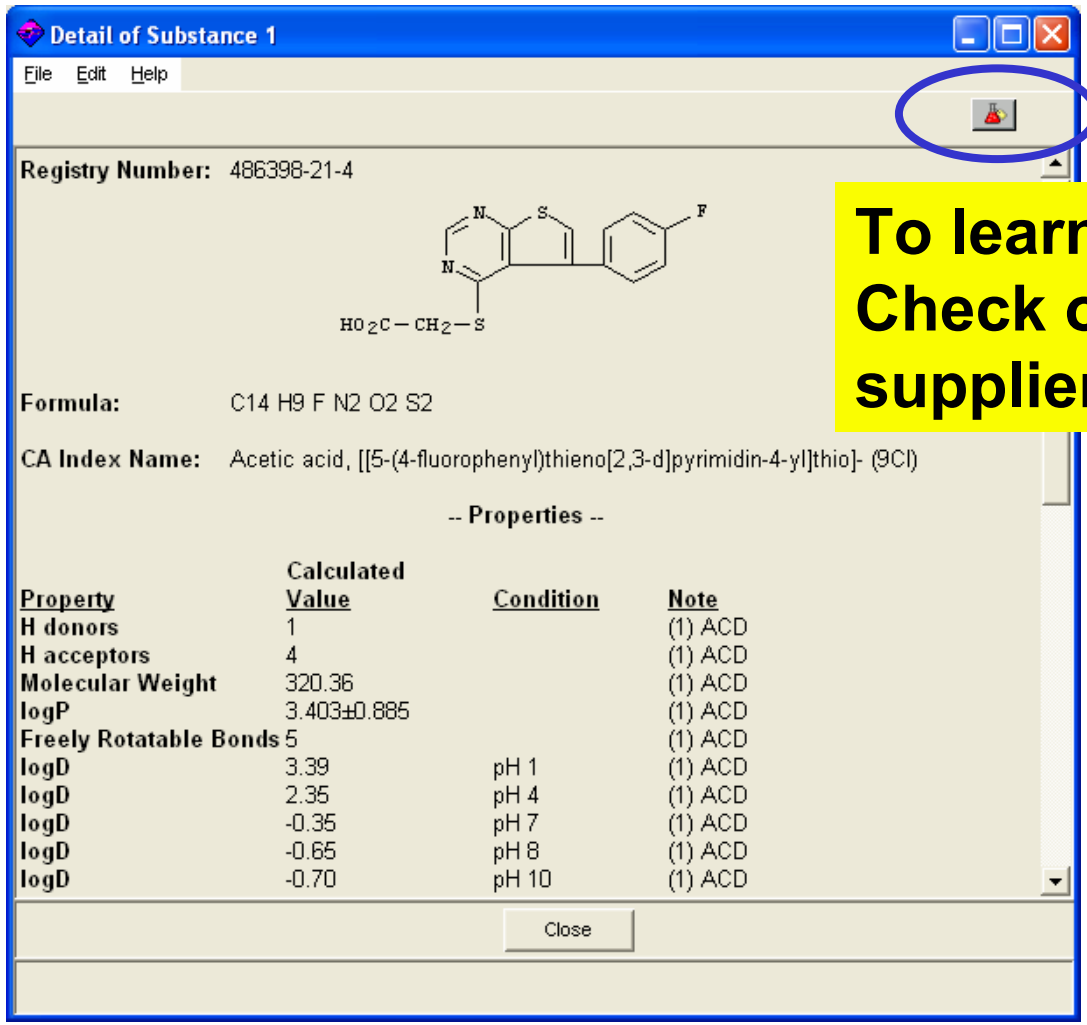
- CAS analysts added new information on 9.76 million substances in 2002
  - 8.1 m sequences
  - 1.66 m non-sequences
- 3.3 m new substances had >=1 reference(s) in CAplus
  - 2.5 m sequences
  - 0.8 m non-sequences
- 10,000 substances updated/added daily
  - New references from both patents and journals
  - Additional structure information
  - New chemical names, *eg* trade names

SciFinder SCHOLAR 2002

# CAS records substance occurrences in many different situations

- The majority of these substances have one or more associated references
- Some may be encountered showing no literature references
- Possible cases are outlined on the following slides

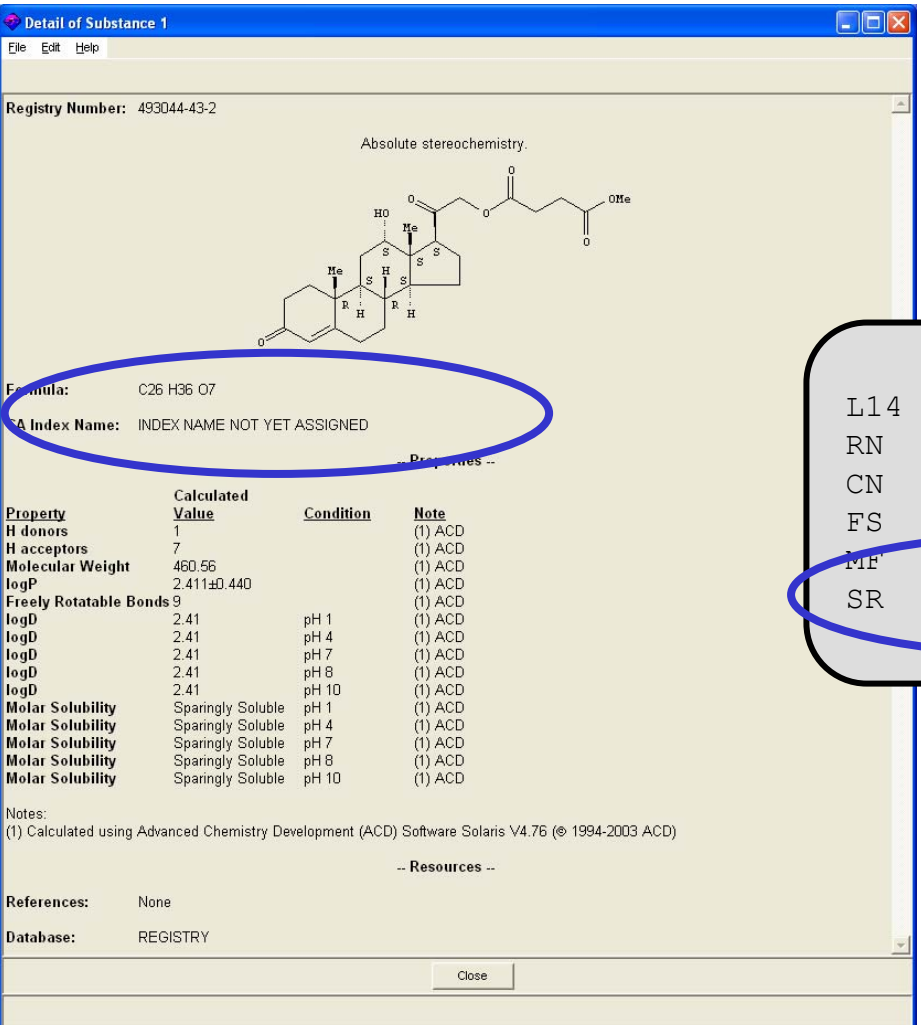
# Substance only cited in CHEMCATS®




**To learn more: Check out the supplier collection**

SciFinder SCHOLAR 2002

# Substance was very recently registered - no name/file information available yet




```
L14   ANSWER 3 OF 25528  REGISTRY  COPYRIGHT 2003 ACS
RN    493044-43-2  REGISTRY
CN    INDEX NAME NOT YET ASSIGNED
FS    STEREOSEARCH
MF    C26 H36 O7
SR    Reaction Database
```

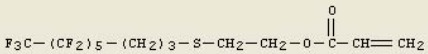
**To learn more: Check periodically or contact CAS for additional information**

# Substance only registered as a component

**Detail of Substance 1**

File Edit Help

**Registry Number:** 493046-07-4



**Formula:** C14 H13 F13 O2 S

**CA Index Name:** 2-Propenoic acid, 2-[(4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl)thio]ethyl ester (9CI)

-- Properties --

| Property | Calculated Value | Condition | Note |
|---|---|---|---|
| H donors | 0 | | (1) ACD |
| H acceptors | 2 | | (1) ACD |
| Molecular Weight | 492.30 | | (1) ACD |
| logP | 6.760±0.952 | | (1) ACD |
| Freely Rotatable Bonds | 13 | | (1) ACD |
| logD | 6.76 | pH 1 | (1) ACD |
| logD | 6.76 | pH 4 | (1) ACD |
| logD | 6.76 | pH 7 | (1) ACD |
| logD | 6.76 | pH 8 | (1) ACD |
| logD | 6.76 | pH 10 | (1) ACD |
| Molar Solubility | Sparingly Soluble | pH 1 | (1) ACD |
| Molar Solubility | Sparingly Soluble | pH 4 | (1) ACD |
| Molar Solubility | Sparingly Soluble | pH 7 | (1) ACD |
| Molar Solubility | Sparingly Soluble | pH 8 | (1) ACD |
| Molar Solubility | Sparingly Soluble | pH 10 | (1) ACD |

Notes:
(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 (© 1994-2003 ACD)

-- Resources --

**References:** None

**Database:** REGISTRY

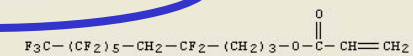
Close

**Detail of Substance 2**

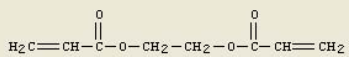
File Edit Help

**Registry Number:** 493046-06-3

Component Registry Number: 493046-05-2
Formula: C14 H11 F15 O2



Component Registry Number: 2274-11-5
Formula: C8 H10 O4



Component Registry Number: 80-05-7
Formula: C15 H16 O2

**Formula:**

**CA Index Name:**

**Class Identifier:**

**Polymer Class Term:**

**References:**

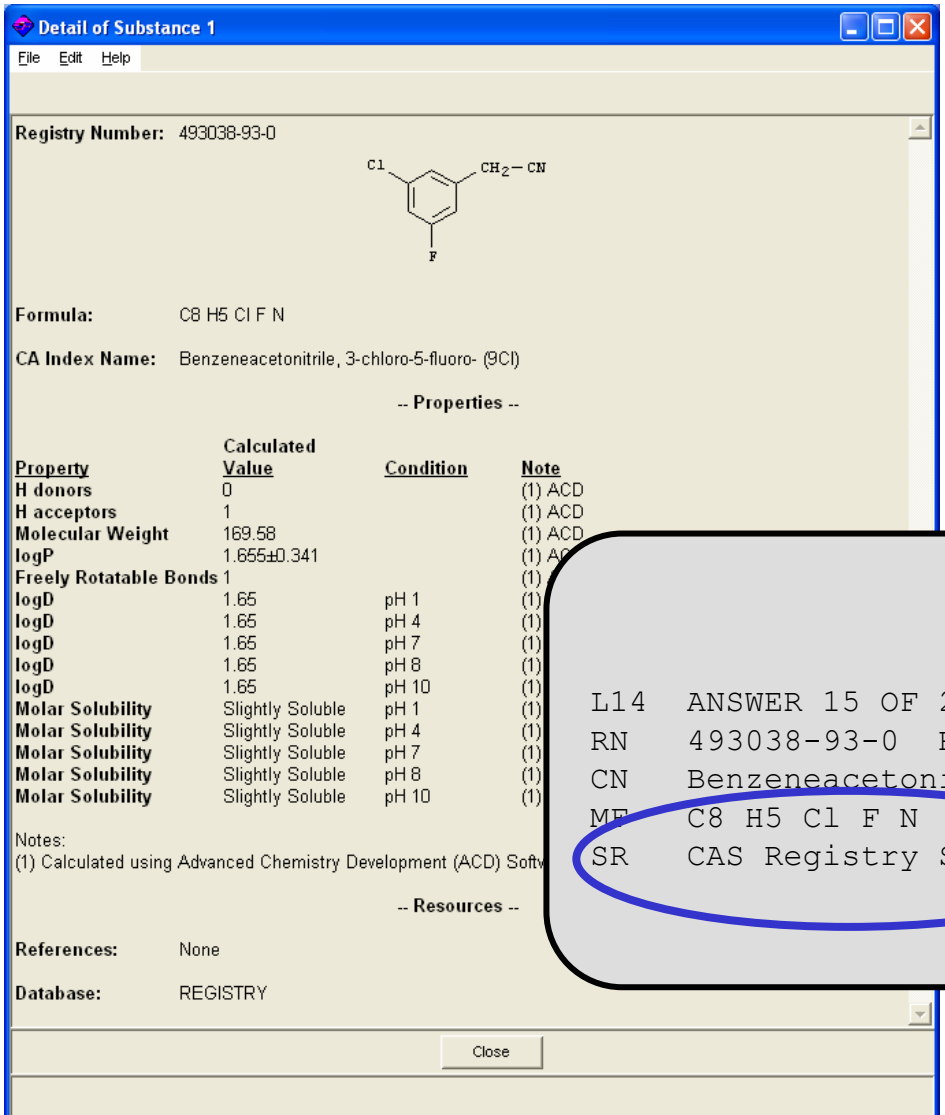
**STN Files:**

**Database:** REGISTRY

Close

**To learn more: Conduct a "family" search to locate substances in which the compound of interest is a component**

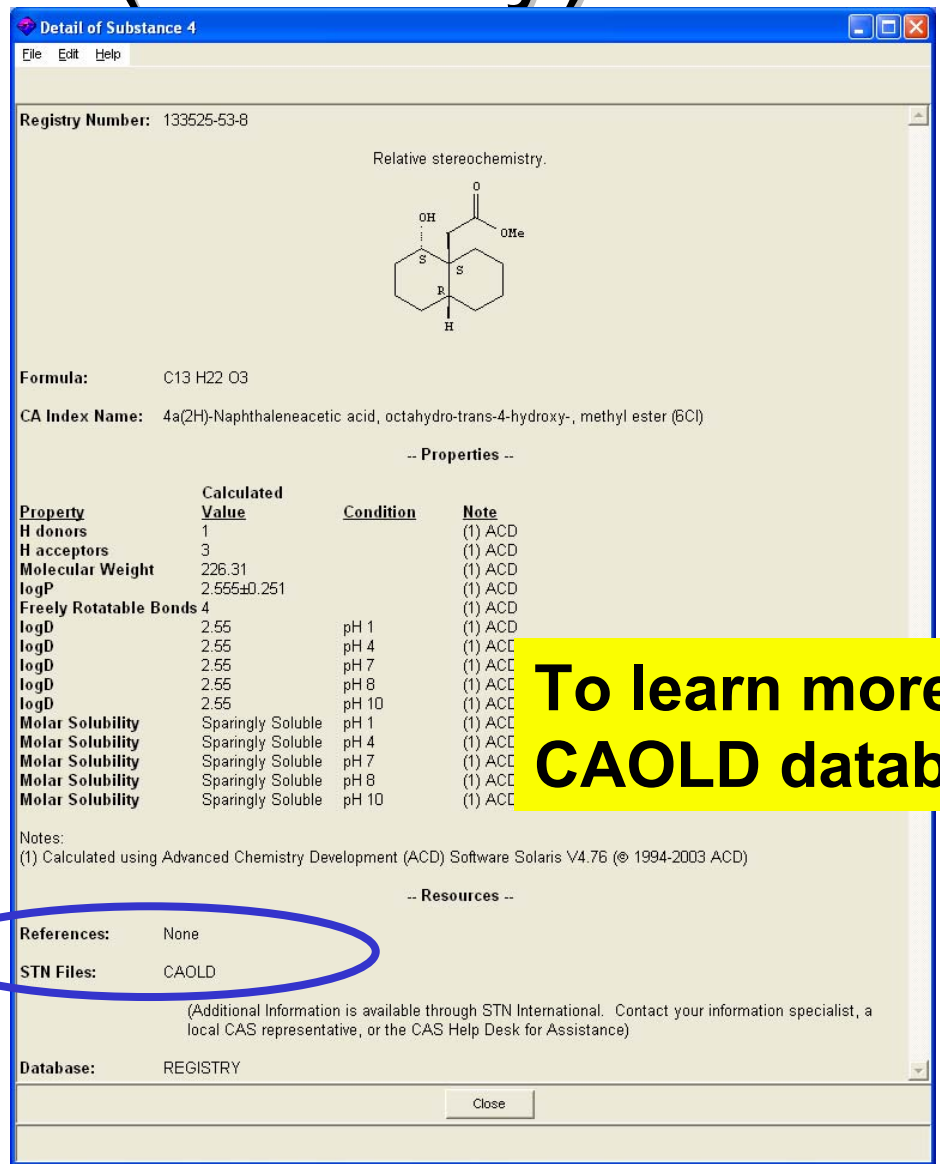
# Registration by CAS Registry Services℠




**To learn more: The majority of these are proprietary registrations for which additional information is not available**

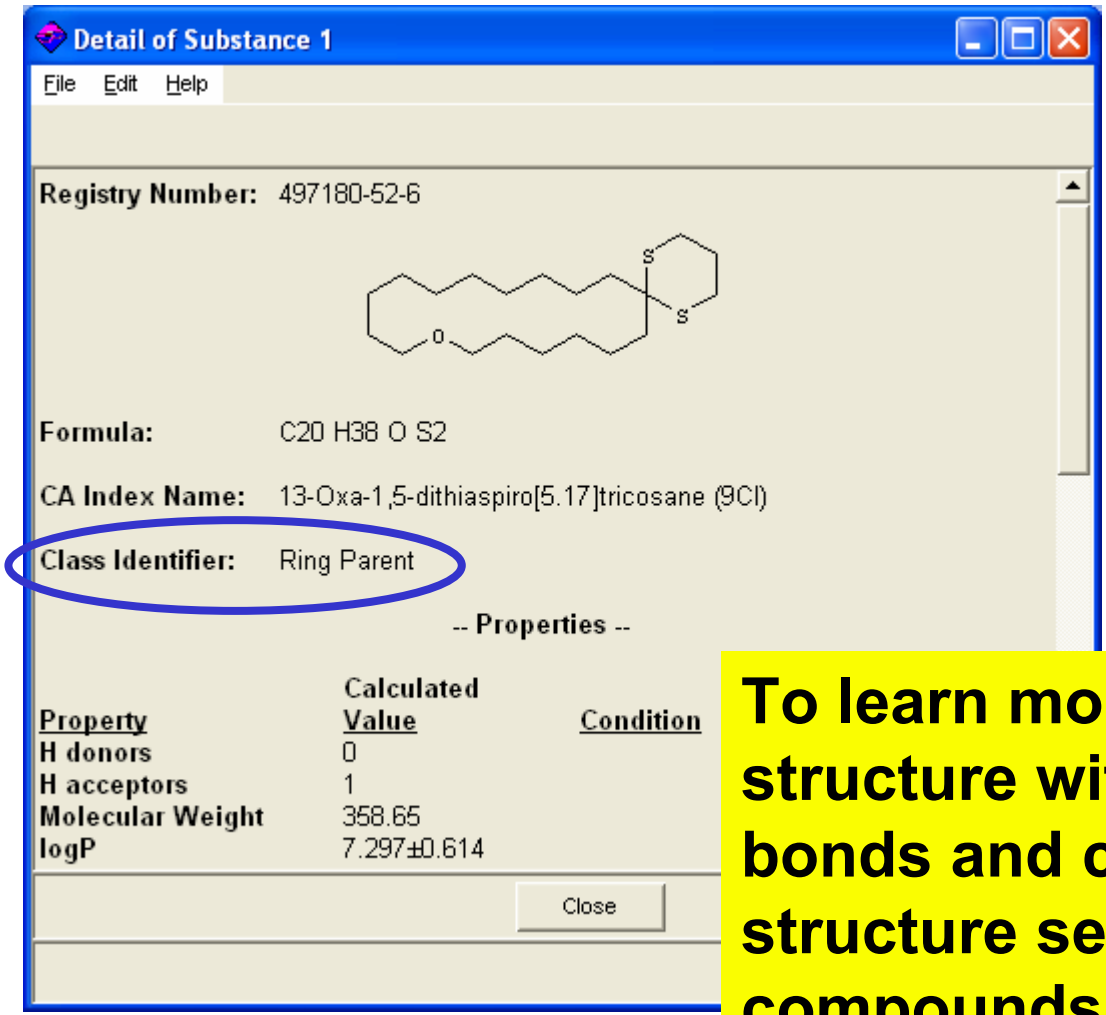
```
L14   ANSWER 15 OF 25528  REGISTRY  COPYRIGHT 2003 ACS
RN    493038-93-0  REGISTRY
CN    Benzeneacetonitrile, 3-chloro-5-fluoro- (9CI)  (CA INDEX NAME)
MF    C8 H5 Cl F N
SR    CAS Registry Services
```

# Substance only cited in CAOLD$^{SM}$ (currently)



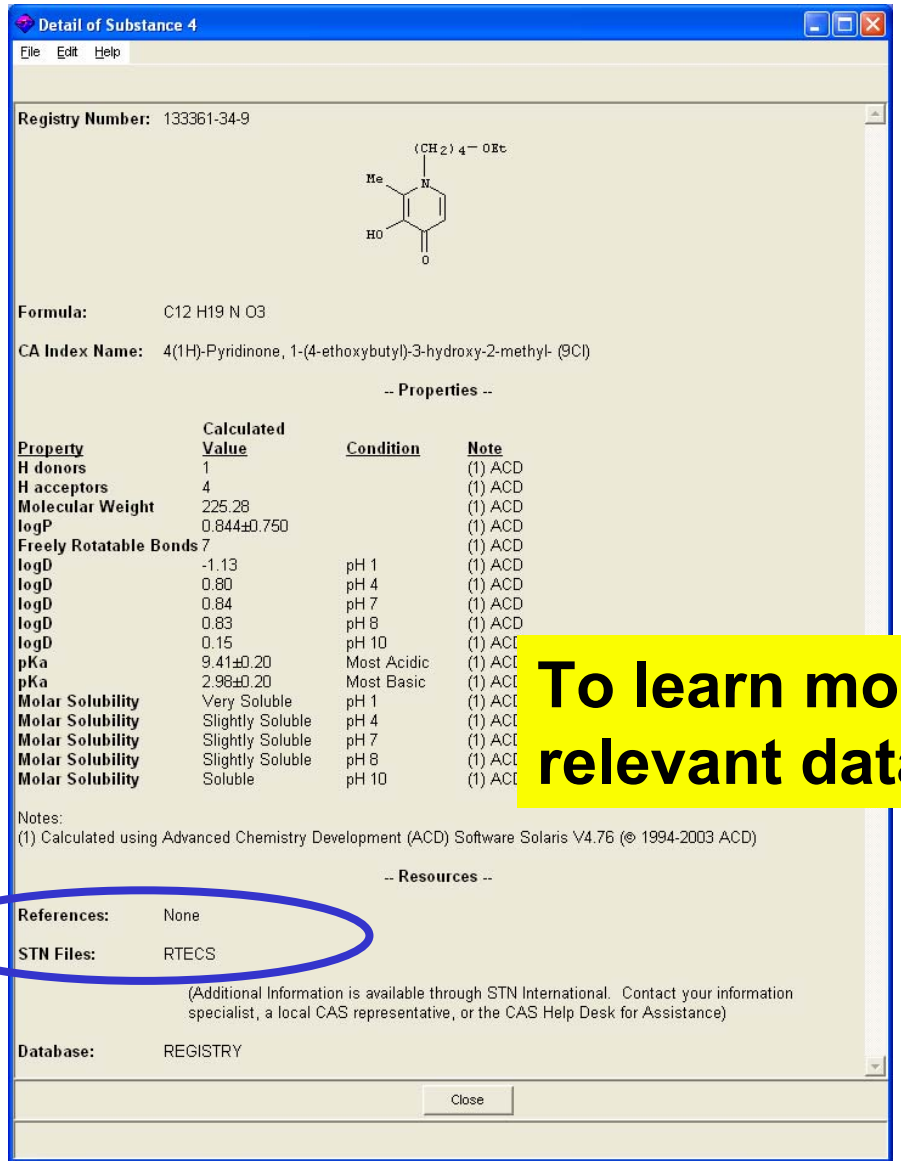

**To learn more: Check the CAOLD database on STN®**

# Substance is a Ring Parent



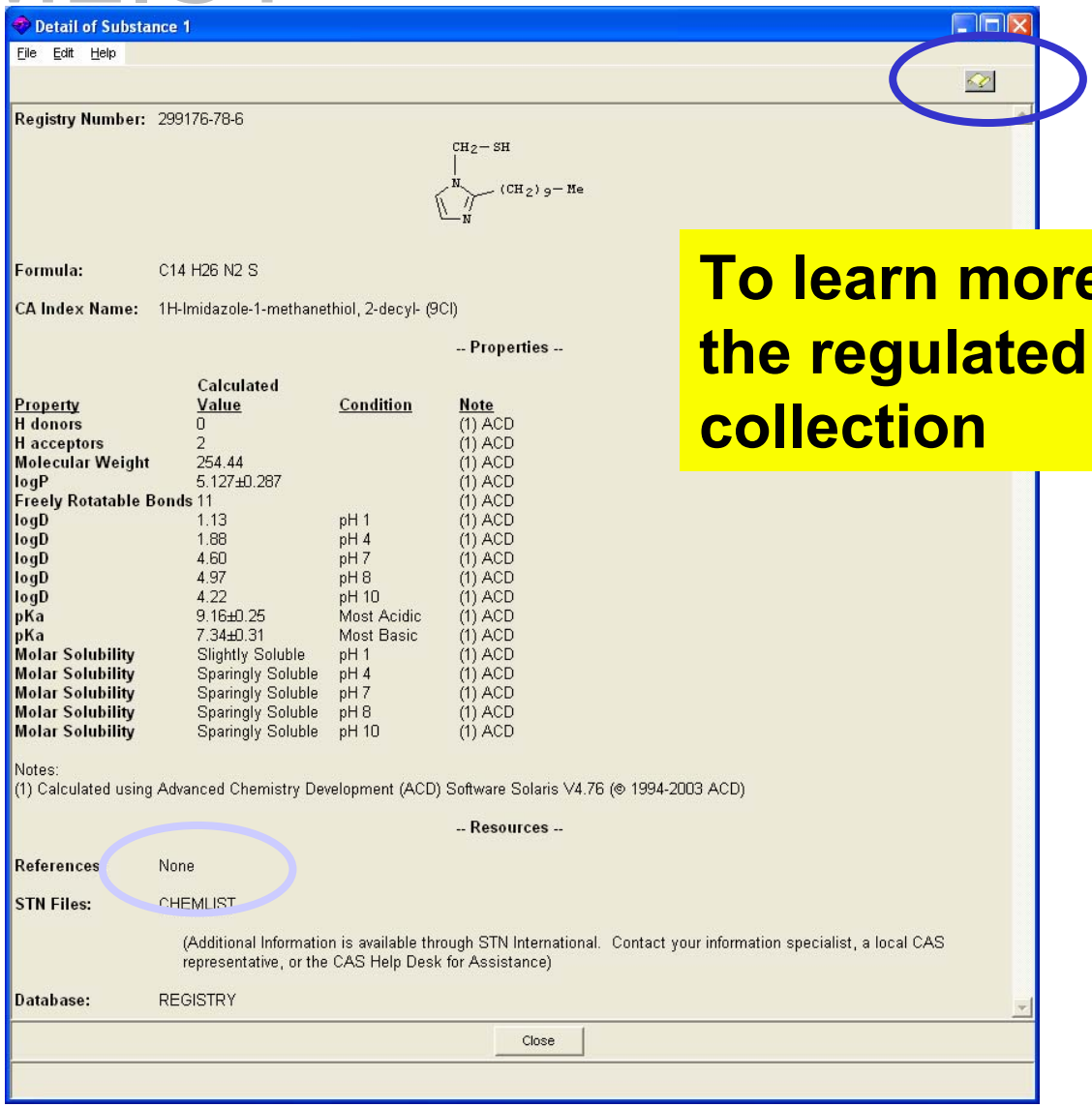

**To learn more: Create a structure with unspecified bonds and conduct a structure search to locate compounds containing this ring system**

# Substance only cited in another STN database




**To learn more: Consult the relevant database on STN**

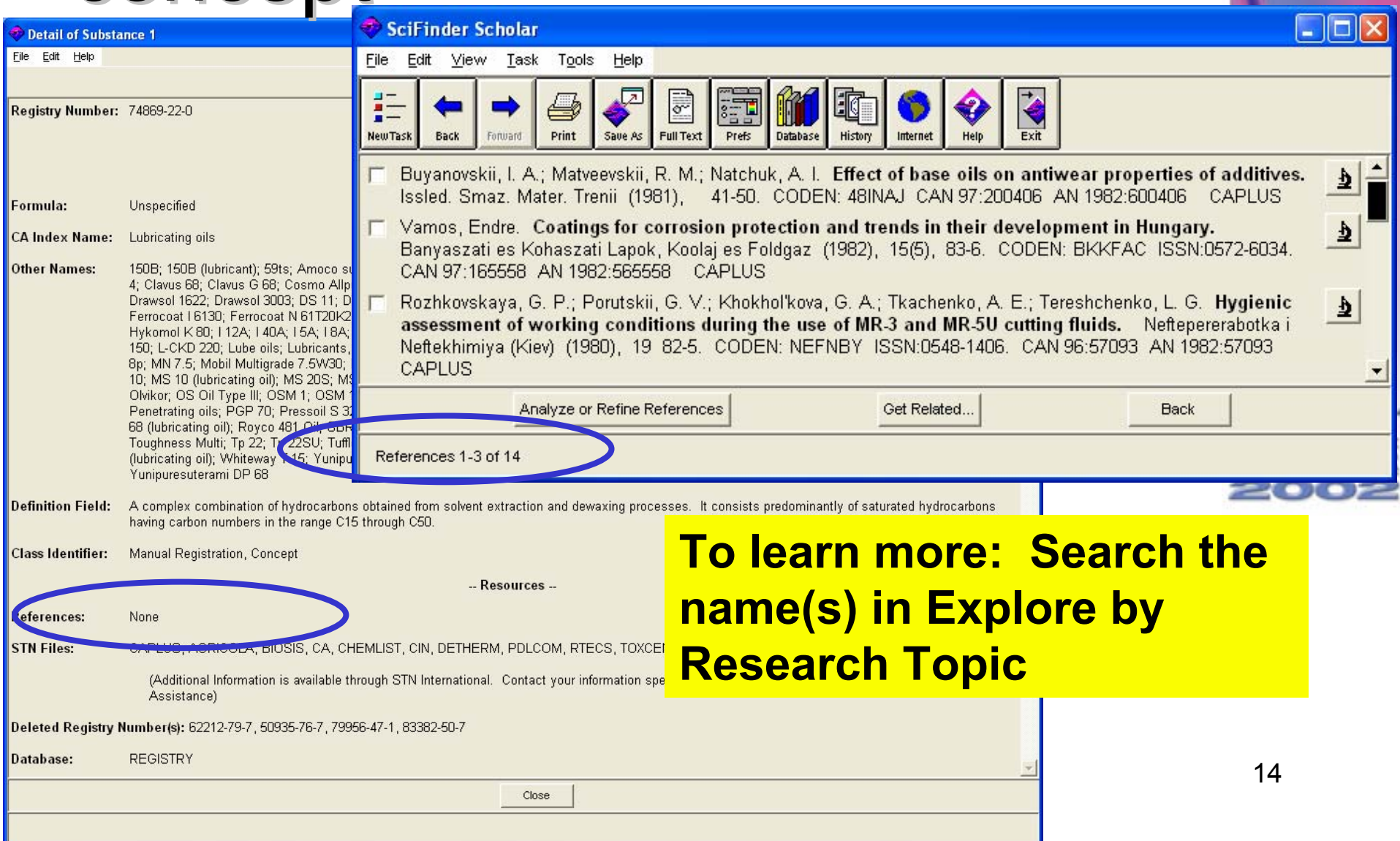
# Substance only cited in CHEMLIST®




**To learn more: Check out the regulated chemicals collection**

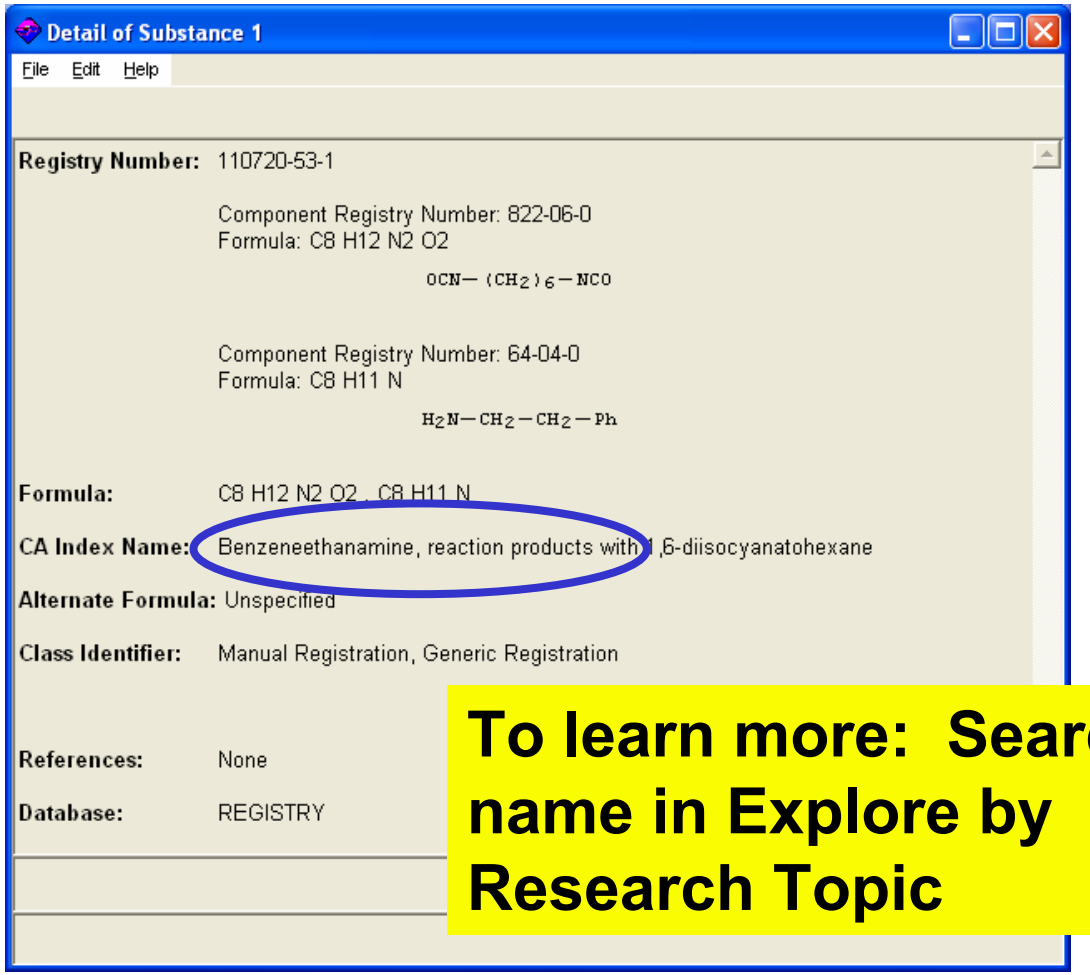
SciFinder SCHOLAR 2002

# Substance registered as a concept



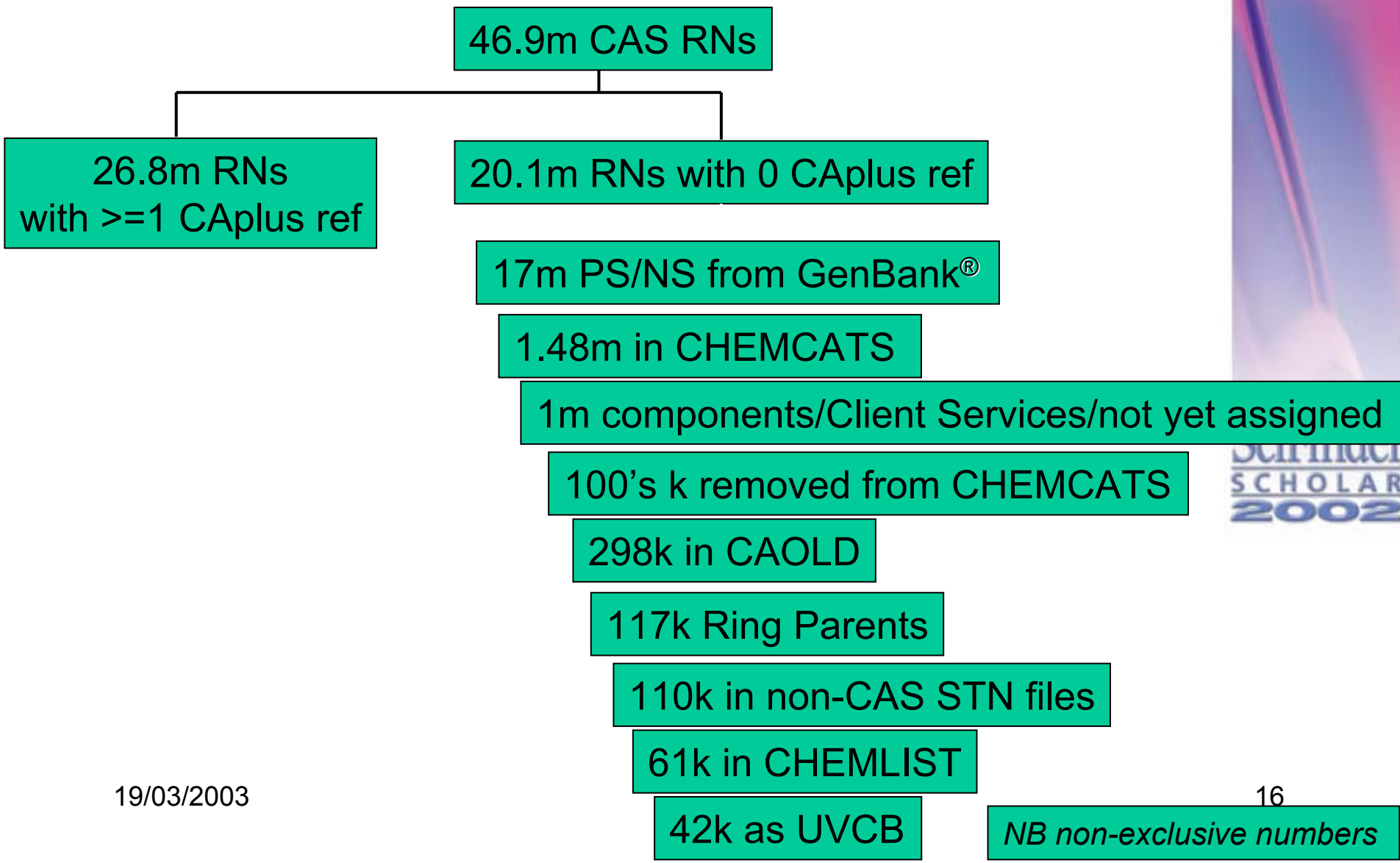

**To learn more: Search the name(s) in Explore by Research Topic**

# Substance only registered as a generic entry



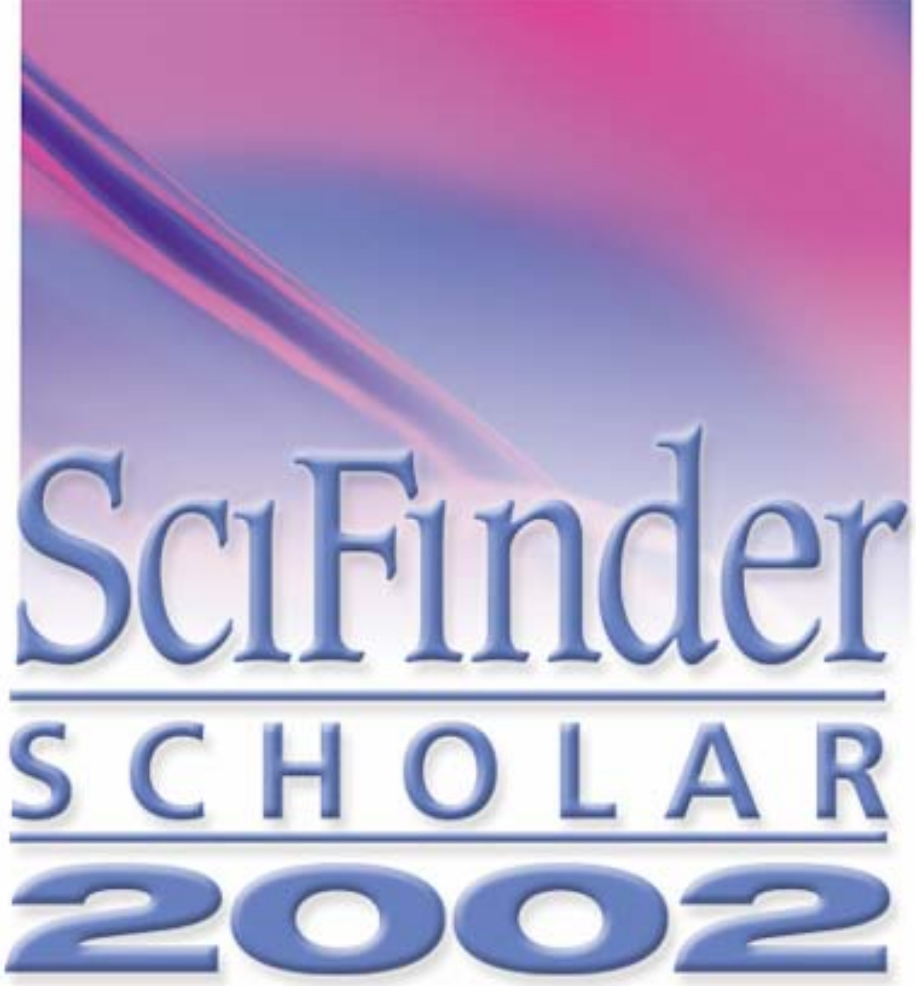

**To learn more: Search the name in Explore by Research Topic**

# Reference summary



# Summary

- The majority of substances in the CAS REGISTRY are derived from literature or patent references
- Many sequences may show no associated references (*eg* GenBank author submissions)
- Some small molecules may show no associated references
- Further information can generally be derived from the detailed display in SciFinder® Scholar™ or on STN

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# Substances with no references in CAS Registry

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