Searching surfactants and detergents on STN

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Agenda

- Surfactant subject indexing CAplus[SM]
- Surfactant substance indexing in REGISTRY
- Extending searches to include DWPI[SM]

Surfactants in CAplus and REGISTRY

1. General Indexing Policies
2. Classification Code
3. Controlled Terms and Linking Terms
4. General Substance Indexing Policies
5. Surfactant Classification
6. Examples:
   - Anionic Surfactants
   - Cationic Surfactants
   - Nonionic Surfactants
   - Amphoteric Surfactants
7. Summary

1. General Indexing Policies

The various aspects of surfactants that are covered by CAS

- Preparation of surfactants
- Chemistry of surfactants and surfactant compositions
- Physical chemistry of surfactants
- Formulations with surfactants (e.g. detergent formulations)
- Uses of surfactants

1. General Indexing Policies

Surfactants are indexed when they are:

- the novelty of a patent
- the focus of a research paper
- reported in the literature with new data
- prepared and characterized
- prophetic substances in the example part of a patent
- of interest for a particular application

1. General Indexing Policies

- Surfactants are not indexed when they are:
  - incidental to the main study (e.g. as an emulsifier in emulsion polymerization with no emphasis on the emulsifier)
  - common constituents in detergent formulations are not indexed when the interest is in the overall composition or in other constituents

1. General Indexing Policies

- Detergent formulations are indexed:
  - with their ingredients (RNs) and an appropriate text modification, e.g. “cleaning composition”
  - with the RN of the mixture when the constituents are deliberately admixed and remain discrete in the medium

2. Classification Code (/CC)

Section Code 46 (since 1967)

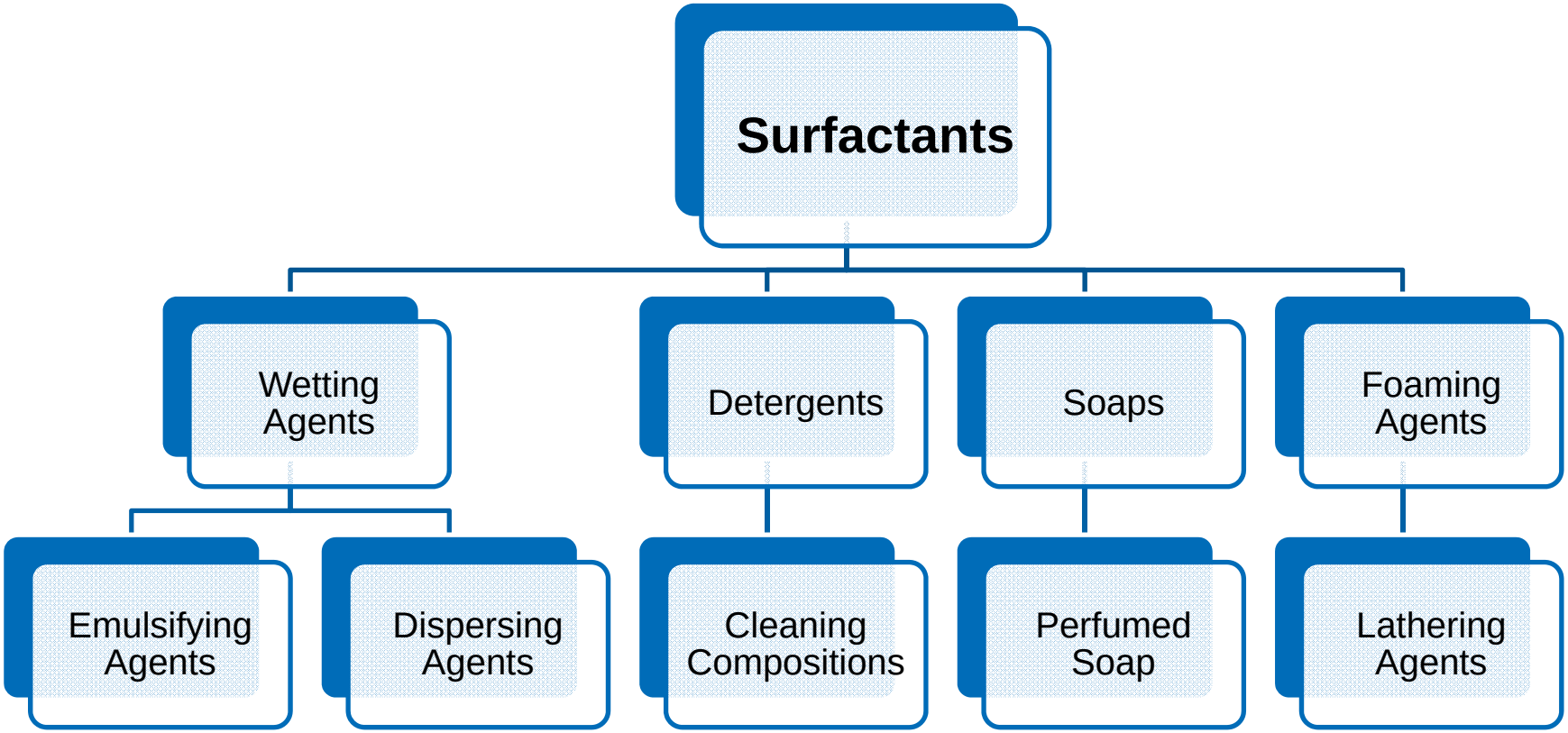
There are several old sections for this topic.

Remember: Some CA section titles and numbers have changed over time.

Use the CA Section thesaurus in the /cc field to find the history of that section.

3. Controlled Terms and Linking Terms

Controlled Term Hierarchy



4. General Substance Indexing Policies

The indexing of individual surfactants depends on how they can be handled for registration. They are indexed:

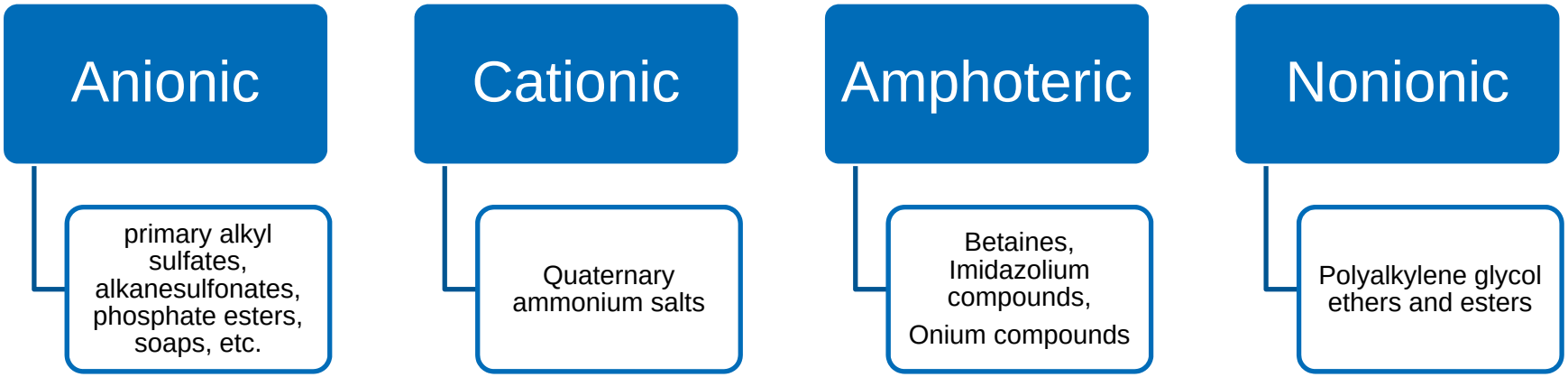
- At their own Registry Number when fully defined.
- At the Registry Number for only a portion of the molecule when part of it (usually alkyl or aryl portion) is unspecified, specified in terms of a C range, or unstructurable.
- Without any Registry Number when no portion of the molecule is sufficiently defined for registration.

4. General Substance Indexing Policies

Trade names for surfactants may be:

- Registered as trade names (without a structure)
- Cross-referred to a chemical name and registered (with a structure)
- Cross-referred to a controlled-term substance heading (e.g. Alcohols) with structural information provided in the text modification
- Cross-referred to a controlled-term use heading such as detergents.

5. Surfactant Classification



6. Examples - Anionic Surfactants

Example: Alkylarenesulfonates

Fully defined and fully structurable alkylarenesulfonates are indexed at their CAS Registry Number. Variations in linearity, position of ring substitution, and salt specification will, however, result in different Registry Numbers for the same basic substance. Indexing will reflect how the substance is described by the author.

6. Examples - Anionic Surfactants

Example: Alkylarenesulfonates

Docecylbenzenesulfonate – linear alkyl assumed

```
RN 27176-87-0 REGISTRY
IN  Benzenesulfonic acid, dodecyl-

RN 25155-30-0 REGISTRY
IN Benzenesulfonic acid, dodecyl-, sodium salt

RN 2211-98-5 REGISTRY
IN Benzenesulfonic acid, 4-dodecyl-, sodium salt
```

Search Tip: For comprehensiveness, the RN of all relevant variants of registration should be included in a search. Also, the RN of the unsubstituted Benzenesulfonic acid should be searched with appended "D" and linked to "alkyl".

6. Examples - Anionic Surfactants

Example: Alkylarenesulfonates

Partial Registration

Partially defined or partially structurable alkylarenesulfonates can be searched using the Registry Number for only a portion of the molecule. The unstructurable or undefined portion must be searched as derivative information in the text modification at the Registry Number.

6. Examples - Anionic Surfactants

Example: Alkylarenesulfonates

Partial Registration

Na alkylbenzenesulfonate

Preferred indexing with: Benzenesulfonic acid [98-11-3]
(The salt is not included in the RN)

Typical CA File index entry:
98-11-3D, Benzenesulfonic acid, alkyl derivs., sodium salt

6. Examples - Anionic Surfactants

Example: Fatty Alcohol Sulfates

Full Registration

Fully defined and fully structurable fatty alcohol sulfates are indexed at their CAS Registry Number.

No Registration

Partially defined or partially structurable alkyl sulfates generally have no portion of the molecule indexed using a Registry Number. The entire molecule must be searched as text terms in CAplus.

6. Examples - Anionic Surfactants

Anionic Surfactants - Full Registration

Find studies for the toxicity of Sodium laurylsulfonate

```
=> FIL REG

=> E SODIUM LAURYLSULFONATE/CN
E1              1     SODIUM LAURYLSARCOSINE/CN
E2              1     SODIUM LAURYLSULFONAMIDOACETATE/CN
E3              1 --> SODIUM LAURYLSULFONATE/CN
E4              1     SODIUM LAURYLTRIOXYETHYLENE SULFATE/CN
E5              1     SODIUM LAVRATE/CN

=> S E3
L1              1 "SODIUM LAURYLSULFONATE"/CN
```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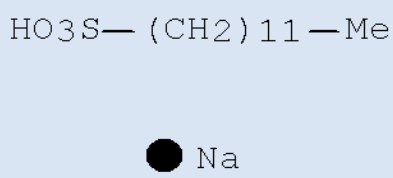
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2011 ACS on STN
RN 2386-53-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Dodecanesulfonic acid, sodium salt (1:1) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Dodecanesulfonic acid, sodium salt (8CI, 9CI)
CN Dodecanesulfonic acid, sodium salt (7CI)
OTHER NAMES:
CN Acme SLS
O o o



CN Sodium laurylsulfonate
CN Sodium n-dodecylsulfonate
CN Stepanol PCK
DR 12640-85-6, 163883-58-7, 139874-16-1
MF C12 H26 O3 S . Na
CI COM
LC STN Files: AGRICOLA, ANABSTR o o o
CRN (1510-16-3)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3892 REFERENCES IN FILE CA (1907 TO DATE)
37 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3953 REFERENCES IN FILE CAPLUS (1907 TO DATE)

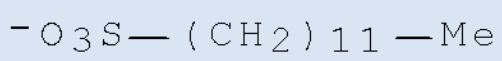
6. Examples - Anionic Surfactants

For comprehensiveness, Registry Number for laurylsulfonate should also be included:

```
=> E LAURYLSULFONATE/CN
E13             1     LAURYLSULFATE GLYCINE SALT/CN
E14             1     LAURYLSULFOBETAINE/CN
E15             1 --> LAURYLSULFONATE/CN
E16             1     LAURYLSULFONIC ACID/CN
E17             1     LAURYLSULFONIC ACID SODIUM SALT/CN

=> S E15
L2              1 LAURYLSULFONATE/CN
```

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2011 ACS on STN
RN 38480-64-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Dodecanesulfonic acid, ion(1-) (CA INDEX NAME)
OTHER NAMES:
CN Dodecylsulfonate
CN Dodecylsulfonate(1-)
CN Laurylsulfonate
MF C12 H25 O3 S
CI COM
LC STN Files: ANABSTR, BIOSIS, BIOTECHNO o o o



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

139 REFERENCES IN FILE CA (1907 TO DATE)
23 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
139 REFERENCES IN FILE CAPLUS (1907 TO DATE)

5. Examples - Anionic Surfactants

```
=> FIL CAP

=> S L1/ADV
          3953 L1
        947951 ADV/RL
L3           17 L1/ADV
                  (L1 (L) ADV/RL)

=> S L2/ADV
           139 L2
        947951 ADV/RL
L4             1 L2/ADV
                  (L2 (L) ADV/RL)
```

6. Examples - Anionic Surfactants

Anionic Surfactants - No Registration

Find studies on tallow-alkyl sulfate surfactants

```
=> FIL CAP
=> S TALLOW (L) ALKYL (W) SULFATE? (L) (SURFACTANT?
OR    DETERGENT? OR EMULSIF?)
L1          148 TALLOW (L) ALKYL (W) SULFATE? (L)
                (SURFACTANT? OR DETERGENT? OR
                 EMULSIF?)
```

Some references may also be found using the RN for sulfuric acid

```
=> S 7664-93-9d (L) TALLOW (L) ALKYL
L5           16 7664-93-9D (L) TALLOW (L) ALKYL
=> S L5 NOT L1
L8            9 L5 NOT L1
```

6. Examples - Cationic Surfactants

Example: Quaternary Ammonium Compounds

Full Registration

Fully defined and fully structurable quaternary ammonium compounds are indexed at their CAS Registry Number.

No Registration

Partially defined or partially structurable quaternary ammonium compounds generally have no portion of the molecule indexed using a Registry Number. The entire molecule must be searched as text terms in CAplus.

6. Examples - Cationic Surfactants

Cationic Surfactants - Full Registration

Cetyltrimethylammonium chloride

```
=> FIL REG

=> E CETYLTRIMETHYLAMMONIUM CHLORIDE/CN
E1              1     CETYLTRIMETHYLAMMONIUM CATION/CN
E2              1     CETYLTRIMETHYLAMMONIUM CHLORATE/CN
E3              1 --> CETYLTRIMETHYLAMMONIUM CHLORIDE/CN
E4              1     CETYLTRIMETHYLAMMONIUM CHLORIDE COMPD.
                       WITH P-PHENYLPHENOL (1:1)/CN
E5              1     CETYLTRIMETHYLAMMONIUM CHLORIDE
                       HEMIHYDRATE/CN

=> S E3
L1               1 "CETYLTRIMETHYLAMMONIUM CHLORIDE"/CN
```

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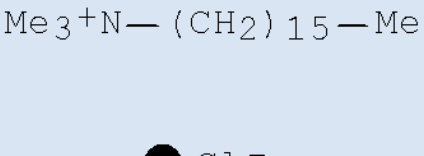
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2011 ACS on STN
RN 112-02-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Hexadecanaminium, N,N,N-trimethyl-, chloride (1:1)
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Hexadecanaminium, N,N,N-trimethyl-, chloride (9CI)
CN Ammonium, hexadecyltrimethyl-, chloride (8CI)
CN Hexadecyltrimethylammonium chloride (6CI)
OTHER NAMES:
CN 1631CL
CN Adogen 444
CN Adogen 444-29
O O O
CN Cetyltrimethylammonium chloride



6. Examples - Cationic Surfactants

Cationic Surfactants - No Registration

Use controlled term “Quaternary ammonium compounds” linked with nomenclature term.

Example: Coco alkyl quaternary ammonium compounds

```
=> E QUATERNARY AMMONIUM COMPOUNDS/CT
E#   FREQUENCY     AT      TERM
--   ---------     --      ----
E1         100      2      QUATERNARY AMMONIUM COMPDS./CT
E2           0      2      QUATERNARY AMMONIUM COMPDS. (L)
                             BENZYLDIMETHYLTALLOW ALKYL,
                             CHLORIDES/CT
E3       51669     96 --> QUATERNARY AMMONIUM COMPOUNDS/CT
```

There are several linking terms

```
=> E E3+LT
E109     51669   -->  Quaternary ammonium compounds/CT
E110               LT   Quaternary ammonium compounds (L)
                        (2-((2-((2-carboxyethyl)(2-hydroxyethyl)amino)ethyl)ami
                        no)-2-oxoethyl)coco alkyldimethyl, inner salts/CT
E111               LT   Quaternary ammonium compounds (L)
                        (2-ethylhexyl)(hydrogenated coco alkyl)dimethyl,
                        chlorides/CT
E112               LT   Quaternary ammonium compounds (L)
                        (2-ethylhexyl)(hydrogenated rape-oil alkyl)dimethyl,
                        chlorides/CT
E115               LT   Quaternary ammonium compounds (L)
                        (2-ethylhexyl)dimethyltallow alkyl, chlorides/CT
E116               LT   Quaternary ammonium compounds (L)
                        (2-hydroxy-C12-14-alkyl)trimethyl, chlorides/CT
E144               LT   Quaternary ammonium compounds (L) C17-20-alkyl/CT
E155               LT   Quaternary ammonium compounds (L) alkyl/CT

=> S QUATERNARY AMMONIUM COMPOUNDS/CT (L) COCO AND (SURFACTANT? OR
DETERGENT? OR  EMULSIF?)
L3          365 QUATERNARY AMMONIUM COMPOUNDS/CT (L) COCO AND (SURFACTANT? OR
                DETERGENT? OR EMULSIF?)
```

Answers in CAplus

All in one index field:

```
IT   Quaternary ammonium compounds
     RL: AGR (Agricultural use); BIOL (Biological study); USES
       (Uses)
       (coco alkyltrimethyl, chlorides, Arquad C 50,
        surfactant; herbicide compns. containing specific
       sulfonium urea compound and adjuvants for weed control)
```

Different index fields

```
IT   Quaternary ammonium compounds
     RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (alkylbenzyldimethyl, chlorides, coco-; biocidal solution
        comprising chlorhexidine salt, alkyl dimethylbenzyl ammonium halide,
        dialkyl dimethylammonium halide, and acid)
IT   Surfactants
        (amphoteric; biocidal solution comprising chlorhexidine salt, alkyl
        dimethylbenzyl ammonium halide, dialkyl dimethylammonium halide, and
        acid)
```

6. Examples - Nonionic Surfactants

Example: Ethoxylated Fatty Alcohols

Full Registration

Fully defined and fully structurable polyethylene glycol ethers with fatty alcohols are indexed at their CAS Registry Number.

Partial Registration

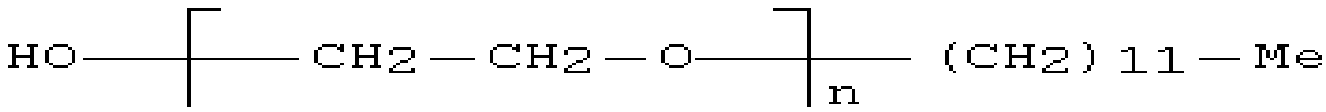
Partially defined or partially structurable polyethylene glycol ethers with fatty alcohols can be searched as derivative information at Registry Number for only the polyethylene glycol portion. The undefined or unstructurable portion (fatty alcohol) entire molecule must be searched as text terms in CAplus.

6. Examples - Nonionic Surfactants

Nonionic Surfactants - Full Registration

Polyethylene glycol monodecyl ether

```
RN   9002-92-0  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Poly(oxy-1,2-ethanediyl), .alpha.-dodecyl-.omega.-
       hydroxy-  (CA INDEX NAME)
```



Post treated polymers, like esters or salts will be indexed in Registry

6. Examples - Nonionic Surfactants

Nonionic Surfactants - Full Registration

Two index entries are made:

1. Polyethylene glycol [25322-68-3] linked with text term “alkyl ethers”
2. Alcohols (Controlled term) linked with “ethoxylated”

As not always both entries are made in one record, search with both queries. Refine with the number of the Alkyl-Carbon atoms

```
=> s (POLYETHYLENE GLYCOL (L) C11-15(W)ALKYL
ETHERS) OR (ALCOHOLS/CT (L) C11-15(W)ETHOXYLATED)
L16          62 (POLYETHYLENE GLYCOL (L) C11-15 (W)ALKYL
                ETHERS) OR (ALCOHOLS/CT (L) C11-15 (W)
                ETHOXYLATED)
```

L10 ANSWER CAPLUS COPYRIGHT 2011 ACS on STN
AN 2003:590042 CAPLUS
DN 140:129966
TI Fundamental insight into the mechanism of oxygen delignification
AU Chen, Sheng-Li; Lucia, Lucian A.
CS Institute of Paper Science and Technology..
SO Cellulose Chemistry and Technology . . .
IT Alcohols, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(C11-15, ethoxylated, surfactant;
application of polyethylene glycol ether surfactants in
oxygen bleaching of kraft pulps)
IT Polyoxyalkylenes, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(C11-15-alkyl ethers,
surfactant; application of polyethylene glycol
ether surfactants in oxygen bleaching of kraft pulps)
IT 25322-68-3D, Polyethylene glycol, C11-
15-alkyl ethers 60828-78-6
RL: TEM (Technical or engineered material use); USES (Uses)
(surfactant; application of polyethylene glycol
ether surfactants in oxygen bleaching of kraft pulps)

6. Examples - Amphoteric Surfactants

Example - Betaines

Full Registration

Fully defined and fully structurable betaines are indexed at their CAS Registry Number.

No Registration

Partially defined or partially structurable betaines are indexed at controlled terms: “Betaines” or “Onium compounds”, or on the compound class heading.

6. Examples - Amphoteric Surfactants

Betaines – No Registration

Imidazolium surfactants

```
=> FIL CAP
=> E BETAINES+ALL
E13      14007   BT3  Chemical compounds/CT
E14      56497     BT2  Organic compounds/CT
E15       8494       BT1  Onium compounds/CT

E16       5697         -->  Betaines/CT

                         HNTE Valid heading during volume 1 (1907) to present.
E17                      UF   Trialkyl(carboxyalkyl) betaines/CT
E18                      UF   Trialkyl(carboxyalkyl)ammonium inner salts/CT
E19          0           NT1  Acetyl-L-carnitine/CT
E20          0           NT1  Carnitine/CT
E21          0           NT1  Cocoamidopropyl betaine/CT
E22          0             NT2  Lauramidopropylbetaine/CT
E23          0           NT1  Glycine betaine/CT
E24          0           NT1  Lauryldimethylaminoacetic acid betaine/CT
E25        835           NT1  Sulfobetaines/CT
E26          0             NT2  3-((3-Cholamidopropyl)dimethylammonio)-1-propan
                                esulfonate/CT
********** END **********
```

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```
=> E IMIDAZOLIUM COMPOUNDS/CT
E#    FREQUENCY     AT      TERM
--    ---------     --      ----
E27           0      2      IMIDAZOLIUM COMPOUND RECEPTORS (L) I1/CT
E28           0      2      IMIDAZOLIUM COMPOUND RECEPTORS (L) I2/CT
E29         535      2 --> IMIDAZOLIUM COMPOUNDS/CT
```

```
=> E E29+ALL
E39         535    -->  Imidazolium compounds/CT
                        HNTE Valid heading during volumes 31-125 (1937-1996) only.

E40                     NEW  Onium compounds (L) imidazolium compds./CT

********** END **********
```

The Linked term is in the text modification

```
IT    Onium compounds
      RL: MOA (Modifier or additive use); USES (Uses)
         (imidazolium compds.; water permeability modifiers
         for fibers for nonwoven fabrics)
```

Slide continous on the next page

```
=> S E16,E39,E40

L1          7772 (BETAINES/CT OR "IMIDAZOLIUM COMPOUNDS"/CT OR "ONIUM
                 COMPOUNDS (L) IMIDAZOLIUM COMPDS."/CT)
```

(Set plurals on)

```
=> S L1 AND (SURFACTANT OR DETERGENT)

L2          3581 L1 AND (SURFACTANT OR DETERGENT)
```

Done: 07/2011

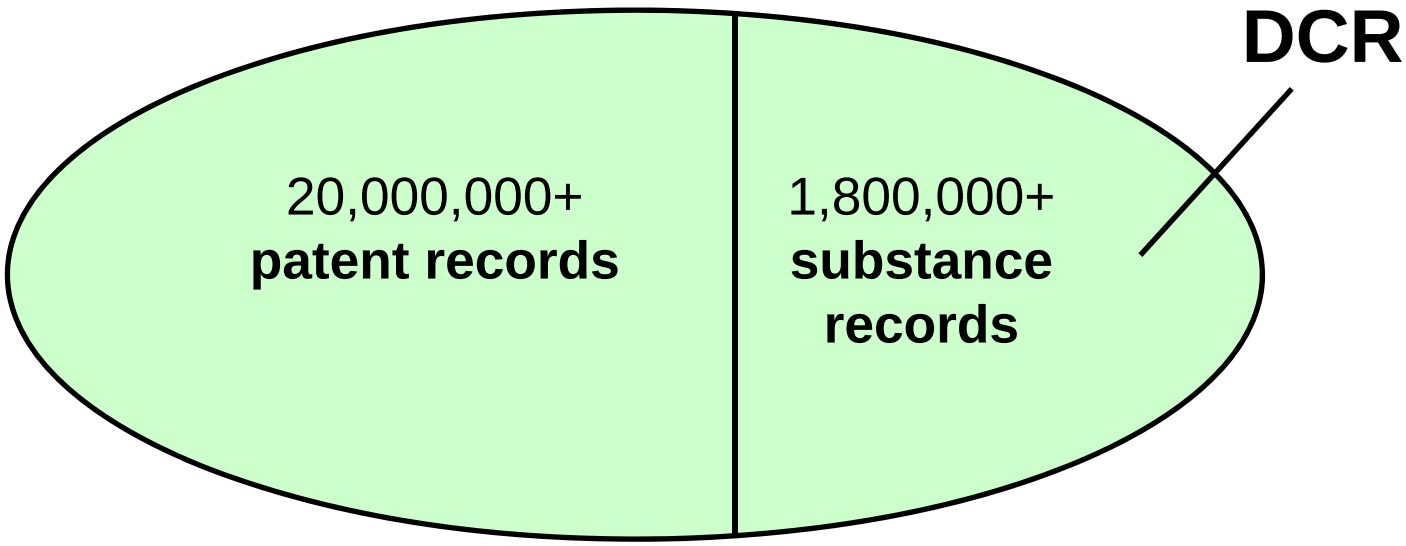
```
L3          3203 L2 AND BETAINES/CT
L4           211 L2 AND "ONIUM COMPOUNDS (L) IMIDAZOLIUM
                    COMPDS."/CT
L5           279 L2 AND "IMIDAZOLIUM COMPOUNDS"/CT
```

7. Summary

- Use the CA thesaurus to find out the right terminology. The analysts have to index as precise as possible
- Use linking terms together with the controlled term to specify your surfactant
- Search for the Registry Number when the substance is fully defined
- Use the CAS RN for structurable portion of incompletely described compounds.
- Use controlled terms for incompletely described compounds, like betaines, alcohols, fatty acids
- Search in MARPAT for generic substances

DWPI Chemistry Resource (DCR)

- DCR is a chemical structure database covering specific chemical structures indexed in DWPI bibliographic patent records
- An integral part of DWPI on STN since 1999
- Available to all users of DWPI



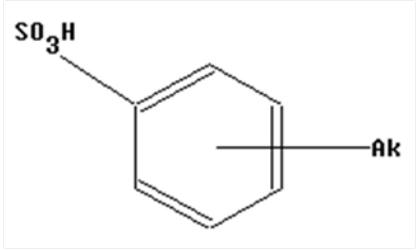
DCR coverage

- Specific chemical compounds indexed by Thomson Reuters from basic patents in DWPI
- DWPI patents classified in Pharmaceutical (B), agrochemical (C) and/or general chemical (E)
- Comprehensive coverage began in 4/1999
- Selective coverage for approximately
  - 20,000 substances from 1/1987 to date
  - 2,100 substances from 7/1981 to date

CAS and DWPI search example

Search Question:

Find patents describing the use of sodium alkyl benzene sulfonate(s) of formula (I), as surfactants, detergents, or emulsifiers:

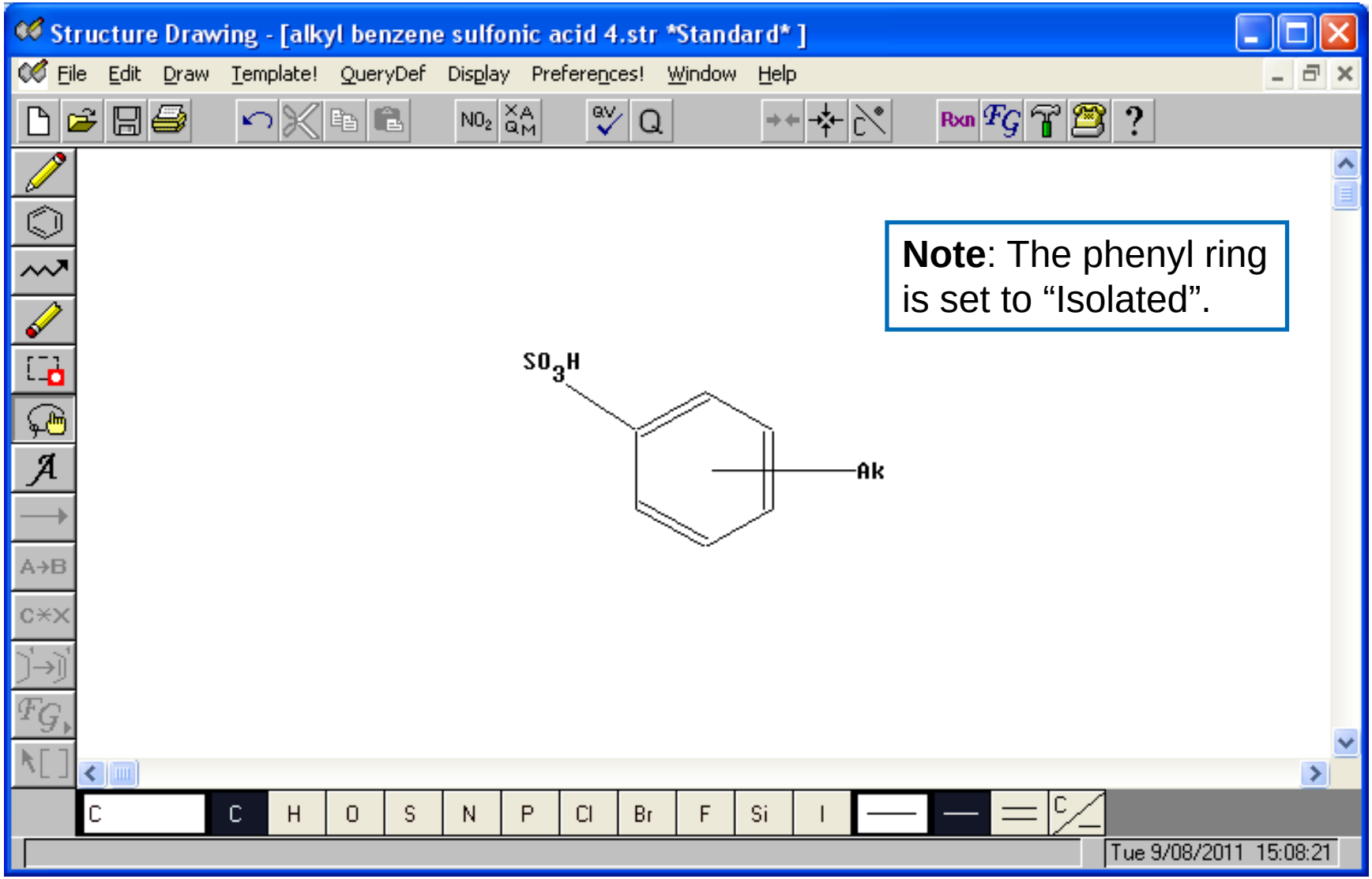


(I)

Ak= Alkyl

No further substitution is allowed.

CAS and DWPI search example



Upload and search the query in REGISTRY

```
=> FILE REGISTRY

=>
Uploading C:\ . . . . \Queries\alkyl benzene sulfonic acid 4.str

L1      STRUCTURE UPLOADED

=> S L1 CSS SAM

=> D SCAN

=> S L1 CSS FUL
FULL SEARCH INITIATED 16:34:24 F
. . . .
L2         32728 L1 CSS FUL

=> S L2 AND NA/ELS NOT PMS/CI
L3           290 S L2 AND NA/ELS NOT PMS/CI
```

The structure query (previous slide) is uploaded via STN Express (L1).

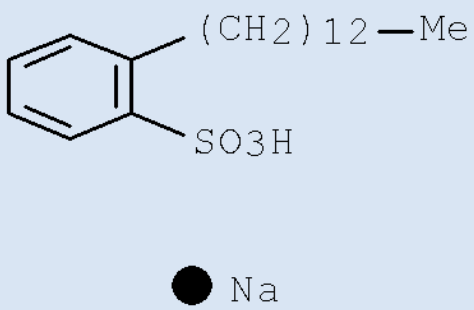
It's a good idea to conduct a free-of-charge preview sample search, and review answers using the free-of-charge format SCAN.

A closed substructure search (CSS) is used to limit further substitution (L2).

Limit to sodium salts and non-polymeric answers (L3).

Review the answers retrieved using D SCAN

```
=> D SCAN L3

L3   290 ANSWERS   REGISTRY  COPYRIGHT 2011 ACS on STN
IN   Benzenesulfonic acid, 2-tridecyl-, sodium salt (1:1)
MF   C19 H32 O3 S . Na
```



The search retrieves a precisely defined group of compounds (L3).

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

L3   290 ANSWERS   REGISTRY  COPYRIGHT 2011 ACS on STN
IN   Benzenesulfonic acid, 3-propyl-, sodium salt (1:1)
MF   C9 H12 O3 S . Na
. . . .
```

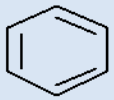
Search for incompletely defined structures (IDS)

```
=> S BENZENESULFONIC ACID (P) SODIUM (P) SALT
L4       17804 S BENZENESULFONIC ACID (P) SODIUM (P) SALT

=> S L4 AND C H O S/ELF AND 3/O AND 1/S AND 2/NC AND
   NA/ELS AND IDS/CI NOT PMS/CI
L5         251 S L4 AND C H O S/ELF AND 3/O AND 1/S AND 2/NC AND
               NA/ELS AND IDS/CI NOT PMS/CI

=> S L3 OR L5
L6         539 S L3 OR L5
```

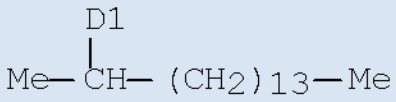
Incompletely defined (IDS/CI) sodium alky benzene sulfonates may be included for a more comprehensive search (L6).

Review the answers retrieved using D SCAN

```
=> D SCAN L6

L6    539 ANSWERS   REGISTRY  COPYRIGHT 2011 ACS on STN
IN    Benzenesulfonic acid, (1-methylpentadecyl)-, sodium salt
      (7CI, 9CI)
MF    C22 H38 O3 S . Na
CI    IDS
```



D1—SO3H



Me—CH(D1)—(CH2)13—Me

● Na

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

The search now includes some important, but incompletely defined structures (IDS) (L6).

Retrieve the corresponding CAplus records

```
=> FILE HCAPLUS

=> S L6
L7          19493 S L6

=> S 98-11-3D (L) ALKYL(W)DERIV? (L) SODIUM(W)SALT?
L8           2481 S 98-11-3D (L) ALKYL(W)DERIV? (L) SODIUM(W)SALT?

=> S L7 OR L8
L9          21701 S L7 OR L8

=> S L9 (L) (SURFACTANT? OR DETERGENT? OR EMULSIF? OR
   CLEAN? OR SOAP?)
L10          8008 S L9(L)(SURFACTANT? OR DETERGENT? OR EMULSIF? OR
                  CLEAN? OR SOAP?)

=> S L10 AND P/DT
L11          5141 S L10 AND P/DT
```

The 539 substance records (L6) correspond to 19,493 bibliographic records in HCAplus (L7).

Add relevant non-specific derivatives of benzene sulfonic acid (RN 98-11-3) (L9).

Limit the HCAplus search to surfactant and detergent uses and patents (L11).

Example: CAplus answer retrieved

```
=> D L11 BIB HITIND 3

L11  ANSWER 3 OF 5141  HCAPLUS  COPYRIGHT 2011 ACS on STN
AN   2011:936722  HCAPLUS  Full-text
DN   155:183088
TI   Polycarbonate resin compositions containing impact modifiers formed
     from size-controlled latex particles and their moldings
IN   Imada, Akira
PA   Fuji Xerox Co., Ltd., Japan
SO   Jpn. Kokai Tokkyo Koho, 26pp.
     CODEN: JKXXAF
DT   Patent
LA   Japanese
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     --------------      ----   --------    -------------------    --------
PI   JP 2011144247        A     20110728    JP 2010-5292           20100113
PRAI JP 2010-5292                20100113
IPCI C08L0069-00 [I,A]; C08L0055-02 [I,A]; C08L0051-00 [I,A]; . . . .
CC   37-6 (Plastics Manufacture and Processing)
     Section cross-reference(s): 38
IT   25155-30-0, Sodium dodecylbenzenesulfonate  26353-67-3,
     Formaldehyde-β-naphthalenesulfonic acid copolymer
     RL: NUU (Other use, unclassified); USES (Uses)
        (emulsifiers; polycarbonate resin compns. containing impact
        modifiers formed from size-controlled latex particles and providing
        impact-resistant moldings)
```

HITIND display format, shows only the indexing with the hit search terms.

Repeat the structure search in DCR

```
=> FILE WPIX
```

Access the Derwent World Patents Index (DWPI) (files WPINDEX, WPIDS or WPIX).

```
=> S L1 CSS FUL
FULL SEARCH INITIATED 16:44:44 FILE 'WPIX'
. . . .
L12          1855 L1 CSS FUL
```

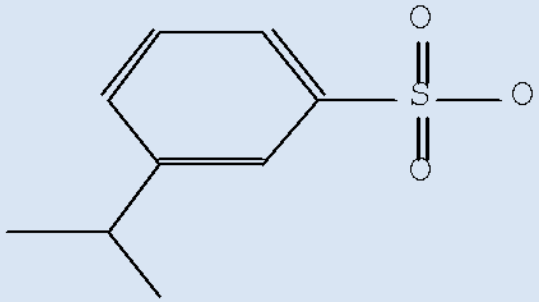
Repeat the structure search (L12) using the same query (L1).

```
=> S L12 AND NA/ELS
L13            43 L12 AND NA/ELS
```

Limit to sodium salts (L13).

Review the answers retrieved using D SCAN

```
=> D SCAN L13

L13  43  ANSWERS  WPIX      COPYRIGHT 2011 THOMSON REUTERS on STN
CN.P SODIUM CUMENE SULFONATE
CN.S sodium cumene sulfonate
MF   Na . C9 H12 O3 S

     CM   1

     Na

     CM   2
```




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

The search retrieves a precisely defined group of compounds (L13).

Retrieve the corresponding DWPI records

```
=> S L13/DCR
L14          4488 S L13/DCR

=> S L14(P)(Q601 OR Q602 OR Q603 OR Q608 OR Q336 OR Q272
   OR Q273 OR Q616)/M0,M2,M3
L15           684 S L14(P)(Q601 OR Q602 OR Q603 OR Q608 OR Q336 OR
                  Q272 OR Q273 OR Q616)/M0,M2,M3
```

The 43 substance records (L13) correspond to 4,448 bibliographic records in DWPI (L14).

Limit the DWPI search to surfactant and detergent uses (below) (L15).

Q616 = Surfactant.
Q272 = Non-soap detergent.
Q273 = Soap compositions.
Q336 = Cleaning compositions.

Q601 = Anticaking.
Q602 = Antifoam.
Q603 = Antistatic.
Q608 = Foaming agent; Foam stabilizer.

Retrieve the unique DWPI records

```
=> TRANSFER L11 1- PNK
L16              TRA L11 1- PNK  :
L17        4768 SEA L16/PNK

=> S L15 NOT L17
L18         449 S L15 NOT L17
```

Transfer PNK from CAplus (L11) to retrieve the corresponding records in DWPI (L17).

Retrieve the unique DWPI records (L18).

Example: unique DWPI answer retrieved

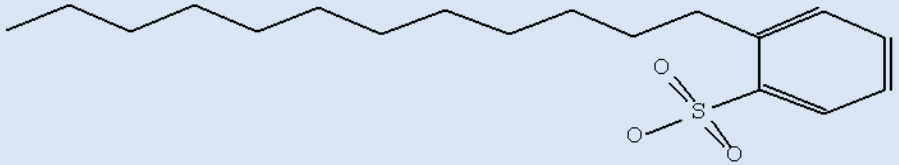
```
=> D L18 BIB HITCMC FRAGHITSTR 2

L18  ANSWER 2 OF 449  WPIX COPYRIGHT 2011       THOMSON REUTERS on STN
AN   2011-H44227 [201145]   WPIX  Full-text
TI   Servicing wellbore involves placing composition comprising surfactant,
     brine, and oleaginous fluid in annular space of wellbore, where
     composition forms microemulsion under low shear conditions
DC   E19; H01
IN   HARRISON D J; VAN ZANTEN R
PA   (HALL-C) HALLIBURTON ENERGY SERVICES INC;
CYC  113
PIA  US 20110160103  A1 20110630 (201145)* EN
     WO 2011080506   A1 20110707 (201145)  EN
ADT  US 20110160103 A1 US 2009-649819 20091230; WO 2011080506 A1
     WO 2010- GB2342 20101229
PRAI US 2009-649819       20091230
CMC  UPB   20110718
     M3 *19*   A111 A960 C710 G011 G100 K0 K4 K431 K432 M225 M231 M240 M281
               M320 M411 M510 M520 M531 M540 M782 Q412 Q616 R023  M905 M904
               DCN: RACZ8F-K RACZ8F-M RAVIYP-K RAVIYP-M
               DCR: 840197-K 840197-M
     M3 *20*   A111 A960 C710 G012 G100 K0 K4 K431 K432 M225 M231 M240 M281
               M320 M411 M510 M520 M531 M540 M630 M782 Q412 Q616 R023  M905
               M904
               DCN: RAXA2T-K RAXA2T-M
               DCR: 1814674-K 1814674-M
     M3 *21*   A111 A960 C710 G013 G100 K0 K4 K431 M225 M231 M240 . . . .
```

HITCMC display format, shows only the indexing with the hit search terms.

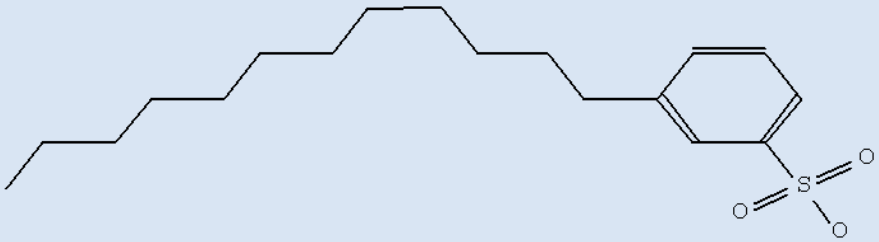
Q616 = Surfactant.

Example: unique DWPI answer retrieved (cont.)

```
AN.S DCR-840197
CN.S Sodium; 2-dodecyl-benzenesulfonate
SDCN RACZ8F; RAVIYP

     CM   1

     Na

     CM   2
```



```
AN.S DCR-1814674
SDCN RAXA2T

     CM   1

     Na

     CM   2
```



```
. . . .
```

The fragmentation code hit structure (FRAGHITSTR) display shows the hit DCR structure from the HITCMC paragraphs (previous slide).

DWPI Classifications (/DC) and Manual Codes (/MC) for detergents and surfactants

- D24 /DC – Soap
  - Metal salts of fatty acids used for cleaning
- D25 /DC – Detergents
  - Other than soap (D24) and used for cleaning
- D11+*NT* /MC
  - Detergents, soaps, glycerol
- D08-B13 /MC
  - Surfactants in cosmetics
- A08-S+*NT* /MC
  - Surfactant additives in polymer science
- B12-M09 /MC
  - Surfactants in pharmaceutical formulations

Summary

- Surfactant subject indexing CAplus
- Surfactant substance indexing in REGISTRY
- Extending searches to include DWPI

Acknowledgement

The CAS database related slides were prepared by:

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DWPI resources

- DWPI on STN User Documentation

  http://www.stn-international.com/stn_dwpi.html

  – DWPI on STN Reference Manual
  – DWPI on STN Workshop Manual
  – DWPI Classification (DC) guide
  – Summary table of member level data coverage
  – Global Patent Sources – DWPI coverage in detail
  – Chemistry, Engineering and Polymer User Guides
- DWPI on STN database summary sheet

  http://www.stn-international.com/wpindex.html

Recorded STN e-Seminars are available to watch at your own pace….

- FIZ Karlsruhe recorded e-Seminars:

  http://www.stn-international.com/recorded_events.html
  - Introduction to Derwent World Patents Index (DWPI)
  - Searching DWPI Chemistry Resource (DCR)

- CAS recorded e-Seminars:

  http://www.cas.org/support/stngen/stntraining/recorded.html
  - Revisiting the basics of structure searching
  - STN: Advanced Structure Searching
  - Structure drawing in STN

For more information …

CAS
E-mail: help@cas.org
Support and Training:
www.cas.org

FIZ Karlsruhe
helpdesk@fiz-karlsruhe.de
Support and Training:
www.stn-international.de

STN is available through FIZ Karlsruhe, Germany and Chemical Abstracts Service, U.S.A.