



STN®: Polymers in Scientific Literature

Agenda

- Polymer information in STN® databases
- Introduction to polymer indexing in CAS REGISTRYSM
- How to search for polymers in scientific literature based on
 - CAS Registry Number® (CAS RN) identifiers
 - Chemical Names
 - Polymer Class Terms
 - Properties
 - Structures

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Polymer information on STN is found in both substance and bibliographic databases

- More than one million substances in REGISTRY are polymers
 - Updated daily with new polymers
 - A CAS RN is assigned to each polymer
- Search REGISTRY to find RNs for polymers
- Search those RNs in CAplusSM, APOLLIT, RAPRA, TEXTILETECH, WSCA, WTEXTILES or other STN databases to find references

Hint: Use the REGISTRY **LC** field to identify other STN databases containing records indexed with CAS RNs for polymers of interest.

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What is a polymer?

- A polymer is a large molecule built by the repetition of small, simple chemical units
- The starting materials for polymers are called monomers
- The repetition of the chemical units may be linear, branched, or interconnected to form three-dimensional networks

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Addition polymers usually contain only carbon atoms in the backbone

- Formed from monomers containing double bonds
- No atoms are lost during polymerization
- Some of the most common types of polymers are

- Vinyl
- Acrylic
- Styrene

```
RN  9003-53-6  REGISTRY
...
CN  Polystyrene
...

CM  1

CRN 100-42-5
CMF C8 H8

H2C=CH-Ph
```

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Condensation polymers usually include heteroatoms in the backbone

- Formed from two or more monomers containing reactive groups
 - Isocyanate
 - Carboxylic acid
 - Hydroxy
- Common types
 - Polyesters
 - Polyamides
 - Polyurethanes
- Small molecules (water or ammonia) are usually lost during polymerization

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Polymers are represented two ways in REGISTRY

- Starting Materials
 - Polymer is indexed based on the component monomers that will combine to form the polymer
- Final Product
 - Polymer is recorded based on the Structural Repeating Unit (SRU) of the polymer
- Primary registration is monomer-based
 - Each component monomer has its own CAS RN
 - Each combination of components has an overall RN
- A supplemental SRU record, having its own RN, may also be indexed

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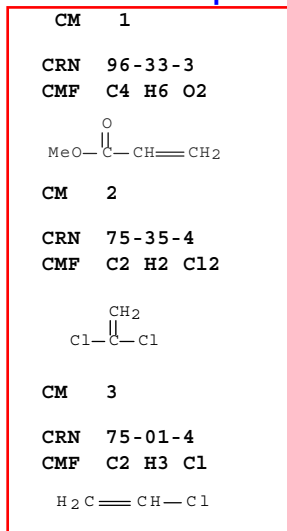
Component monomer-based REGISTRY record for an addition polymer

```
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 28572-91-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propenoic acid, methyl ester, polymer with chloroethene and
1,1-dichloroethene (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Acrylic acid methyl ester, polymer with chloroethylene and
1,1-dichloroethylene (8CI)
...
OTHER NAMES:
CN Ixan PA 331
CN Methyl acrylate-vinyl chloride-vinylidene chloride copolymer
...
CN Vinylidene chloride-vinyl chloride-methyl acrylate polymer
MF (C4 H6 O2 . C2 H3 Cl . C2 H2 Cl2)x
CI PMS
PCT Chloropolymer, Polyacrylic, Polyvinyl
LC STN Files: CA, CAPLUS, CHEMLIST, IFICDB, IFIPAT, IFIUDB,
TOXCENTER,USPAT2, USPATFULL, USPATOLD
```

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Addition polymer records show all of the component monomers and CRNs



There are 3 monomer components for this polymer

- CM1
- CM2
- CM3

For each component, the record lists

- CM 1 = Component Number
- CRN = Component Registry Number
- CMF = Component Molecular Formula
- Component structure

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Structural Repeating Unit (SRU) records are supplied in certain circumstances

- Monomer-based records for polymers may be supplemented with a SRU entry when
 - SRU structure is well documented by the author
 - The SRU can be confidently assumed because only one structure is chemically possible
- Some commonly occurring polymers are registered only as SRUs
 - Polyethylene glycol (PEG) (25322-68-3)
 - Polypropylene glycol (PPG) (142901-89-1)

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REGISTRY record for a polymer based on a Structural Repeating Unit

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 24968-12-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Poly(oxy-1,4-butanediylloxycarbonyl-1,4-phenylenecarbonyl)
(CA INDEX NAME)

OTHER NAMES:

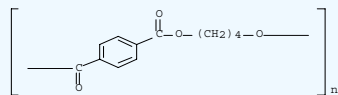
CN 1,4-Butanediol-dimethyl terephthalate copolymer, SRU
CN 1,4-Butanediol-dimethyl terephthalate polymer, SRU
CN 1,4-Butanediol-divinyl terephthalate copolymer, SRU

•••

MF (C12 H12 O4)_n
CI PMS
PCT Polyester

MF = Molecular Formula
CI = Substance Class Identifier
(PMS for Polymers)
PCT = Polymer Class Term

RELATED POLYMERS AVAILABLE WITH POLYLINK



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REGISTRY record for a polymer with a publicly unknown structure

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 365544-04-3 REGISTRY
•••
ED Entered STN: 31 Oct 2001
CN Fatty acids, C16-18 and C18-unsatd., branched and linear, diesters with polyethylene glycol (CA INDEX NAME)
MF Unspecified
CI PMS, MAN, CTS
PCT Manual registration
SR CAS Client Services
LC STN Files: CHEMLIST
Other Sources: TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

The structures of some polymers are not known by the public.

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REGISTRY record for a polymer known only by a trade name

```
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 501004-43-9 REGISTRY
ED Entered STN: 31 Mar 2003
CN Resamine CU 8433HV (9CI) (CA INDEX NAME)
ENTE A polycarbonate-polyurethane (Dainichiseika)
MF Unspecified
CI PMS, MAN
PCT Manual registration
SR CA
LC STN Files: CA, CAPLUS
```

```
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
      1 REFERENCES IN FILE CA (1907 TO DATE)
      1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
```

Some polymers may be publicly known only by a trade name.

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DISPLAY Editor Notes (/ENTE) to find information for trade name polymers

- There are more than 65,000 Editor Notes in REGISTRY for polymer trade names

```
L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 11141-00-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN SP 1045 (CA INDEX NAME)
OTHER NAMES:
CN Schenectady SP 1045
ENTE A dimethylol phenolic resin curative; has been identified as
butylphenol-formaldehyde copolymer, p-nonylphenol-
formaldehyde copolymer, p-octyl-formaldehyde copolymer and
2,6-bis(hydroxymethyl)phenol (Schenectady Chemicals, Inc.)
MF Unspecified
CI COM, MAN
```

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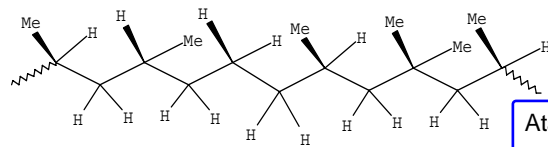
Some factors affect polymer registration

- Different stereochemistry
 - Atactic polypropylene (NS) RN: 9003-07-0
 - Isotactic polypropylene RN: 25085-53-4
 - Syndiotactic polypropylene RN: 26063-22-9
- Presence of end-groups
 - Only for SRUs
- Different architectures
 - Block, graft, alternating polymer forms
 - Considered only since 1987

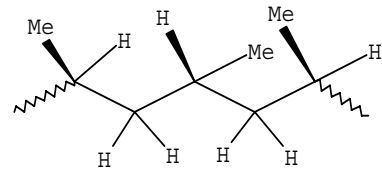
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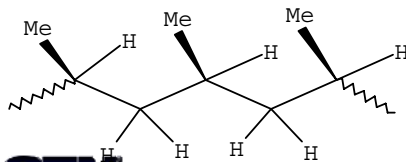
Tacticity refers to the stereochemical arrangement of groups along the backbone



Atactic polymers have a random arrangement.



Syndiotactic polymers have an alternating arrangement.



Isotactic polymers have an arrangement where groups occur on the same side throughout.

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Polymer architecture refers to the arrangement of mers

-AAAABBBBAAAABBAAAA-

-AAAAAAAAABBBBBBBBBB-

Block (segmented) polymers contain groups of mers in the backbone.

BBBBB

BBBBB

BBBBB

-AAAAXAAAAXAAAAXAAA-

Graft (comb) polymers contain groups of mers attached to a backbone.

-ABABABABABAB-

Alternating polymers contain backbones in which every other mer is the same.

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Some factors do not affect polymer registration

- Molecular weight
- Monomer ratio in addition polymers
 - e.g., 60:40 and 90:10 ethylene-vinyl chloride copolymers have the same CAS RN
- Head-to-head vs. head-to-tail arrangements
- Blends
 - Polymer blends are indexed using the CAS RNs for each of the specific polymers in the blend

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Post-treatment refers to the modification of polymers after the backbone has formed

- A post-treated polymer may be in REGISTRY in its modified form as
 - An unique substance
 - Or it may not
 - If a post-treated polymer is not in REGISTRY, search the indexing in CAPlus associated with the RN for the polymer being treated
 - e.g., 9003-53-6D

"D" for derivative is appended to the CAS RN for the known portion of the modified polymer.

```
=> FIL CAP
=> S 9003-53-6D/IT
L2      12184 9003-53-6D/IT

=> D IT
...

IT 9002-98-6 9003-53-6D,
Polystyrene, chloromethylated derivs.
```

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How to locate CAS Registry Numbers for polymers

- Search the REGISTRY database for
 - Chemical names
 - Polymer names
 - Component monomer names
 - Monomer Component Registry Numbers (/CRN)
 - Use the POLYLINK command for comprehensive retrieval of all RNs for condensation polymers
 - Polymer Class Terms
 - Structures
 - Monomer structures
 - SRUs

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Find polymers by searching the chemical name

- EXPAND and SEARCH names in REGISTRY in the Chemical Name (/CN) index
- Various name formats are possible
 - Trade names
 - Final polymer name
 - All of the monomer names
- Name searching works best with
 - Homopolymers
 - Simple copolymers

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Locate polymers by searching for the trade name

- Verify trade names
 - EXPAND the trade name in REGISTRY in the chemical name (/CN) index before searching
- Use variations on
 - Spelling
 - Spacing
 - Punctuation

```
=> FILE REGISTRY  
=> E PET/CN  
=> E SARAN SL 112/CN
```

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Search for the final name of a polymer

- Format final polymer names
 - Begin each name with the prefix “poly”
 - Enclose multiple-word monomers in parentheses
- Verify final polymer names
 - EXPAND in REGISTRY in the chemical name (/CN) field before searching

```
=> FILE REGISTRY
=> E POLYETHYLENE/CN
=> E POLY(TETRAFLUORO-1,3-DITHIETANE)/CN
```

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Search for polymers based on the names of their component monomers

- Use this technique when
 - You know the monomer reactants
 - You can name each monomer accurately
- Format monomer names by
 - Placing the monomers in alphabetical order
 - Separating the monomers with hyphens
 - Following the name with “polymer” or “copolymer”
- Verify the name by EXPANDING in the /CN field

```
=> FILE REGISTRY
=> E ACRYLIC ACID-METHYL METHACRYLATE-
    STYRENE COPOLYMER/CN
```

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Polymers may be found by using the RNs of the component monomers

Search Question:

Find references directed to copolymers of terephthalic acid and 1,4-butylene glycol used in resistors.

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Monomer name search example

To locate polymers when names of starting monomers are known...

- Step 1. Identify CAS RNs for each monomer
- Step 2. Isolate polymers with the monomers of interest
 - Search CAS RNs in the /CRN field
 - Refine by Number of Components
- Step 3. Search the answer set in CPlus

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SEARCH each component name separately to find Component RN

```
=> FILE REGISTRY
=> SET EXPAND CONTINUOUS
=> E TEREPHTHALIC ACID/CN
E1          1      TEREPHTHALHYDROXIMOYL CHLORIDE/CN
E2          1      TEREPHTHALHYDROXYAMOYL CHLORIDE-4,4`...
              THIOL POLYMER/CN
E3          1 --> TEREPHTHALIC ACID/CN
● ● ●

=> S E3;D
L1          1 "TEREPHTHALIC ACID"/CN

L1 ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN  100-21-0  REGISTRY
CN  1,4-Benzenedicarboxylic acid (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN  Terephthalic acid (7CI, 8CI)
OTHER NAMES:
● ● ●
```

SEARCH and DISPLAY
in one step by stacking
the commands.

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SEARCH each component name separately to find Component RN (cont'd)

```
=> E 1,4-BUTYLENE GLYCOL/CN
E#      FILE          FREQUENCY  TERM
--      ---          -
E13     REGISTRY      1          1,4-BUTYLENE DIMETHACRYLATE-N-
              ((R)-1-TETRALIN
              YL)ACRYLAMIDE POLYMER/CN
E14     REGISTRY      1          1,4-BUTYLENE DINITRATE/CN
E15     REGISTRY      1 --> 1,4-BUTYLENE GLYCOL/CN
● ● ●

=> S E15;D
L2          1 "1,4-BUTYLENE GLYCOL"/CN

L2 ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN  110-63-4  REGISTRY
CN  1,4-Butanediol (8CI, 9CI)  (CA INDEX
OTHER NAMES:
CN  1,4-Butylene glycol
● ● ●
```

The second component,
1,4-butylene glycol is
now searched.

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SEARCH the RN for each component and limit by number of components

```
=> SELECT RN L1;SEL RN L2
E25 THROUGH E25 ASSIGNED
E26 THROUGH E26 ASSIGNED
```

```
=> D SEL
```

```
● ● ●
```

```
E25   REGISTRY   1   100-21-0/BI
E26   REGISTRY   1   110-63-4/BI
```

```
=> S E25/CRN AND E26/CRN
```

```
L3           2665 100-21-0/CRN AND 110-63-4/CRN
```

```
=> S L3 AND 2/NC
```

```
L4           1 L3 AND 2/NC
```

SELECT RN extracts the CAS RN for each component monomer and assigns it an E-number. SEARCH for records having both RN numbers in the Component Registry Number (/CRN) fields.

Limit the answers to substances having exactly 2 as the number of components.

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The same final polymer may result from different combinations of starting materials

DIACID + DIOL

CAS RN 26062-94-2
1,4-Benzenedicarboxylic acid,
polymer with 1,4-butanediol

DIACID HALIDE + DIOL

CAS RN 59822-52-5
1,4-Benzenedicarbonyl dichloride,
polymer with 1,4-butanediol

DIESTER + DIOL

CAS RN 52237-47-5
1,4-Benzenedicarboxylic acid, diethyl ester,
polymer with 1,4-butanediol

POLYESTER

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Use POLYLINK to obtain a complete set of related condensation polymers

- What does the POLYLINK command do?
 - Finds a “family” of linked CAS RNs
 - Obtains all related records for a condensation polymer that also has a related SRU entry
 - Retrieves the SRU and all related monomer-based CAS RNs
 - Creates a new answer set that encompasses the original CAS RNs plus the CAS RNs linked to the original answer set

Use POLYLINK on

- Individual CAS RNs
- E-numbers containing a RN
- REGISTRY answer sets

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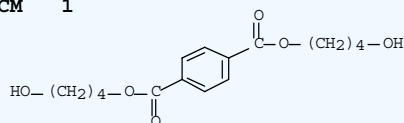
POLYLINK retrieves additional relevant polymer records

```
=> POLYLINK L4
L5          16 POLYLINK L4

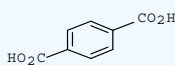
=> D SCAN
L5  16 ANSWERS  REGISTRY COPYRIGHT  2008 ACS on STN
IN  1,4-Benzenedicarboxylic acid, polymer with bis(4-
    hydroxybutyl) 1,4-benzenedicarboxylate (9CI)
MF  (C16 H22 O6 . C8 H6 O4)x
CI  PMS
```

****RELATED POLYMERS AVAILABLE WITH POLYLINK****

CM 1



CM 2



POLYLINK retrieves 15 additional CAS RNs.

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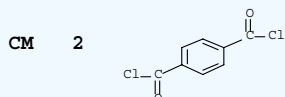
POLYLINK retrieves additional monomer-based records...

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

L5 16 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,4-Benzenedicarbonyl dichloride, polymer with 1,4-butanediol
(9CI)
MF (C8 H4 Cl2 O2 . C4 H10 O2)x
CI PMS, COM

****RELATED POLYMERS AVAILABLE WITH POLYLINK****

CM 1
HO—(CH₂)₄—OH



This record would have been missed if only a chemical name search was performed.

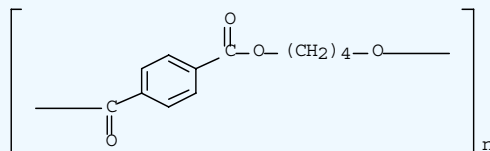
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...in addition to final polymer (SRU) records

L5 16 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Poly(oxy-1,4-butanediylloxycarbonyl-1,4-phenylenecarbonyl)
(9CI)
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT
MF (C₁₂ H₁₂ O₄)_n
CI PMS, COM

****RELATED POLYMERS AVAILABLE WITH POLYLINK****



Polymer Structural Repeating Unit

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

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Find the corresponding references in CAPlus

```
=> FILE CAPLUS
=> S L5 AND RESISTOR
L6          14 L7 AND RESISTOR
=> D 1 IBIB HIT
L8 ANSWER 1 OF 14 CAPLUS COPYRIGHT 20
ACCESSION NUMBER:      2008:773407 CAP
TITLE:                  Heat generating bodies
INVENTOR(S):           Nakajima, Keizo; Ishii, Takahito
PATENT ASSIGNEE(S):    Matsushita Electric Industrial Co., Ltd.,
                        Japan
SOURCE:                Japan Kokai Tokkyo Koho, 13pp.
                        CODEN: JKXXAF
DOCUMENT TYPE:         Patent
LANGUAGE:              Japanese
IT  24937-78-8, Ethylene-vinyl acetate copolymer 24968-12-5,
    Polybutylene terephthalate 25038-59-9
    RL: TEM (Technical or engineered material use); USES (Uses)
        (heat generating bodies containing polymeric resistors and
        resin coatings)
```

A Japanese patent publication disclosing resistors comprised of the monomers of interest.

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Polymer Class Terms (PCTs) describe broad classes of polymers

- Each term represents the structural characteristics of the polymer backbone
 - Linkages already present within the monomer backbone
 - Linkages present in the SRU backbone
 - Linkages formed in the polymerization process
- PCTs can be searched along with other terms
 - Text terms
 - Component RNs
 - Structures

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Polymers are also found by searching the broader Polymer Class Terms

Search Question:

Find references discussing fluoropolymers used as antifriction coatings.

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Polymer Class Term search strategy

To find references describing broad classes of polymers...

- Step 1. Search relevant Polymer Class Terms in REGISTRY
- Step 2. Identify Controlled Terms for coatings in CAplus
- Step 3. Combine both sets of results
- Step 4. Expand and Search CAplus substance class terms

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Find CAS RNs using Polymer Class Terms in REGISTRY

```
=> FILE REGISTRY
...
=> E FLUOROPOLYMER/PCT 5
E#      FILE              FREQUENCY  TERM
--      -
E1      REGISTRY          54664     EPOXY RESIN/PCT
E2      REGISTRY          11507     FLPO/PCT
E3      REGISTRY          11507     --> FLUOROPOLYMER/PCT
E4      REGISTRY          85610     MANC/PCT
E5      REGISTRY          166006    MANR/PCT

=> S FLUOROPOLYMER/PCT
L1      11507  FLUOROPOLYMER/PCT
```

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Two Polymer Class Terms are represented by this answer

```
L1  ANSWER 351 OF 11507  REGISTRY COPYRIGHT 2008 ACS on STN
RN  944477-77-4  REGISTRY
ED  Entered STN: 13 Aug 2007
CN  Ethene, 1-[difluoro[1,1,2,2-tetrafluoro-2-
    (trifluoromethoxy)ethoxy]methoxy]- 1,2,2-trifluoro-,
    polymer with 1,1-difluoroethene (CA INDEX NAME)
MF  (C6 F12 O3 . C2 H2 F2)x
CI  PMS
PCT Fluoropolymer, Polyvinyl
SR  CA
LC  STN Files:  CA, CAPLUS

    CM  1

    CRN 369371-47-1
    CMF C6 F12 O3
```

This polymer is in both the fluoropolymer and polyvinyl classes.

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Explore the CA Lexicon thesaurus for antifriction coating synonyms

```

=> FILE CAPLUS
=> E ANTI-FRICTION COATINGS/CT 5
E#  FREQUENCY  AT  TERM
---  -
E1      0      3  ANTI-FRICTION ABRASION-R
E2      0      2  ANTI-FRICTION AGENTS/CT
E3      0      2  --> ANTI-FRICTION COATINGS/CT
E4      0      2  ANTI-FRICTION LUBRICATING OIL ADDITIVES/CT
E5     4357     5  ANTI-FRICTION MATERIALS/CT
=> E E3+ALL
E13      0      --> Antifriction coatings/CT
E14      USE Coating materials (L) antifriction/CT
***** END *****
=> E E14+ALL
E25     19513  BT2 Materials/CT
E26     299919 BT1 Coating materials/CT
E27      --> Coating materials (L) antifriction/CT
E28      OLD Antifriction materials (L) coatings/CT
E29      UF Antifriction coatings/CT
E30      UF Antifriction nonstick coatings/CT
E31      UF Tribological coatings/CT
***** END *****

```

Utilize the complete controlled terminology thesaurus to retrieve additional related terms.

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Search CPlus for fluoropolymers used as antifriction coatings

```

=> S L1/USES
L2      68852 L1/USES
        (L1 (L) USES/RL)

=> S L2 (L) ANTI-FRICTION (L) (COATING OR MATERIAL)
L3      285 L2 (L) ANTI-FRICTION (L) (COATING OR MATERIAL)

```

/USES is a CAS Role that limits answer set L1 to CPlus references that describe a use of a fluoropolymer in the answer set.

Adding text terms further limits the answer set to references that describe the use of a fluoropolymer in an antifriction coating or antifriction material context. The (L) connector requires that all terms are in the same field of the database record.

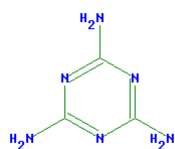
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Find references to classes of polymers containing a known monomer structure

Search Question:

Locate references relating to a fast-curing, thermosetting phenolic laminating resin having a pH of about 7.0 - 9.0 and based on this monomer:



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Strategy to find a class of polymers based on a known monomer

To find references describing classes of polymers based on a known monomer...

- Step 1. Locate the PCT for the class of polymers
- Step 2. Draw the structure of interest
- Step 3. Locate substances matching both requirements
- Step 4. Refine results using text terms

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Locate the Polymer Class Term of interest

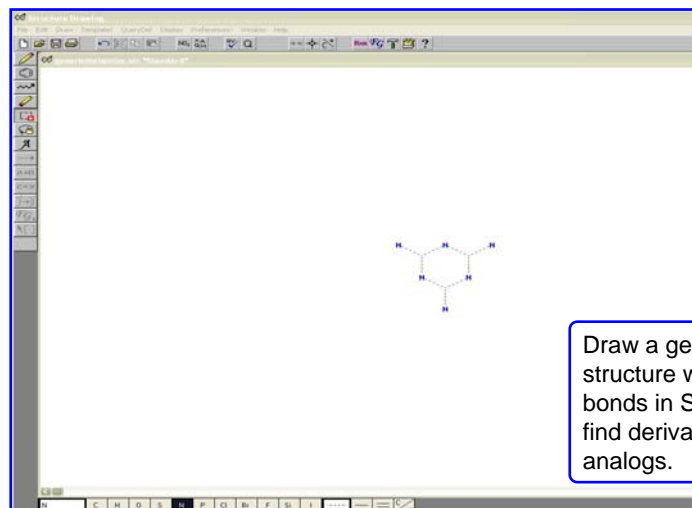
```
=> FIL REG
...
=> E PHENOLIC RESIN/PCT 5
E#      FILE          FREQUENCY  TERM
--      -
E1      REGISTRY      308947    PETH/PCT
E2      REGISTRY      84816     PETH F/PCT
E3      REGISTRY      17731    --> PHENOLIC RESIN/PCT
E4      REGISTRY      3852     PHZ/PCT
E5      REGISTRY      2994     PHZ F/PCT

=> S E3
L1      17731 "PHENOLIC RESIN"/PCT
```

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Draw the structure in the STN Express® Drawing Window



Draw a generic melamine structure with unspecified bonds in STN Express to find derivatives and analogs.

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Run a subset search for the generic melamine structure

```
=>
Uploading C:\Documents and Settings\STN Express
8.3\Queries\PolymerEx\genericmelamine.str
```

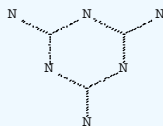
•••

L2 STRUCTURE UPLOADED

```
=> D
```

L2 HAS NO ANSWERS

L2 STR



```
=> S L2 SUB=L1 FULL
```

•••

L3 1153 SEA SUB=L1 SSS FUL L2

Search the melamine structure with the L1 REGISTRY subset of phenolic resins Polymer Class Terms.

STN

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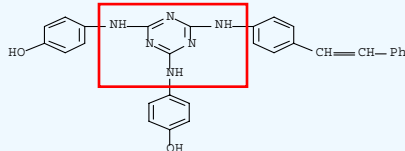
Browse substance answers to see if the polymers match your intended search

```
L3 1153 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
RN 30756-81-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Formaldehyde, polymer with 4,4'-[[6-[[4-(2-phenylethenyl)phenyl]amino]-1,3,5-
triazine-2,4-diy]diimino]bis[phenol] (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Phenol, 4,4'-[[6-(p-styrylanilino)-s-triazine-2,4-diy]diimino]di-,
polymer with formaldehyde (8CI)
CN Phenol, 4,4'-[[6-[[4-(2-phenylethenyl)phenyl]amino]-1,3,5-triazine-2,4-
diyl]diimino]bis-, polymer with formaldehyde (9CI)
MF (C29 H24 N6 O2 . C H2 O)x
CI PMS
PCT Phenolic resin, Polyamine, Polystyrene
```

CM 1

CRN 47794-21-8

CMF C29 H24 N6 O2



The melamine structure and two phenol groups are represented in component 1 of this 2-component polymer.

STN

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Crossover to CAPLUS and limit the search with text terms

=> FILE CAPLUS

•••

=> S L3 AND ?LAMINAT? AND PH(S) (7 OR 8 OR 9)

•••

L4 19 L3 AND ?LAMINAT? AND PH(S) (7 OR 8 OR 9)

=> D HIT 1

L5 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2008 ACS on

TI Environmentally friendly thermosetting resins decorative laminated boards.

AB The resins are prepared by mixing 60-100 parts 11 parts phenol, adjusting pH to 7-8 with 30% adding 3-10 parts melamine and 10-22 parts urea 40-60 min, adding 1-4 parts polyvinyl alc., stirring for 10-15 min, adjusting pH to 4.6-6 with 30% aqueous HCO₂H solution, adding 8-17 parts urea, keeping temperature at 60-75, adjusting pH to 7.5-8 with 30% aqueous NaOH solution when viscosity reaches 14-16 s, adding 3-6 parts urea, stirring for 10-15 min, cooling, and discharging. The resins are light-red transparent liqs. with low formaldehyde content, and have improved flexibility and water resistance when used for manufacture of flame retardant boards.

This publication discusses an environmentally friendly thermosetting resin for high pressure decorative laminated boards.

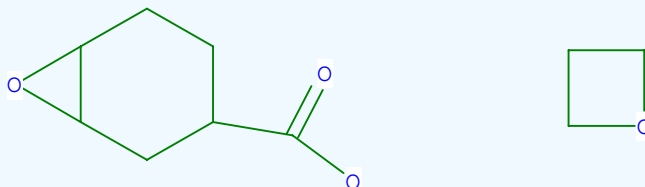
STN

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Locating polymers by structure

Search Question:

Find references discussing polymers containing these structural fragments in their starting materials for dental composites:



STN

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Monomer structure search strategy

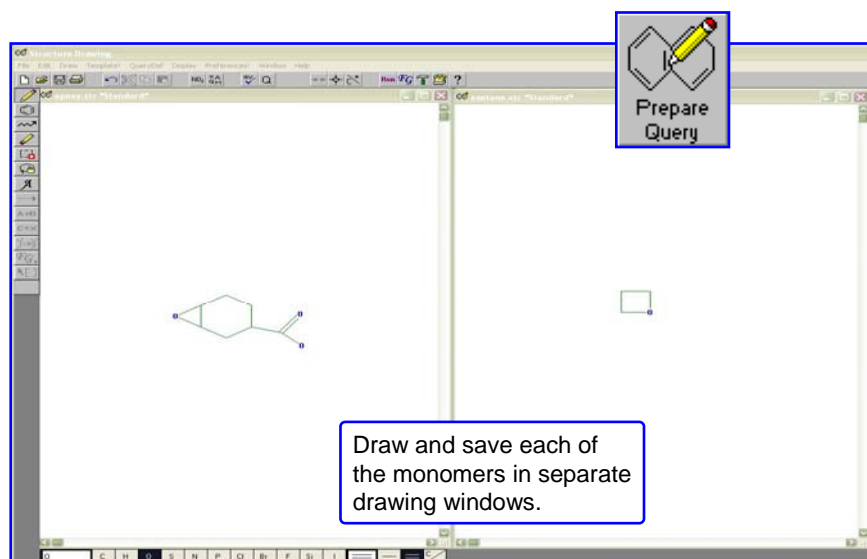
To locate polymers with known monomer structures...

- Step 1. Draw two (2) separate structures
- Step 2. Save *one* structure with the polymer filter
- Step 3. Upload structures in REGISTRY
- Step 4. Combine structure and filter L-numbers with the AND operator to find answers with the fragments
- Step 5. Find references in CPlus

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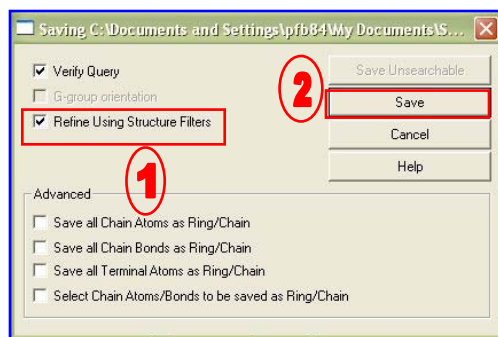
Draw two different structures



STN

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Save the structures and be sure to refine using a Structure Filter



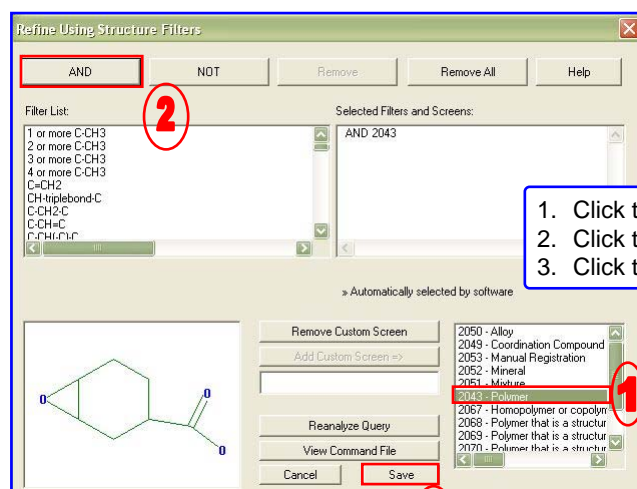
1. Check the appropriate box to add a polymer filter to the structure query.

2. Click the "Save" button.

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Add the Polymer filter (screen 2043) to one structure query



1. Click the Polymer screen.

2. Click the "AND" button.

3. Click the "Save" button.

STN

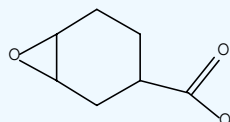
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Upload the epoxy structure in REGISTRY

- Each structure is uploaded individually

```
=> FILE REGISTRY
=>
Uploading ...

L1      STRUCTURE UPLOADED
=> D L1
L1 HAS NO ANSWERS
L1      STRUCTURE
```



STN

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Upload the oxetane structure

```
=> ....Testing the current file.... screen
=> screen 2043
L2      SCREEN CREATED

=>
Uploading...

L3      STRUCTURE UPLOADED

=> QUE L3 AND L2
L4      QUE L3 AND L2
```

A filter is a SCREEN command.

```
=> D L4
L4 HAS NO ANSWERS
L2      SCR 2043
L3      STR
```

IMPORTANT! Note the L-numbers of the SCREEN command and the structure.



STN

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Run a SAMPLE substructure search using AND to combine

```
=> S L1 AND L2 AND L3 SSS SAM
SCREENS AND STRUCTURES MUST BE GROUPED
Structures and screens are processed separately in queries
which contain both types of search terms...
```

```
=> S L1 AND L3 AND L2 SSS SAM
```

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH  **COMPLETE**
PROJECTED ITERATIONS:   7598 TO  10122
PROJECTED ANSWERS:     640 TO   1520
L5                      50 SEA SSS SAM L1 AND L3 AND L2
```

When combining multiple structure queries and L-numbers containing screens, the order of combination is important. The L-number containing the screen(s) should be placed last.

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Run FULL substructure search and use POLYLINK

```
=> S L1 AND L3 AND L2 SSS FULL
100.0% PROCESSED      8622 ITERATIONS      865 ANSWERS
SEARCH TIME: 00.00.01
L6                      865 SEA SSS FUL L1 AND L3 AND L2
```

```
=> POLYLINK L6
L7                      865 POLYLINK L6
```

L1 = epoxy structure fragment
L2 = polymer screen
L3 = oxetane structure fragment

POLYLINK does not find any additional linked polymers.

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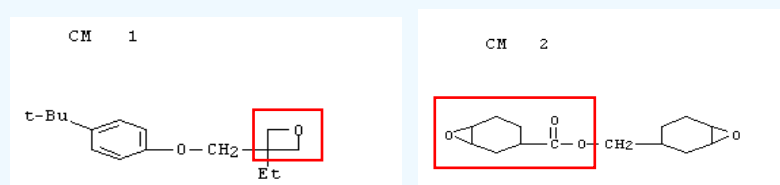
DISPLAY results

=> D SCAN

IN 7-Oxabicyclo[4.1.0]heptane-3-carboxylic acid, 7-oxabicyclo[4.1.0]hept-3-ylmethyl ester, polymer with 3-[[4-(1,1-dimethylethyl)phenoxy]methyl]-3-ethyloxetane

MF (C16 H24 O2 . C14 H20 O4)x

CI PMS



STN

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Crossover to CAPLUS and refine with /BIOL role

=> FILE CAPLUS

•••

=> S L7/BIOL

L12 6 L7/BIOL

The BIOL role is a broad role assigned to biological uses and studies.

=> D BIB HITSTR

L12 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2008:215200 CAPLUS Full-text

DN 148:269529

TI Dental restorative filling composite materials

IN Hara, Tadashi; Suzuki, Takeshi

PA Tokuyama Dental Corp., Japan

SO Japan Kokai Tokkyo Koho, 20pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2008037776	A	20080221	JP 2006-212087	20060803

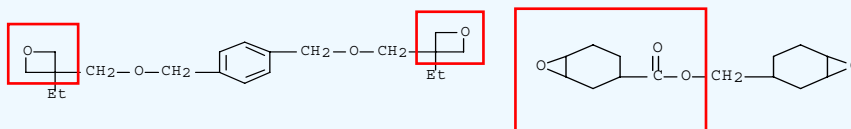
STN

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The HITSTR display shows the structure diagram searched in your query

IT 167488-43-9P
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (dental restorative filling composite materials)
 RN 167488-43-9 CAPLUS
 CN 7-Oxabicyclo[4.1.0]heptane-3-carboxylic acid, 7-oxabicyclo[4.1.0]hept-3-ylmethyl ester, polymer with 3,3'-[1,4-phenylenebis(methyleneoxymethylene)]bis[3-ethyloxetane] (CA INDEX NAME)

CM 1	CM 2
CRN 142627-97-2	CRN 2386-87-0
CMF C20 H30 O4	CMF C14 H20 O4



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Summary

- Search component monomer names in the **Chemical Name** index (**/CN**) in REGISTRY to find CAS RNs
- Search monomer RNs as **Component Registry Numbers** (**/CRN**) to find polymer records
- Use **POLYLINK** to find records for all condensation polymer monomer combinations and SRUs
- Use the **CAplus thesaurus** to enhance comprehensiveness
- Use **Polymer Class Terms (PCT)** and **CAplus substance class indexing** to find broad classes of polymers

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Upcoming e-Seminars

The screenshot shows the CAS STN website interface. At the top, the CAS logo is displayed with the tagline "A Division of the American Chemical Society". Below the logo is a navigation menu with links for Home, About CAS, Our Expertise, Solutions, Products & Services, Support, News & Events, Meeting Center, Training Center, Event Center, Support Center, More Services, and My WebEx. The main content area is titled "All e-Seminars" and features the STN logo. There are search filters for Product (STN), Category (All), and Language (All), with a "Display" button. A note indicates "All event times in: Eastern ST". A table lists upcoming seminars:

Date & Time	Event	Category	Subcategory
November 2008			
November 25, 2008 13:00 - 14:00 Eastern ST	STN: Polymers in Scientific Literature	Polymers	Intermediate Enroll
December 2008			
December 11, 2008 9:00 - 10:00 Eastern ST	STN: Polymers in Scientific Literature	Polymers	Intermediate Enroll
December 16, 2008 13:00 - 14:00 Eastern ST	STN: Dealing with Large Answer Sets	Search Techniques	Intermediate Enroll
January 2009			
January 8, 2009 9:00 - 10:00 Eastern ST	STN: Dealing with Large Answer Sets		Enroll

Don't forget to register!
<http://casevents.webex.com>

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CAS[®]
e-Seminars

STN: Polymers in Scientific
Literature