

# STN<sup>®</sup>

## Polymer Searching in CAS REGISTRY<sup>SM</sup>

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# Topics

- How polymers are “registered” in CAS REGISTRY
- Search for polymer information based on
  - Text search
  - Molecular Formula
  - Structures
- Search for post-treated polymers in CAplus<sup>SM</sup>

# How CAS defines a polymer

- A macromolecule formed by linking together 10 or more smaller molecules (monomers)
- REGISTRY also identifies smaller “mers”, e.g., dimers, trimers, tetramers
- Types of polymers covered in REGISTRY include homopolymers, copolymers, addition, condensation, block, alternating, and graft polymers

# Classes of polymers included in REGISTRY

- Synthetic
  - Polyamides, e.g., for nanocomposites
  - Polycarbonates, e.g., for impact resistance
  - Polyurethanes, e.g., for coatings
- Naturally occurring
  - Amino acids, e.g., peptides and proteins
  - Nucleic acids, e.g., probes or primers
  - Oligosaccharides, e.g., bulking agents

# More than 1.4 million polymers are included in REGISTRY

- REGISTRY is updated daily with new polymers
- A unique CAS Registry Number<sup>®</sup> (CAS RN) is assigned to each polymer that is registered
- To identify STN bibliographic databases containing records indexed with RNs for polymers of interest, check the REGISTRY Number Locator field (LC)

# There are two main types of polymer records in REGISTRY

- Primary registration is monomer-based
  - The polymer containing component monomers has a CAS Registry Number (RN)
  - Each component monomer has its own Component Registry Number (CRN)
- A supplemental Structural Repeating Unit (SRU) may also be indexed
  - The SRU will have a unique RN

# Component monomer-based REGISTRY record for a polymer

RN 28572-91-0 REGISTRY  
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)

CN Ethene, 1,1-dichloro-, polymer with chloroethene and methyl  
2-propenoate (9CI)

● ● ●

OTHER NAMES:

CN Ixan PA 331

CN Methyl acrylate-vinyl chloride-vinylidene chloride polymer

● ● ●

CN Vinylidene chloride-vinyl chloride-methyl acrylate copolymer

MF (C4 H6 O2 . C2 H3 Cl . C2 H2 Cl2)x

CI PMS

PCT Chloropolymer, Polyacrylic, Polyvinyl

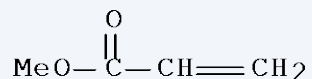
LC STN Files: CA, CAPLUS, CHEMLIST, IFICDB, IFIPAT, IFIUDB,

# Component monomer-based REGISTRY record for a polymer (cont.)

CM 1

CRN 96-33-3

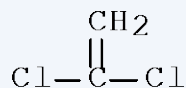
CMF C4 H6 O2



CM 2

CRN 75-35-4

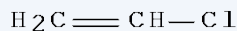
CMF C2 H2 Cl2



CM 3

CRN 75-01-4

CMF C2 H3 Cl



There are 3 monomer components, identified as

- CM1
- CM2
- CM3

For each component, the record lists

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

CRNs are searchable in the /CRN field

CMFs are searchable in the Basic Index



# Polymer Structural Repeating Unit (SRU) records

- Monomer-based records for condensation polymers can be supplemented with a structural repeating unit (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 mainly as SRUs
  - Polypropylene glycol (PPG) (142901-89-1)

# REGISTRY record for a polymer based on the Structural Repeating Unit

RN 24968-12-5 REGISTRY  
CN Poly(oxy-1,4-butanediloxycarbonyl-1,4-phenylenecarbonyl)  
(CA INDEX NAME)

## OTHER NAMES:

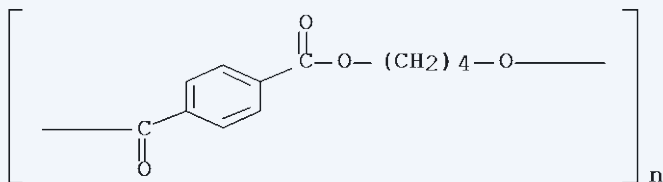
CN 1,4-Butanediol-dimethyl terephthalate copolymer, SRU  
CN 1,4-Butanediol-dimethyl terephthalate polymer, SRU  
CN 1,4-Butanediol-divinyl terephthalate copolymer, SRU

MF (C12 H12 O4)<sub>n</sub>

CI PMS, COM

PCT Polyester

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



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

21559 REFERENCES IN FILE

357 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

21577 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# Locate polymers by chemical name

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

# Polymer Name Search

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

```
=> FILE REGISTRY
```

```
=> E POLYETHYLENE/CN
```

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

```
=> E POLY(LACTIC ACID-GLYCOLIC ACID)/CN
```

```
=> E METHYL ACRYLATE-VINYL CHLORIDE-VINYLDENE CHLORIDE COPOLYMER/CN
```

## Use POLYLINK to obtain a complete set of related *condensation* polymers

- Obtains all related records for a condensation polymer that has a SRU record
- Retrieves the SRU record and all corresponding monomer-based RN records
- Creates a new answer set that encompasses all linked polymer records

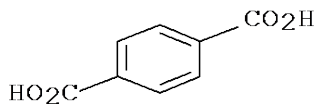
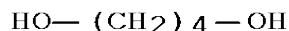
Use POLYLINK on

- Individual Registry Numbers
- E-numbers containing a RN
- REGISTRY answer set L-numbers

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

## DIACID + DIOL

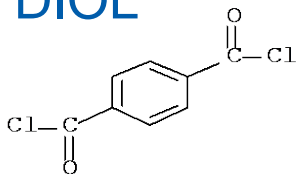
**CAS RN 26062-94-2**



1,4-Benzenedicarboxylic acid,  
polymer with 1,4-butanediol

## DIACID HALIDE + DIOL

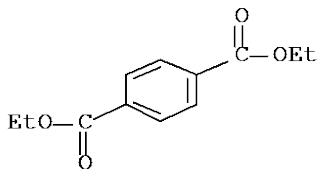
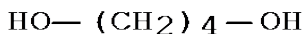
**CAS RN 59822-52-5**



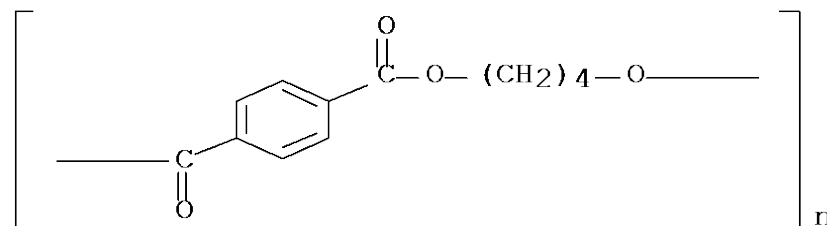
1,4-Benzenedicarbonyl dichloride,  
polymer with 1,4-butanediol

## DIESTER + DIOL

**CAS RN 52237-47-5**



1,4-Benzenedicarboxylic acid, diethyl ester,  
polymer with 1,4-butanediol



## POLYESTER

**CAS RN 24968-12-5**

Poly(oxy-1,4-butanediylloxycarbonyl-  
1,4-phenylenecarbonyl)

Use POLYLINK from any  
starting RN and retrieve all the  
associated records that make  
the same final polymer.

# Polymer class terms (PCT) in REGISTRY

Specific polymers with structures are classified into broad classes of polymers in the PCT field

```
RN 297134-63-5 REGISTRY
ED Entered STN: 19 Oct 2000
CN Poly(oxy-1,4-butanediyl),  $\alpha$ -hydro- $\omega$ -hydroxy-, polymer with
  1,6-diisocyanatohexane and fluoroethene, block (9CI) (CA
  INDEX NAME)
OTHER NAMES:
CN 1,6-Hexamethylene diisocyanate-poly(tetramethylene glycol)-
  vinyl fluoride block copolymer
MF (C8 H12 N2 O2 . (C4 H8 O)n H2 O . C2 H3 F)x
CI PMS
PCT Fluoropolymer, Polyether, Polyurethane, Polyurethane formed,
  Polyvinyl
SR CA
LC STN Files: CA, CAPLUS
```

# EXPAND Polymer Class Terms in REGISTRY

=> E POLY/PCT 20

E1	2858	PNUC/PCT
E2	40085	POLF/PCT
E3	0	--> POLY/PCT
E4	17824	POLYACETYLENE/PCT
E5	431552	POLYACRYLIC/PCT
E6	45326	POLYAMIC ACID/PCT
E7	45106	POLYAMIC ACID FORMED/PCT
E8	101870	POLYAMIDE/PCT
E9	76906	POLYAMIDE FORMED/PCT
E10	57064	POLYAMINE/PCT
E11	18402	POLYAMINE FORMED/PCT
E12	1683	POLYANHYDRIDE/PCT
E13	1146	POLYANHYDRIDE FORMED/PCT
E14	7409	POLYAZOMETHINE/PCT
E15	3868	POLYAZOMETHINE FORMED/PCT
E16	2489	POLYBENZIMIDAZOLE/PCT
E17	1141	POLYBENZIMIDAZOLE FORMED/PCT
E18	4211	POLYBENZOXAZOLE/PCT
E19	2793	POLYBENZOXAZOLE FORMED/PCT
E20	1542	POLYCARBODIIMIDE/PCT

FORMED is added when polymerization of monomers creates a specific type of bond.



# Polymer class information in CPlus

Polymer classes also appear as indexing terms with modifying text and CAS Roles

IT Polyurethanes, uses

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(polyester-, coatings; moisture-permeable water-resistant camouflaging fabrics manufactured by printing fabrics with camouflaging patterns exhibiting multistep IR reflection and coating the fabrics with polyurethanes and manufacture)

IT Fluoropolymers, uses

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(polyurethane-, coatings; moisture-permeable water-resistant camouflaging fabrics manufactured by printing fabrics with camouflaging patterns exhibiting multistep IR reflection and coating the fabrics with polyurethanes and manufacture)

# Search Example: Text search for polymers

A pharmaceutical composition comprising:

- (a) a bioerodible water insoluble polymer matrix comprising a polyester polymer, wherein the polymer matrix has a melting point of less than 60.degree. C.; and
- (b) an active agent dispersed within the polymer matrix, wherein the composition is formulated for controlled release the active agent to a target site for a pre-determined period of time.

# Search strategy

1. Search Polymer Class Terms to find polyesters in REGISTRY
2. Search controlled terms to find polyesters in CAplus
3. Combine answer sets and refine using CAS Roles and text
4. Option: TRANSFER hit Registry Numbers to REGISTRY, limit by melting point range
5. Display references

# Find polyester class term in REGISTRY

**=> FILE REGISTRY**

**=> E POLYESTER/PCT**

E1	1594	POLYCYANURATE/PCT
E2	1575	POLYCYANURATE FORMED/PCT
E3	254264	--> POLYESTER/PCT
E4	205858	POLYESTER FORMED/PCT
E5	366086	POLYETHER/PCT
E6	103071	POLYETHER FORMED/PCT
E7	4267	POLYHYDRAZIDE/PCT
E8	3298	POLYHYDRAZIDE FORMED/PCT
E9	71311	POLYIMIDE/PCT
E10	45106	POLYIMIDE FORMED/PCT
E11	6599	POLYIONENE/PCT
E12	2721	POLYIONENE FORMED/PCT

**=> S POLYESTER/PCT**

L1 254264 POLYESTER/PCT

# Look up polyesters as a controlled term in ZCAplus

```
=> FILE ZCAPLUS
```

```
=> E POLYESTERS/CT
```

E#	FREQUENCY	AT	TERM
--	-----	--	----
E1	0	2	POLYESTERIFICATION/CT
E2	0	3	POLYESTERIMIDES/CT
E3	296923	99	--> POLYESTERS/CT
E4	0	11	POLYESTERS (L) ACRYLATE-TERMINATED/CT

● ● ●

```
=> E E3+ALL
```

```
E20 296923 --> Polyesters/CT
      HNTE Valid heading during volume 31 (1937) to
            present.
      NOTE Polymers containing ester or thio groups in
            the backbone are indexed here or at one of its
            narrower terms. Polymers formed by addition
            polymerization from unsaturated esters, such
            as butyl 2-propenoate or ethenyl propanoate,
            with resulting pendent ester groups are
            indexed at the named esters or at Esters.
```

● ● ●

# Search both Registry Numbers and controlled terminology in HCAplus

=> FILE HCAPLUS

=> S L1

L2 483070 S L1

=> S E20+NT, PFT

L3 519394 POLYESTERS+NT, PFT/CT

=> S L2 OR L3; D SCAN HIT

L4 720581 S L2 OR L3

IT **34346-01-5**, Poly(lactic-co-glycolic acid)

RL: AMX (Analytical matrix); ANST (Analytical study)  
(development and validation of reversed-phase HPLC method  
for detn. Of exenatide in poly(lactic-co-glycolic acid)  
microspheres)

IT **Polyesters**

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(polyoxyalkylene-; biomaterials comprising hydroxy  
carboxylate-polyethylene glycol copolymer and specified siRNA)

- L2 = answers from Registry Number crossover of polyester class term
- L3 = answers from polyester controlled terms in HCAplus

# Refine search using CAS Roles, truncation, and proximity

```
=> S L4 (L) ((THU/RL OR PAC/RL OR PKT/RL) OR (?PHARMA? OR ?DRUG? OR THERAP?))
```

```
L5      79042 L4 (L) ((THU/RL OR PAC/RL OR PKT/RL) OR (?PHARMA? OR ?DRUG? OR THERAP?))
```

```
=> S L5 (L) (BIODEGRAD? OR BIO DEGRAD? OR BIOEROD? OR BIO EROD?)
```

```
L6      4674 L5 (L) (BIODEGRAD? OR BIO DEGRAD? OR BIOEROD? OR BIO EROD?)
```

```
=> S L6 (L) (WATER OR AQUEOUS) (5A) INSOL?
```

```
L7      7 L6 (L) (WATER OR AQUEOUS) (5A) INSOL?
```

# Option: Limit results to substances having the claimed melting point range

```
=> FILE REGISTRY
=> TRA L7 HIT RN 1-
L8          TRA L7 1- RN HIT : 37 TER
L9          37 SEA L8

=> S L9 AND MP<60
L10         16 S L9 AND MP<60
```

```
=> D HIT 5
```

```
RN 50974-93-1 REGISTRY
```

CODE	VALUE	TYPE	NOTE
------	-------	------	------

MP	52.6 deg C	Experimental	(1) CAS
----	------------	--------------	---------

MP	48 deg C	Experimental	(2) CAS
----	----------	--------------	---------

MP	36 deg C	Experimental	(2) CAS
----	----------	--------------	---------

(1) Asplund, J. O. Basse; Macromolecules 2006 V39(13) P4380-4385  
CAPLUS

(2) Helminen, Antti O.; Journal of Polymer Science, Part A:  
Polymer Chemistry 2003 V41(23) P3788-3797 CAPLUS

The **TRANSFER (TRA)** command extracts fields of information to be searched in another database. In this case, only HIT RNs of polyesters are crossed back to REGISTRY.

Alternatively, display format **QRD** to see the substance identification information, plus the query related fields.



# Crossover to HCAplus and find references

```
=> FILE HCAPLUS  
  
=> S L7 AND L10  
L11          5 S L7 AND L10  
  
=> S L7 NOT L10  
L12          2 S L7 NOT L10
```

- L7 = 7 answers from text search
- L10 = RNs with a reported melting point < 60° C

# Display references where the polyester has a reported melting point < 60° C

=> D L11 IBIB ABS HITIND 1-5

TITLE: Sustained release of water-insoluble simvastatin from biodegradable hydrogel augments bone regeneration  
AUTHOR(S): Tanigo, Tomomi; Takaoka, Ryohei; Tabata, Yasuhiko  
CORPORATE SOURCE: Department of Biomaterials, Field of Tissue Engineering, Institute for Frontier Medical Sciences, Kyoto University, 53 Kawara-cho Shogoin, Sakyo-ku  
SOURCE: Journal of Controlled Release (2010), 143(2), 201-206  
CODEN: JCREEC; ISSN: 0168-3659

AB Drug delivery technol. is a practically promising way to enhance the therapeutic efficacy of drugs. However, there remain some properties of material to be improved for drug delivery, such as the biodegradability and biocompatibility. In this study, we demonstrate that a biodegradable hydrogel of gelatin can achieve the sustained release of water-insol. simvastatin. ● ● ●

IT 26161-42-2D, grafted to gelatin 26811-96-1D,  
Poly(L-lactic acid), grafted to gelatin  
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(sustained release of water-insol. simvastatin from biodegradable hydrogel augments bone regeneration)

# Display references where the polyester does not have a reported melting point < 60° C in REGISTRY

=> D L12 IBIB ABS HITIND 1-2

TITLE: Characteristic of hyaluronic acid derivative films cross-linked by polyethylene glycol of low water content

AUTHOR(S): Chen, Jinghua; Chen, Jingtao; Xu, Zheng; Gu, Qisheng

CORPORATE SOURCE: College of Publishing and Printing, University of Shanghai for Science and Technology, Shanghai, 200093, Peop. Rep. China

SOURCE: Journal of Medical Colleges of PLA (2008), 23(1), 15-19

LANGUAGE: English

AB Objective: To test the characteristics of hyaluronic acid (HA) deriv. cross-linked by polyethylene glycol films of low water content. Methods: The cross-linked HA film with 200 .mu.m thickness was got at atm. Pressure at 25 .degree.C for 5 d. ● ● ●

IT **9004-61-9**, Hyaluronic acid 25322-68-3, Polyethylene glycol

RL: TEM (Technical or engineered m **use**); BIOL (Biological study); USE (hyaluronic acid hydrogel cross low water content, slow degrdn. face in white fac indicating that HA mols. can be cross-linked with PEG to produce **water-insol., biodegradable** hydrogel material)

No melting point has been recorded for hyaluronic acid in REGISTRY.

# Search Example: Molecular formula, trade name and POLYLINK search for polymers

The pharmaceutical composition of claim 1, wherein the polymer matrix comprises a polymer having the formula  $(C_6H_{10}O_2)_x \cdot (C_5H_8O_4)$  where x is such that the polymer has an average molecular weight of about 1000.

## Specification

[0025] In a preferred embodiment, the polymer matrix includes the polyester polymer 2-oxepanone, polymer with 2,2-bis(hydroxymethyl)-1,3-propanediol. This polymer is also known as epsilon-caprolactone polymer with pentaerythritol and has the chemical formula  $(C_6H_{10}O_2)_x \cdot C_5H_{12}O_4$ , where x is such that the polymer has an average molecular weight of about 1000. This polymer is commercially available from Solvay Chemicals, Inc. as CAPA® 4101.

# Search strategy

1. **EXPAND** and **SEARCH** the complete molecular formula in the molecular formula (/MF) field
2. **EXPAND** and **SEARCH** trade names in the chemical name (/CN) field
3. Use **POLYLINK** to find condensation polymers related to the SRU record
4. **SEARCH** component molecular formulas in the Basic Index to find polymers with >2 components
5. Combine answer sets in REGISTRY and crossover to HCAplus
6. Refine using CAS Roles and text

# EXPAND and SEARCH the complete molecular formula in the /MF field

```
=> FILE REGISTRY
```

```
=> E (C6H10O2)X.C5H8O4/MF
```

```
E1          1      (C6H10O2)X.C5H8O3.H3O4P/MF
```

```
E2          1      (C6H10O2)X.C5H8O3.XH3O4P/MF
```

```
E3          1 --> (C6H10O2)X.C5H8O4/MF
```

```
E4          1      (C6H10O2)X.C5H9BR3O/MF
```

```
● ● ●
```

```
=> S E3
```

```
L1          1 "(C6H10O2)X.C5H8O4"/MF
```

- **EXPAND** complete molecular formulas in the /MF field
- Polymer molecular formulas are in Hill system order, with the repeating units enclosed in parentheses, followed by X
- The molecular formulas of non-repeating portions of the polymer are combined and included at the end of the MF without parentheses

# Display results

=> D L1

RN 234113-99-6 REGISTRY

ED Entered STN: 21 Aug 1999

CN 2-Oxepanone, homopolymer, hydrogen pentanedioate (9CI) (CA INDEX NAME)

MF (C6 H10 O2)x . C5 H8 O4

PCT Polyester, Polyester formed

SR CA

LC STN Files: CA, CAPLUS

CM 1

CRN 110-94-1

CMF C5 H8 O4

CM 2

CRN 24980-41-4

CCI PMS

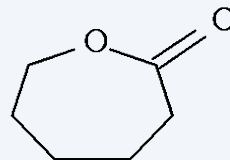
(C6 H10 O2)x

HO<sub>2</sub>C—(CH<sub>2</sub>)<sub>3</sub>—CO<sub>2</sub>H

CM 3

CRN 502-44-3

CMF C6 H10 O2



# EXPAND and SEARCH trade names in the complete chemical name (/CN) field

```
=> E (C6H10O2)X.C5H12O4/MF
E1      1      (C6H10O2)X.C5H12O.C3H
E2      2      (C6H10O2)X.C5H12O2/MF
E3      0 --> (C6H10O2)X.C5H12O4/MF
E4      1      (C6H10O2)X.C5H14NO4P.
E5      1      (C6H10O2)X.C5H6O2/MF
```

• • •

```
=> E CAPA 4101/CN
```

```
E1      1      CAPA 316-MDI COPOLYMER/CN
E2      1      CAPA 316-VESTAGON B 1540 COPOLYMER/CN
E3      1 --> CAPA 4101/CN
```

• • •

```
=> S E3
```

```
L2      1 "CAPA 4101"/CN
```

- **EXPAND**ing on the molecular formula disclosed in the specification finds no hits
- **EXPAND** and **SEARCH** on the trade name to find the substance disclosed in the specification



=> D L2

RN 55798-91-9 REGISTRY

CN Poly[oxy(1-oxo-1,6-hexanediyl)],  $\alpha$ -hydro- $\omega$ -hydroxy-, ester with 2,2-bis(hydroxymethyl)-1,3-propanediol (4:1) (CA INDEX NAME)

OTHER NAMES:

CN **Capa 4101**

CN Caprolactone homopolymer, SRU, pentaerythritol ester

CN Poly( $\epsilon$ -caprolactone), pentaerythritol-initiated, sru

CN Poly( $\epsilon$ -caprolactone), SRU, tetraester with pentaerythritol

CN Polycaprolactone, sru, ester with pentaerythritol

• • •

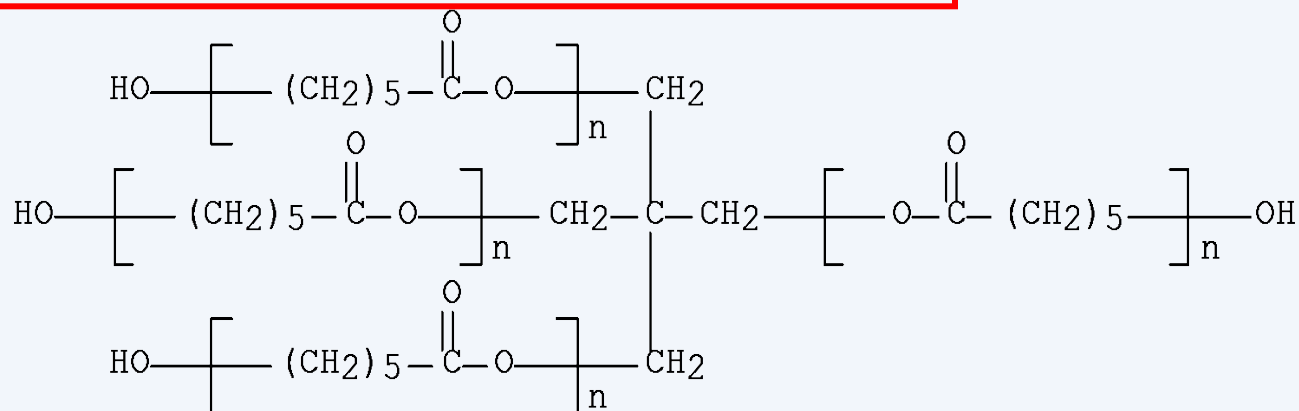
MF (C6 H10 O2)<sub>n</sub> (C6 H10 O2)<sub>n</sub> (C6 H10 O2)<sub>n</sub> (C6 H10 O2)<sub>n</sub> C5 H12 O4

CI PMS, COM

PCT Polyester

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL

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



# Use POLYLINK to find polymers related to the SRU record

=> POLYLINK L2

L3 4 POLYLINK L2

=> S L1 OR L3

L4 5 L1 OR L3

=> S C6H10O2

L5 29809 C6H10O2

=> S L5 AND (C5H8O4 OR C5H12O4)

L6 312 L5 AND (C5H8O4 OR C5H12O4)

=> D SCAN

IN Pentanedioic acid, polymer with ethyl 2-methyl-2-propenoate, 1,6-hexanediol and N-methyl-2-propenamamide, graft (9CI)

MF (C6 H14 O2 . C6 H10 O2 . C5 H8 O4 . C4 H7 N O)x

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Search molecular formulas (without spaces) in the Basic Index to find substances that may have more than 2 components.

# Combine answer sets in REGISTRY and crossover to HCAplus

=> S L4 OR L6

L7 314 L4 OR L6

=> S L7 AND PMS/CI

L8 313 L7 AND PMS/CI

=> FILE HCAPLUS

=> S L8 (L) ((THU/RL OR PAC/RL OR PKT/RL) OR (?PHARMA? OR ?DRUG? OR "THERAP?"))

L9 37 L8 (L) ((THU/RL OR PAC/RL OR PKT/RL) OR (?PHARMA? OR ?DRUG? OR THERAP?))

=> S L9 (L) (BIODEGRAD? OR BIO DEGRAD? OR BIOEROD? OR BIO EROD?)

L10 11 L9 (L) (BIODEGRAD? OR BIO DEGRAD? OR BIOEROD? ● ● ●

Optional: Since this polymer has a trade name (CAPA 4101) and a common name (epsilon-caprolactone polymer with pentaerythritol), it is a good candidate for searching in STNIndex to locate other polymer files with information about this polymer.

=> D IBIB ABS HITIND 1-11

ACCESSION NUMBER: 2004:60282 HCAPLUS  
DOCUMENT NUMBER: 140:117395  
TITLE: Drug delivery systems for releasing active ingredients based on biodegradable or biocompatible polymers with shape memory effect  
INVENTOR(S): Lendlein, Andreas; Steuer, Susi; Tuleweit, Annika  
PATENT ASSIGNEE(S): Mnemoscience GmbH, Germany  
LANGUAGE: German  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 2004006885	A2	20040122	WO 2003-EP7515	20030710

AB The invention relates to systems for releasing active ingredients by means of shape memory materials. The loading of the shape memory effect matrixes can be performed by dissolving the drug in a solvent, mixing the soln. with the memory effect polymer matrix while the matrix is swelling and removing the swollen matrix from the soln. The matrix can also be loaded by crosslinking the polymer in the presence of the drug.

IT 41706-81-4P, Caprolactone-glycolide copolymer 647016-51-1P  
**647018-62-0P** 647028-84-0P

RL: SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)  
(shape memory effect material; **drug** delivery systems for releasing active ingredients based on **biodegradable** or biocompatible polymers with shape memory effect)

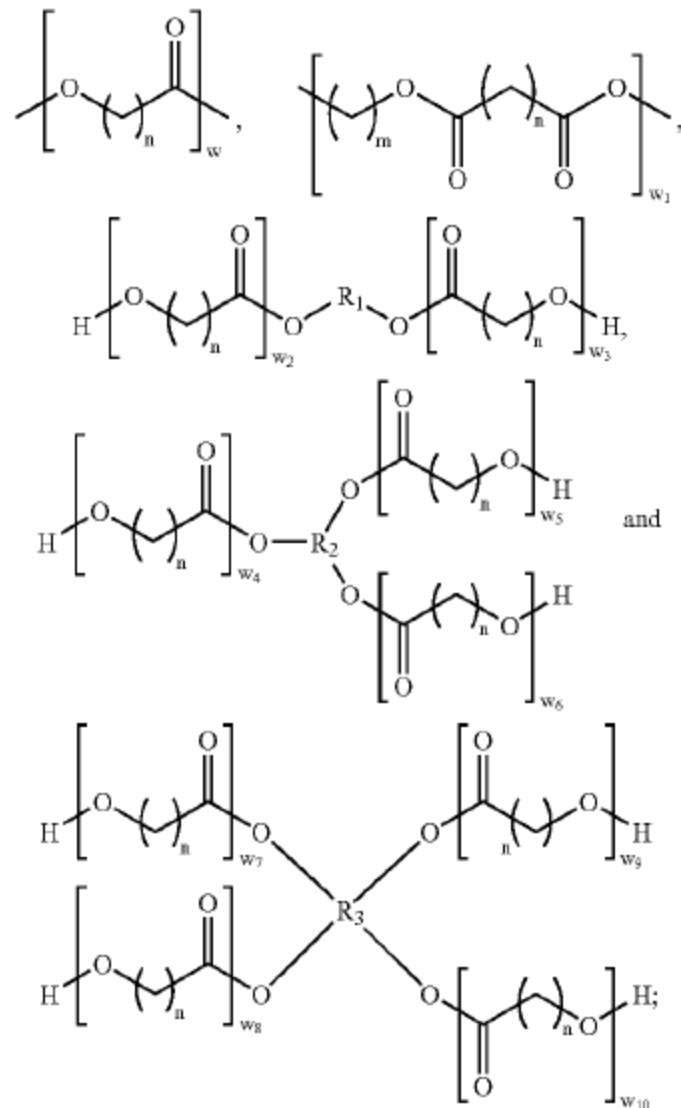
# Structure search for polymers

## Claim 6 from US

### 20080113027:

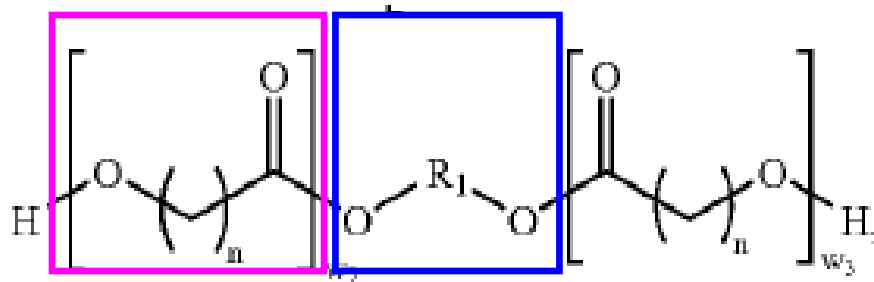
6. The pharmaceutical composition of claim 1, wherein the polymer matrix comprises a polyester polymer selected from the group consisting of:

##STR6## wherein R1, R2 and R3 are independently selected from the group consisting of alkyl and alkoxy diols, triols and tetraols of 2 to 8 carbon atoms; w, w<sub>1</sub> are independently an integer from 4 to 12; w<sub>2</sub>, w<sub>3</sub> are independently an integer from 1 to 12; w<sub>4</sub>, w<sub>5</sub>, w<sub>6</sub>, w<sub>7</sub>, w<sub>8</sub>, w<sub>9</sub> and w<sub>10</sub> are independently an integer from 0 to 12; n is an integer from 4 to 9; and m is an integer from 2 to 8.



# Search strategy

- Draw structure fragments to find monomer-based registrations and SRUs
- Save one fragment with the polymer filter
- Upload and search in CAS REGISTRY
- Option: Refine with Polymer Class Term
- Crossover to HCAPlus
- Refine with CAS Roles and text terms



Structure Drawing

File Edit Draw Template! QueryDef Display Preferences! Window Help

NO<sub>2</sub> XA QM Qv Q Rxn FG ?

Save ONE of the structures with a polymer filter.

alkyldiol polymer exact bonds.str \*Standa...

The screenshot shows the Structure Drawing software interface. On the left, a window displays a chemical structure of a diester polymer sub-unit,  $\text{H}-\text{O}-\left(\text{CH}_2\right)_n-\text{C}(=\text{O})-\text{O}$ , highlighted with a pink box. On the right, another window displays a chemical structure of a diol,  $\text{OH}-\text{Ak}-\text{OH}$ , highlighted with a blue box. The software interface includes a menu bar (File, Edit, Draw, Template!, QueryDef, Display, Preferences!, Window, Help), a toolbar with various drawing tools, and a bottom panel with element selection buttons (C, H, O, S, N, P, Cl, Br, F).

- The bonds to the 2 OH groups were set to EXACT to find diols in the answer set.
- The Ak element count was set to 2-8 C.

# Upload structures and filters (screens)

=> FILE REGISTRY

=>

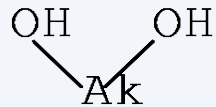
Uploading ● ● ●

L1 STRUCTURE UPLOADED

=> D

L1 HAS NO ANSWERS

L1 STRUCTURE





```
=> ....Testing the current file....$ screen
```

```
ENTER SCREEN EXPRESSION OR (END):end
```

```
=> screen 2043
```

```
L2      SCREEN CREATED
```

```
=>
```

```
Uploading • • •
```

```
L3      STRUCTURE UPLOADED
```

```
=> que L3 AND L2
```

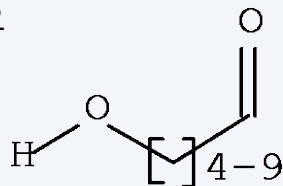
```
L4      QUE L3 AND L2
```

```
=> D
```

```
L4 HAS NO ANSWERS
```

```
L2      SCR 2043
```

```
L3      STR
```



Structures saved with screens upload a script which runs automatically.

Note the individual L-numbers of the screen and the structure.

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

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 287129 TO 301671  
PROJECTED ANSWERS: 39735 TO 45265

L5 50 SEA SSS SAM L1 AND L3 AND L2

**=> S L1 AND L3 AND L2 SSS FULL**

FULL SEARCH INITIATED 15:53:24  
FULL SCREEN SEARCH COMPLETED - 293530 TO ITERATE

100.0% PROCESSED 293530 ITERATIONS 42156 ANSWERS  
SEARCH TIME: 00.00.01

L6 42156 SEA SSS FUL L1 AND L3 AND L2

**=> S L6 AND POLYESTER/PCT**

254471 POLYESTER/PCT

L7 39585 L6 AND POLYESTER/PCT

Combine the two structure queries L1 and L3 with the screen L2 listed last on the command line.

Option: refine with polymer class term.

# Crossover to HCAplus and limit with CAS roles and text

```
=> FILE HCAPLUS
```

```
=> S L7 (L) ((THU/RL OR PAC/RL OR PKT/RL) OR (?PHARMA? OR ?DRUG? OR  
THERAP?))
```

```
L8      985 L7 (L) ((THU/RL OR PAC/RL OR PKT/RL) OR (?PHARMA? OR  
?DRUG? OR THERAP?))
```

```
=> S L8 (L) (BIODEGRAD? OR BIO DEGRAD? OR BIOEROD? OR BIO EROD?)
```

```
L9      164 L8 (L) (BIODEGRAD? OR BIO DEGRAD? OR BIOEROD? OR BIO  
EROD?)
```

=> D L9 BIB ABS HITSTR

TI Implantable medical device coatings with biodegradable elastomer and releasable taxane agent

IN Barnett, Angela R.; Gearhart, Krista N.; Lichti, Jason; Reyes, Priscilla T.; Sarasam, Aparna R.

PA Med Institute, Inc., USA

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
PI WO 2010021757	A2	20100225	WO 2009-US4810	20090824

AB A coated medical device, such as a stent, that elutes a taxane agent in a controlled manner is provided. In one embodiment, the taxane agent is paclitaxel and at least a portion of the paclitaxel is present in a dihydrate solid form. The medical device may be coated with a layer including a taxane agent and a layer of bioabsorbable elastomer over the layer including the taxane agent. • • •

IT **52192-81-1**, Glycerol sebacic acid copolymer

RL: **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)  
(implantable medical device coatings with **biodegradable** elastomer and releasable taxane agent)

CN Decanedioic acid, polymer with 1,2,3-propanetriol (CA INDEX NAME)

CM 1	CM 2
CRN 111-20-6	CRN 56-81-5
CMF C10 H18 O4	CMF C3 H8 O3

HO<sub>2</sub>C—(CH<sub>2</sub>)<sub>8</sub>—CO<sub>2</sub>H

HO—CH<sub>2</sub>— $\begin{array}{c} \text{OH} \\ | \\ \text{CH} \end{array}$ —CH<sub>2</sub>—OH

# Search for post-treated polymers in CAplus

The electrolyte membrane of claim 1, wherein the polymer comprises at least one polymer selected from the group consisting of a perfluorinated sulfonic acid group containing polymer, a sulfonated polyether ether ketone, a sulfonated polyimide, a sulfonated polystyrene, a sulfonated polysulfone, and a sulfonated or phosphated hydrocarbon polymer.

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

- Find post-treated polymers in CAplus
  - Search the RN associated with the polymer being treated, e.g., polystyrene is 9003-53-6
  - Add “D” for “derivative”  
=> **FILE CAPLUS; S 9003-53-6D**
- For large answer sets, search the REGISTRY L-number/D linked to text terms describing the modification  
=> **S L3/D (L) ?SULFON?**

# Summary

- Use Polymer Class Terms (/PCT) and CAplus substance class indexing to find broadly claimed classes of polymers
- Search complete molecular formulas in the molecular formula field (/MF) and component molecular formulas in the Basic Index
- Structure search monomer component fragments or SRU fragments with a polymer screen
- Use CAS roles and text terms to refine polymer searches
- Search post-treated polymer RNs with a “D”

# STN<sup>®</sup>

For more information ...

CAS

E-mail: [help@cas.org](mailto:help@cas.org)

Support and Training:

[www.cas.org](http://www.cas.org)

FIZ Karlsruhe

[helpdesk@fiz-karlsruhe.de](mailto:helpdesk@fiz-karlsruhe.de)

Support and Training:

[www.stn-international.de](http://www.stn-international.de)