

CAS STNnext[®] COFFEE LECTURE

Polymer use cases

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Searching polymers on CAS STNext

Focus on polymer compositions

CAS Registry contains 2.46 mil polymer compounds identified by CAS Registry Numbers (PMS/CI)

CAplus contains 4.9 mil documents in the Macromolecular sections (MAC/CC)

WPIndex contains almost 8 mil patent records in the Derwent section A (A/DC)

IFIALL contains Uniterm and Fragment codes for records prior to 2011.

PQSciTech has 405K documents in the Engineered Materials – Polymers section of the database (/FS)

There are three static files with specialized polymer content on STNext: Apollit (436K refs, -2005), Rapra (1.5 mil refs, -2021) and WSCA (549K refs, -2020)

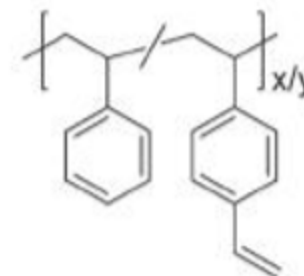
Searching addition polymers

Polymers obtained by opening a double bond, or ring-opening metathesis

Typical classes include polyolefins, polyacrylates, vinyl polymers, fluoropolymers, polyacetylenes, etc.

Monomer-based registration in Registry, even when the publication shows a kind of structural repeating unit

RN **25086-67-3** REGISTRY
CN Benzene, 1,4-diethenyl-, polymer with ethenylbenzene (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzene, ethenyl-, polymer with 1,4-diethenylbenzene (9CI); Benzene, p-divinyl-, polymer with styrene (8CI); Styrene, polymer with p-divinylbenzene (8CI)
OTHER NAMES:
CN 1,4-Divinylbenzene-styrene copolymer; 4-Divinylbenzene-styrene copolymer; p-Divinylbenzene-styrene copolymer; p-Divinylbenzene-styrene polymer; Polysorb 10b; Styrene p-divinylbenzene polymer; Styrene-1,4-divinylbenzene copolymer; Styrene-p-divinylbenzene copolymer
CI PMS, COM
PCT Polystyrene



CM 1

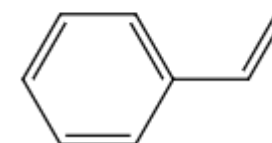
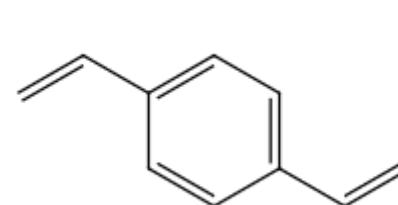
CRN **105-06-6**

CMF C10 H10

CM 2

CRN **100-42-5**

CMF C8 H8



Conducting a search using Component RNs

Limiting to 2-3 components only having styrene functionality

=> S (105-06-6/CRN OR 1321-74-0/CRN) AND 100-42-5/CRN

2308 105-06-6/CRN

16356 1321-74-0/CRN

135172 100-42-5/CRN

L1 7385 (105-06-6/CRN OR 1321-74-0/CRN) AND 100-42-5/CRN

=> S L1 AND 2-3/NC

10740391 2-3/NC

L2 1719 L1 AND 2-3/NC

=> S L2 AND POLYSTYRENE/PCT AND 1/PCT.CNT

241090 POLYSTYRENE/PCT

1073695 1/PCT.CNT

L3 623 L2 AND POLYSTYRENE/PCT AND 1/PCT.CNT

The component 1321-74-0 is for the incompletely defined divinylbenzene

PCT is Polymer Class Term

PCT.CNT is the Polymer Class Term count

Example of a specific polymer

RN **1001098-35-6** REGISTRY

ED Entered STN: 30 Jan 2008

CN 1-Naphthalenamine, N-[(4-ethenylphenyl)methyl]-, polymer with
1,4-diethenylbenzene and ethenylbenzene (CA INDEX NAME)

OTHER NAMES:

CN p-Divinylbenzene-4-(1-naphthylaminomethyl)styrene-styrene copolymer

MF (C19 H17 N . C10 H10 . C8 H8)x

CI PMS

PCT Polystyrene

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

CM 1

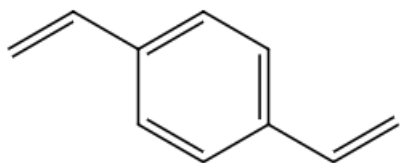
CRN **262591-86-6**

CMF C19 H17 N

CM 2

CRN **105-06-6**

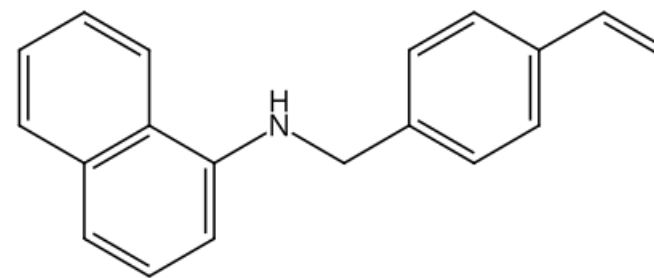
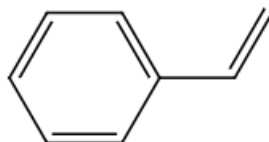
CMF C10 H10



CM 3

CRN **100-42-5**

CMF C8 H8



Blends of polystyrene and polydivinylbenzene

Polymer blends are not covered by the copolymer

Polymer blends follow the indexing rules for a formulation

Each polymer itself will be indexed

Often, these polymer components of a blend will get the role POF (polymer in formulation)

Since the indexing is done at the document level in CAplus, it is not possible to link these two components of the polymer blend

There is a precision issue as these two polymers may be different options to be blended with another polymer

Search strategy for polymer blends

Each polymer searched separately in Registry; combined in CAplus

FILE 'REGISTRY' ENTERED AT 21:34:23 ON 05 APR 2024

L1 1 S POLYSTYRENE/CN
L2 1 S "POLY(DIVINYLBENZENE)"/CN
L3 1 S "POLY(1,4-DIVINYLBENZENE)"/CN

FILE 'CAPLUS' ENTERED AT 21:35:53 ON 05 APR 2024

L4 9 S L1/POF(L)BLEND AND (L2/POF OR L3/POF)(L)BLEND

Example of polymer blend indexing

L4 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2024 ACS on STN

TI Preparation and characterization of composites using blends of
divinylbenzene-based hyperbranched and linear functionalized polymers

SO Polymers for Advanced Technologies (2021), 32(8), 3333-3342

CODEN: PADTE5; ISSN: 1042-7147

IT **9003-53-6**, Poly(styrene)

RL: **POF (Polymer in formulation)**; PRP (Properties); USES (Uses)

(**blend** with hyperbranched poly(divinyl benzene); prepn. and

characterization of composites using **blends** of

divinylbenzene-based hyperbranched and linear functionalized polymers)

IT **9003-69-4 DP**, Divinyl benzene homopolymer, hydrogenated

RL: **POF (Polymer in formulation)**; PRP (Properties); SPN

(Synthetic preparation); PREP (Preparation); USES (Uses)

(**blend** with linear polystyrene benzene); prepn. and

characterization of composites using **blends** of

divinylbenzene-based hyperbranched and linear functionalized polymers)

Defined copolymers only by tradenames

The ENTE field contains a description of the material

=> S STYRENE/ENTE AND (DIVINYLBENZENE OR DIVINYL(W)BENZENE)/ENTE

5779 STYRENE/ENTE

1197 DIVINYLBENZENE/ENTE

89 DIVINYL/ENTE

164 BENZENE/ENTE

49 DIVINYL(W)BENZENE

L4 842 STYRENE/ENTE AND (DIVINYLBENZENE OR DIVINYL(W)BENZENE)/ENTE

Impactful tradename-defined substance

RN **9037-24-5** REGISTRY
ED Entered STN: 16 Nov 1984
CN Amberlyst 15 (CA INDEX NAME)
OTHER NAMES:
CN Amberlyst 15 DRY
CN Amberlyst 15 Wet
CN Amberlyst 15(H)
CN Amberlyst RTM 15
DR **54241-79-1**, **120528-22-5**, **550365-45-2**, **1292765-99-1**
ENTE A sulfonated **styrene** -**divinylbenzene** copolymer cation exchange resin
MF Unspecified
CI PMS, COM, MAN
PCT Manual registration
LC STN Files: BIOSIS, CA, CAPLUS, CASFORMULTNS, CASREACT, CHEMCATS, CHEMLIST, IFIALL, PIRA, TOXCENTER, USPAT2, USPATFULL, USPATOLD

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

4075 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> FILE CAPLUS

=> S L3 OR L4

22062 L3

25634 L4

L5 45905 L3 OR L4

Derwent has a record for the copolymer

DCR number found 360 patents in WPIIndex (of which 130 were unique)

AN DCR-199515 DCR
DCSE 199515-0-0-0
CN.P **STYRENE-DIVINYLBENZENE**-COPOLYMER
SY COPOLYMER, **STYRENE-DIVINYLBENZENE**-;
DIVINYLBENZENE-COPOLYMER, **STYRENE**-; **STYRENE-DIVINYLBENZENE**-COPOLYMER

Substance image not available

CMT Standard polymerA copolymer of **Styrene** with C₁₀H₁₀ divinyl benzene may be ortho, meta or para,.Source-based monomers shown.
MF Polymer
ED Entered STN: 9 Jun 1999
Last updated on STN: 9 Jun 1999
Update DWPI Cross Ref.: 25 Mar 2024

Indexing within the WPIIndex record

PLE codes available to special subscribers

TI Solid-phase microextraction film useful in drug detection, comprises copper mesh surface coated with polystyrene/divinylbenzene polymer microspheres and polydimethylsiloxane

PA (UJIN-C) UNIV JINAN GUANGDONG

PI **CN 113842672** A 20211228 (2022042)* ZH
CN 113842672 B 20230203 (2023016) ZH

IT UPIT 20220530
DCR-199515-CL **DCR-199515-USE**; DCR-13801-CL DCR-13801-DET
DCR-13801-USE; DCR-100569-CL DCR-100569-DET DCR-100569-USE; DCR-107032-CL
DCR-107032-USE; DCR-61643-CL DCR-61643-DET DCR-61643-USE

M1 *02* **M423 M430 M782 P831 Q233 R043 M905**
DCN-RA0439-M DCN-RA0439-K
DCR-199515-M **DCR-199515-K**

PLE UPA 20220530
[1.1] **2004 G0851-R G0840 G0817 D01 D02 D12 D10 D19 D18 D31 D51 D54 D58
D76 D90; G0102 G0022 D01 D02 D12 D10 D19 D18 D31 D51 D53 D58 D76
D88 DCN-R00708 DCR-368; H0022-R H0011; S9999 S1398-R; S9999
S1285-R; P1741; P1774;**

PLE code G0840 is for diolefinic aromatic hydrocarbons

PLE code D90 indicates a carbon count of 9

PLE code K9745 would be for polymer blends

PLE code P1774 is for a styrene-divinylbenzene polymer (retrieves 15,250 documents)

Searching condensation polymers

Monomer-based registration or structural repeating units

Condensation reaction splits off a small molecule (H₂O, HCl, etc) to form the polymeric chain

Mainly for polyesters, polyethers, polycarbonates, polyamines, polyamides, polyimides, polyoxyalkylenes, polyurethanes, polyalkenamers, polysiloxanes, etc.

A structural repeating units (SRUs) can only be created for condensation polymers that are unambiguous (often symmetrical)

CAS Analysts intellectually link SRUs to their monomer-based registrations from a variety of starting materials

The POLYLINK command in Registry is able to retrieve these related polymer registrations

Condensation polymers

Will have a monomer-based registration

RN **29435-48-1** REGISTRY

CN Butanoic acid, 3-hydroxy-, (3R)-, homopolymer (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Butanoic acid, 3-hydroxy-, (R)-, homopolymer; Butyric acid, 3-hydroxy-, D-(-)-, polyesters (8CI)

OTHER NAMES:

CN **(R)-3-Hydroxybutyric acid homopolymer**; D-3-Hydroxybutyric acid homopolymer; Poly((R)-(-)-3-hydroxybutyrate); Poly(D-(3-Hydroxybutyrate)); Poly(D-β-hydroxybutyrate); Poly(D-3-hydroxybutyric acid); Poly-3R-hydroxybutyric acid; Poly[(-)-3-hydroxybutyric acid]; Poly[(R)-3-hydroxybutyrate]; Poly[D(-)-β-hydroxybutyric acid]; Poly[D(-)-3-hydroxybutyric acid]

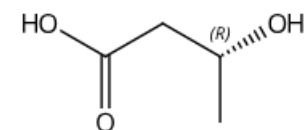
PCT Polyester, Polyester formed

694 REFERENCES IN FILE CA (1907 TO DATE)

29 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

706 REFERENCES IN FILE CAPLUS (1907 TO DATE)

CM 1



Absolute stereochemistry shown
Rotation (-)

Condensation polymers

May also have a structural repeating unit

RN 31759-58-7 REGISTRY

CN Poly[oxy[(1R)-1-methyl-3-oxo-1,3-propanediyl]] (CA INDEX NAME)

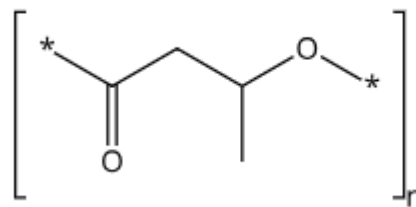
OTHER CA INDEX NAMES:

CN Poly(oxycarbonylpropylene), D- (8CI); Poly[oxy(1-methyl-3-oxo-1,3-propanediyl)], (R)-

OTHER NAMES:

CN (R)- α -hydro- ω -hydroxypoly[oxy(1-methyl-3-oxo-1,3-propanediyl)]; (R)-3-Hydroxybutanoic acid homopolymer, SRU; (R)-3-hydroxybutyrate homopolymer, SRU; (R)-3-Hydroxybutyric acid homopolymer, SRU; (R)-3-Hydroxybutyric acid isotactic homopolymer, SRU; (R)-3-Hydroxybutyric acid, homopolymer isotactic, SRU; Biocycle B 100; Biomer 16F; Biomer B 300; Biomer M 0997; Biomer P 209E; Biomer P 226; Biomer P 300; Biomer PHB P 226; Biomer T 22; Biopol 30; Biopol GO 8; BU 396311; BX-GV 9; D-(-)-Poly(oxycarbonylpropylene); Enmat Y 3000; ENMAT-Y 3000P; Isotactic (R)-3-hydroxybutanoic acid homopolymer, SRU; Isotactic (R)-3-hydroxybutyrate homopolymer, sru; Isotactic (R)-3-hydroxybutyric acid homopolymer, sru; Isotactic β -hydroxybutyric acid homopolymer, sru; L 88; Microbial poly(3-hydroxybutyrate), sru; Microbial poly(hydroxybutyrate), sru; Mirel M 2100; P 226; PHB; PHB-L 88; Poly((R)-(-)-3-hydroxybutyrate); Poly(D- β -hydroxybutyrate), sru; Poly(D-3-hydroxybutyric acid), sru; Poly-(R)- β -hydroxybutyrate, isotactic, SRU; Poly[(-)-3-hydroxybutyric acid] SRU; Poly[(R)- β -butyrolactone], sru; Poly[(R)-3-hydroxybutyrate]; Poly[(R)-3-hydroxybutyrate], sru; Poly[(R)-3-hydroxybutyric acid]; Poly[D(-)-3-hydroxybutyric acid], SRU; Sconacell B; T 19

PCT Polyester



RELATED POLYMERS AVAILABLE WITH POLYLINK

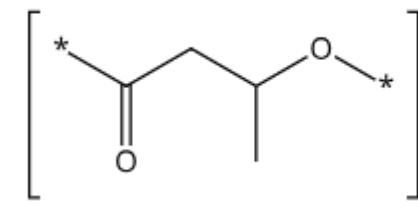
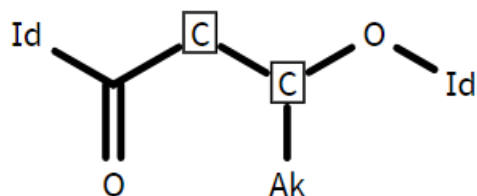
1512 REFERENCES IN FILE CA (1907 TO DATE)

45 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1525 REFERENCES IN FILE CAPLUS (1907 TO DATE)

How to search SRUs by structure

Using the ID dummy node for the repeating nodes



L1 STRUCTURE UPLOADED

=> **s l1 css ful**

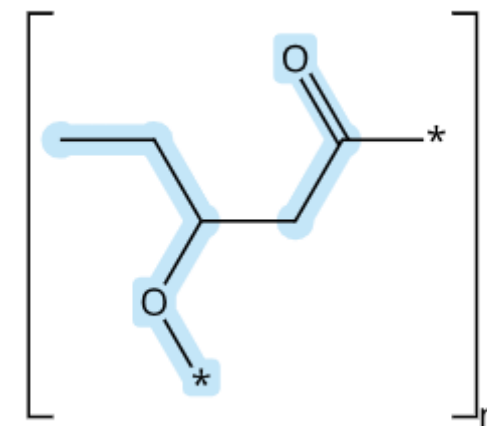
FULL SEARCH INITIATED 06:33:24

100.0% PROCESSED 7374144 ITERATIONS

SEARCH TIME: 00.00.07

L2 55 SEA CSS FUL L1

55 ANSWERS



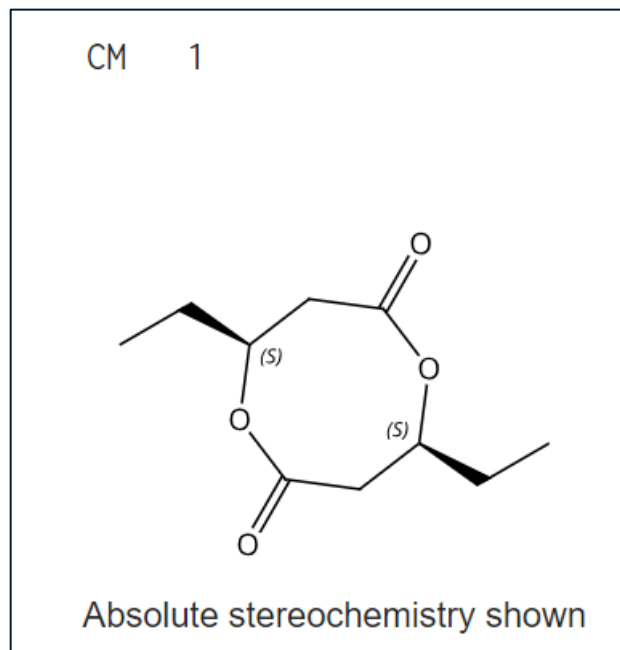
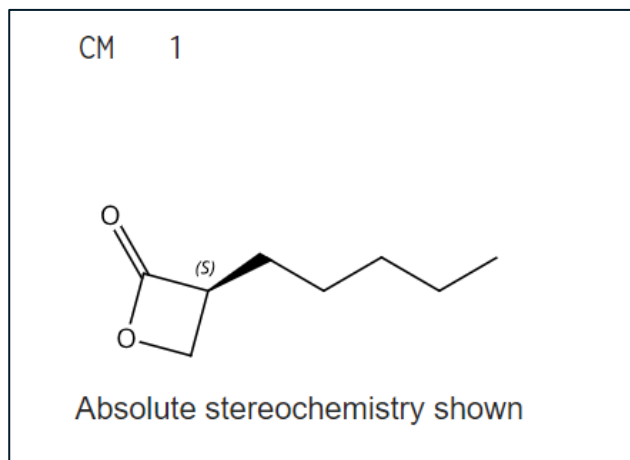
Polylink – moving between Monomer and SRU

Intellectually link monomer and SRU registrations together

Includes your original answer set

Added monomer-based registrations

Shows diversity in polymer building blocks



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L1          STRUCTURE UPLOADED
L2          55 S L1 CSS FUL

=> polylink 12

L3          157 POLYLINK L2

=> s 13 not 12

L4          102 L3 NOT L2
```

When the final polymer is not well-defined

Claim text often use “comprising” indicating additional components

WO 2012/149407

PCT/US2012/035576

- 58 -

CLAIMS

What is claimed is:

1. A method for producing an aqueous polyhydroxyalkanoate (PHA) emulsion from a biobased, biodegradable PHA polymer, copolymer or blends thereof, comprising the steps of:
melting the PHA polymer, copolymer or blends thereof;
2. The method of Claim 1, wherein the aqueous PHA emulsion comprises a 3-hydroxybutyrate polymer, copolymer or blends thereof.

How is this document indexed

It is not the homopolymer, but only the monomer is defined

Based on this claim, indexing is done as a non-specific derivative of the monomer:

```
IT 625-72-9 D, (R)-3-Hydroxybutyric acid, polymers
28728-97-4, Poly(4-hydroxybutyrate), sru 31759-58-7, Microbial
poly(3-hydroxybutyrate), sru 114959-05-6, Poly(4-hydroxybutyrate)
141455-97-2, Microbial poly(3-hydroxybutyrate)
RL: PEP (Physical, engineering or chemical process); POF (Polymer in
formulation); PROC (Process); USES (Uses)
(microbial, blend; process for polyhydroxyalkanoate latex prodn. by
melt emulsification)
```

Subsequent examples did provide specific polymers which were indexed as final polymers

Summary

Comprehensive polymer searching requires significant expertise

Monomer-based registrations for most of the polymers

Structural repeating units for unambiguous condensation polymers

Tradenname-based product definitions

Watch out for incompletely defined monomers

Broad patent claims using 'comprising' terminology

Polymer blends and post-treated polymers require special approach

For full FTO consider outsourcing to specialists, like at CAS IP Services

Derwent files provide additional results

Derwent polymer coding available to special subscribers

Between problems
and progress
are connections
that matter



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