

The logo for SciFinder Scholar 2002 features the text "SciFinder" in a large, blue, serif font with a registered trademark symbol. Below it, "SCHOLAR" is written in a smaller, blue, sans-serif font, and "2002" is in a large, blue, sans-serif font. The text is set against a background of a purple and blue gradient with a diagonal line.

SciFinder®
SCHOLAR
2002



Substances with no references in
CAS Registry

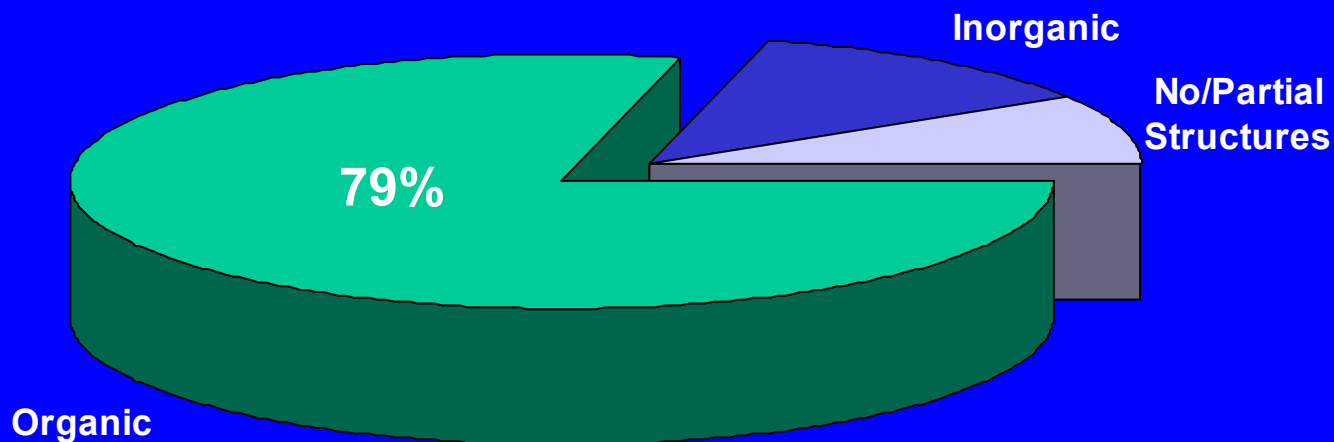
Dr Barry Dunne, SII/CAS
bdunne@cas.org

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)



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

CAS records substance occurrences in many different situations

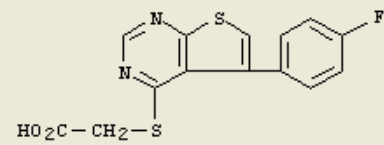
- The majority of these substances have one or more associated references
- Some may be encountered showing no literature references
- Possible cases are outlined on the following slides

Substance only cited in CHEMCATS®

Detail of Substance 1

File Edit Help

Registry Number: 486398-21-4



Formula: C14 H9 F N2 O2 S2

CA Index Name: Acetic acid, [[5-(4-fluorophenyl)thieno[2,3-d]pyrimidin-4-yl]thio]- (9CI)

-- Properties --

Property	Calculated Value	Condition	Note
H donors	1		(1) ACD
H acceptors	4		(1) ACD
Molecular Weight	320.36		(1) ACD
logP	3.403±0.885		(1) ACD
Freely Rotatable Bonds	5		(1) ACD
logD	3.39	pH 1	(1) ACD
logD	2.35	pH 4	(1) ACD
logD	-0.35	pH 7	(1) ACD
logD	-0.65	pH 8	(1) ACD
logD	-0.70	pH 10	(1) ACD

Close

To learn more:
Check out the
supplier collection

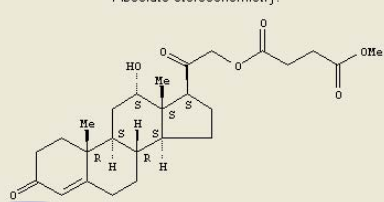
SciFinder
SCHOLAR
2002

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

Detail of Substance 1

Registry Number: 493044-43-2

Absolute stereochemistry.



Formula: C₂₆ H₃₆ O₇

Index Name: INDEX NAME NOT YET ASSIGNED

Property	Calculated Value	Condition	Note
H donors	1		(1) ACD
H acceptors	7		(1) ACD
Molecular Weight	460.56		(1) ACD
logP	2.411±0.440		(1) ACD
Freely Rotatable Bonds	9		(1) ACD
logD	2.41	pH 1	(1) ACD
logD	2.41	pH 4	(1) ACD
logD	2.41	pH 7	(1) ACD
logD	2.41	pH 8	(1) ACD
logD	2.41	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)

References: None

Database: REGISTRY

Close

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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

Registry Number: 493046-07-4

$$\text{F}_3\text{C}-(\text{CF}_2)_5-(\text{CH}_2)_3-\text{S}-\text{CH}_2-\text{CH}_2-\text{O}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}=\text{CH}_2$$

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-tridecafluoronyl)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

Registry Number: 493046-06-3

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

$$\text{F}_3\text{C}-(\text{CF}_2)_5-\text{CH}_2-\text{CF}_2-(\text{CH}_2)_3-\text{O}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}=\text{CH}_2$$

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

$$\text{H}_2\text{C}=\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_2-\text{CH}_2-\text{O}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}=\text{CH}_2$$

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

Formula: (C

CA Index Name: IN

Class Identifier: P

Polymer Class Term:

References: ~

STN Files: C

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 ServicesSM

Detail of Substance 1

File Edit Help

Registry Number: 493038-93-0

Formula: C8 H5 Cl F N

CA Index Name: Benzeneacetonitrile, 3-chloro-5-fluoro- (9CI)

-- Properties --

Property	Calculated Value	Condition	Note
H donors	0		(1) ACD
H acceptors	1		(1) ACD
Molecular Weight	169.58		(1) ACD
logP	1.655±0.341		(1) ACD
Freely Rotatable Bonds	1		(1)
logD	1.65	pH 1	(1)
logD	1.65	pH 4	(1)
logD	1.65	pH 7	(1)
logD	1.65	pH 8	(1)
logD	1.65	pH 10	(1)
Molar Solubility	Slightly Soluble	pH 1	(1)
Molar Solubility	Slightly Soluble	pH 4	(1)
Molar Solubility	Slightly Soluble	pH 7	(1)
Molar Solubility	Slightly Soluble	pH 8	(1)
Molar Solubility	Slightly Soluble	pH 10	(1)

Notes:
(1) Calculated using Advanced Chemistry Development (ACD) Software

-- Resources --

References: None

Database: REGISTRY

Close

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

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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
```

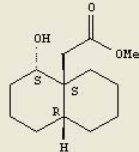
Substance only cited in CAOLDSM (currently)

Detail of Substance 4

File Edit Help

Registry Number: 133525-53-8

Relative stereochemistry.



Formula: C13 H22 O3

CA Index Name: 4a(2H)-Naphthaleneacetic acid, octahydro-trans-4-hydroxy-, methyl ester (6CI)

-- Properties --

Property	Calculated Value	Condition	Note
H donors	1		(1) ACD
H acceptors	3		(1) ACD
Molecular Weight	226.31		(1) ACD
logP	2.555±0.251		(1) ACD
Freely Rotatable Bonds	4		(1) ACD
logD	2.55	pH 1	(1) ACD
logD	2.55	pH 4	(1) ACD
logD	2.55	pH 7	(1) ACD
logD	2.55	pH 8	(1) ACD
logD	2.55	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

STN Files: CAOLD

(Additional Information is available through STN International. Contact your information specialist, a local CAS representative, or the CAS Help Desk for Assistance)

Database: REGISTRY

Close

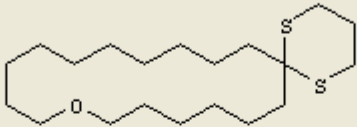
To learn more: Check the
CAOLD database on STN[®]

Substance is a Ring Parent

Detail of Substance 1

File Edit Help

Registry Number: 497180-52-6



Formula: C₂₀ H₃₈ O S₂

CA Index Name: 13-Oxa-1,5-dithiaspiro[5.17]tricosane (9Cl)

Class Identifier: Ring Parent

-- Properties --

Property	Calculated Value	Condition
H donors	0	
H acceptors	1	
Molecular Weight	358.65	
logP	7.297±0.614	

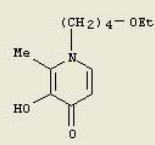
Close

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

Detail of Substance 4

Registry Number: 133361-34-9



Formula: C₁₂ H₁₉ N O₃

CA Index Name: 4(1H)-Pyridinone, 1-(4-ethoxybutyl)-3-hydroxy-2-methyl- (9CI)

-- Properties --

Property	Calculated Value	Condition	Note
H donors	1		(1) ACD
H acceptors	4		(1) ACD
Molecular Weight	225.28		(1) ACD
logP	0.844±0.750		(1) ACD
Freely Rotatable Bonds	7		(1) ACD
logD	-1.13	pH 1	(1) ACD
logD	0.80	pH 4	(1) ACD
logD	0.84	pH 7	(1) ACD
logD	0.83	pH 8	(1) ACD
logD	0.15	pH 10	(1) ACD
pKa	9.41±0.20	Most Acidic	(1) ACD
pKa	2.98±0.20	Most Basic	(1) ACD
Molar Solubility	Very Soluble	pH 1	(1) ACD
Molar Solubility	Slightly Soluble	pH 4	(1) ACD
Molar Solubility	Slightly Soluble	pH 7	(1) ACD
Molar Solubility	Slightly Soluble	pH 8	(1) ACD
Molar Solubility	Soluble	pH 10	(1) ACD

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

-- Resources --

References: None

STN Files: RTECS

(Additional Information is available through STN International. Contact your information specialist, a local CAS representative, or the CAS Help Desk for Assistance)

Database: REGISTRY

Close

To learn more: Consult the relevant database on STN

Substance only cited in CHEMLIST®

Detail of Substance 1

File Edit Help

Registry Number: 299176-78-6

CSC1=CN=C(C1)CCCCCCCCC

Formula: C14 H26 N2 S

CA Index Name: 1H-Imidazole-1-methanethiol, 2-decyl- (9CI)

-- Properties --

Property	Calculated Value	Condition	Note
H donors	0		(1) ACD
H acceptors	2		(1) ACD
Molecular Weight	254.44		(1) ACD
logP	5.127±0.287		(1) ACD
Freely Rotatable Bonds	11		(1) ACD
logD	1.13	pH 1	(1) ACD
logD	1.88	pH 4	(1) ACD
logD	4.60	pH 7	(1) ACD
logD	4.97	pH 8	(1) ACD
logD	4.22	pH 10	(1) ACD
pKa	9.16±0.25	Most Acidic	(1) ACD
pKa	7.34±0.31	Most Basic	(1) ACD
Molar Solubility	Slightly 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

STN Files: CHEMLIST

(Additional Information is available through STN International. Contact your information specialist, a local CAS representative, or the CAS Help Desk for Assistance)

Database: REGISTRY

Close

To learn more: Check out
the regulated chemicals
collection

SciFinder
SCHOLAR
2002

Substance registered as a concept

The screenshot displays the SciFinder Scholar interface. On the left, the 'Detail of Substance 1' window shows the following information:

- Registry Number: 74869-22-0
- Formula: Unspecified
- CA Index Name: Lubricating oils
- Other Names: 150B; 150B (lubricant); 59ts; Amoco s... 4; Clavus 68; Clavus G 68; Cosmo Allp... Drawsol 1622; Drawsol 3003; DS 11; D... Ferrocoat I 6130; Ferrocoat N 61T20K2... Hykomol K 80; I 12A; I 40A; I 5A; I 8A;... 150; L-CKD 220; Lube oils; Lubricants... 8p; MN 7.5; Mobil Multigrade 7.5W30;... 10; MS 10 (lubricating oil); MS 20S; M... Olivkor; OS Oil Type III; OSM 1; OSM... Penetrating oils; PGP 70; Pressoil S 3... 68 (lubricating oil); Royco 481 O; S... Toughness Multi; Tp 22; T... 22SU; Tuff... (lubricating oil); Whiteway 1 15; Yunipu... Yunipuresuterami DP 68
- Definition Field: A complex combination of hydrocarbons obtained from solvent extraction and dewaxing processes. It consists predominantly of saturated hydrocarbons having carbon numbers in the range C15 through C50.
- Class Identifier: Manual Registration, Concept
- References: None
- STN Files: CAPLUS, AGRISOLA, BIOSIS, CA, CHEMLIST, CIN, DETHERM, PDLCOM, RTECS, TOXCE... (Additional Information is available through STN International. Contact your information spe... Assistance)
- Deleted Registry Number(s): 62212-79-7, 50935-76-7, 79956-47-1, 83382-50-7
- Database: REGISTRY

On the right, the SciFinder Scholar window shows a list of references:

- Buyanovskii, I. A.; Matveevskii, R. M.; Natchuk, A. I. **Effect of base oils on antiwear properties of additives.** Issled. Smaz. Mater. Trenii (1981), 41-50. CODEN: 48INAJ CAN 97:200406 AN 1982:600406 CAPLUS
- Vamos, Endre. **Coatings for corrosion protection and trends in their development in Hungary.** Banyaszati es Kohaszati Lapok, Koolaj es Foldgaz (1982), 15(5), 83-6. CODEN: BKKFAC ISSN:0572-6034. CAN 97:165558 AN 1982:565558 CAPLUS
- Rozhkovskaya, G. P.; Porutskii, G. V.; Khokhol'kova, G. A.; Tkachenko, A. E.; Tereshchenko, L. G. **Hygienic assessment of working conditions during the use of MR-3 and MR-5U cutting fluids.** Neftepererabotka i Neftekhimiya (Kiev) (1980), 19 82-5. CODEN: NEFNBY ISSN:0548-1406. CAN 96:57093 AN 1982:57093 CAPLUS

Buttons at the bottom of the SciFinder window include 'Analyze or Refine References', 'Get Related...', and 'Back'. A blue oval highlights the 'References 1-3 of 14' text. A yellow box with black text is overlaid on the bottom right of the image.

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

Substance only registered as a generic entry

Detail of Substance 1

File Edit Help

Registry Number: 110720-53-1

Component Registry Number: 822-06-0
Formula: C8 H12 N2 O2
OCN-(CH2)6-NCO

Component Registry Number: 64-04-0
Formula: C8 H11 N
H2N-CH2-CH2-Ph

Formula: C8 H12 N2 O2 . C8 H11 N

CA Index Name: Benzeneethanamine, reaction products with 1,6-diisocyanatohexane

Alternate Formula: Unspecified

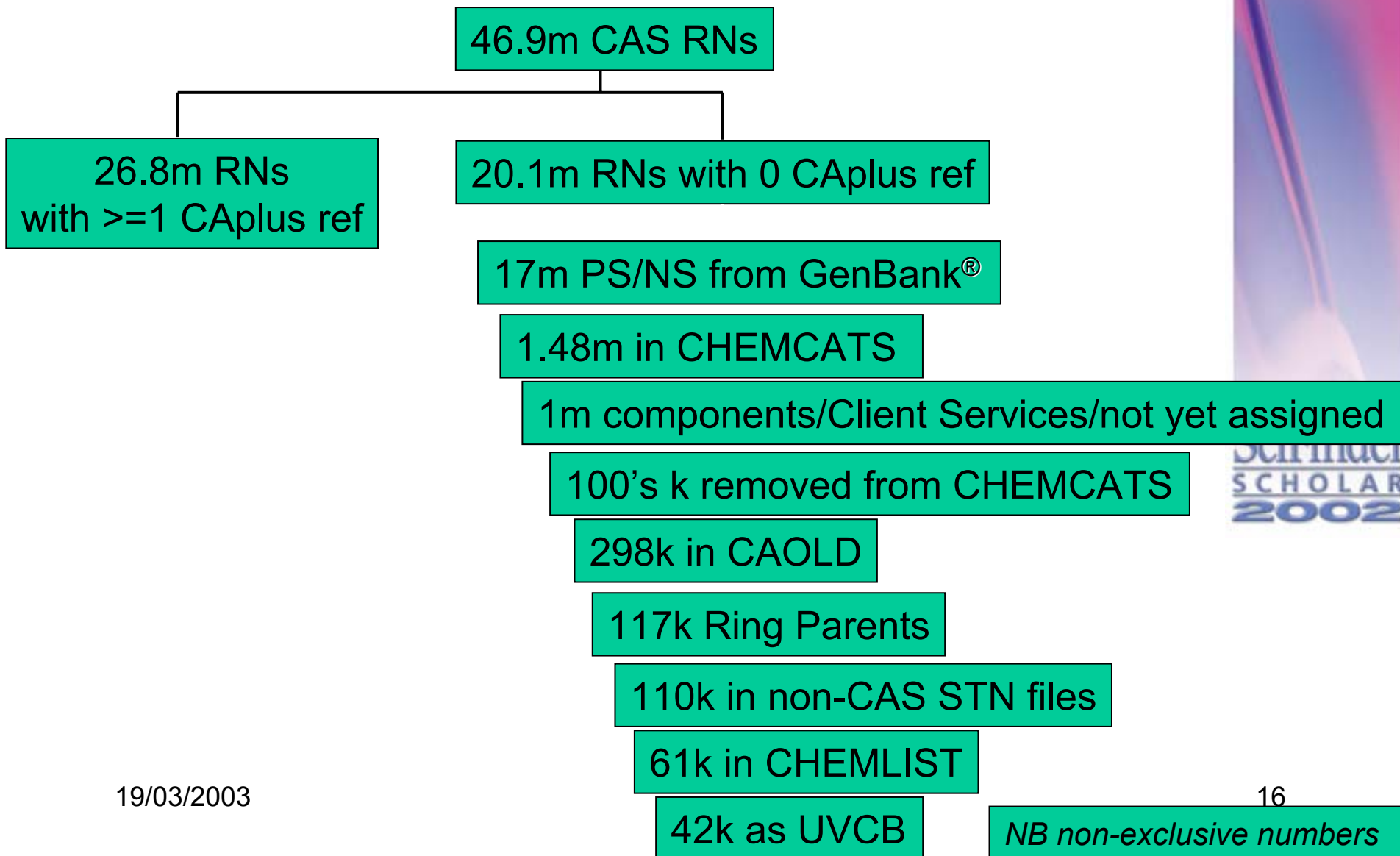
Class Identifier: Manual Registration, Generic Registration

References: None

Database: REGISTRY

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

The logo for SciFinder Scholar 2002. It features the word "SciFinder" in a large, blue, serif font with a registered trademark symbol. Below it, the word "SCHOLAR" is written in a smaller, blue, sans-serif font, separated by a thin blue horizontal line. At the bottom, the year "2002" is displayed in a large, blue, sans-serif font. The background of the logo is a gradient of purple and blue with a diagonal light effect.

SciFinder®
SCHOLAR
2002



Substances with no references in
CAS Registry

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