Finding Polymer Information – Part 1: Basics

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Agenda

• Polymers in CAS Registry
• Searching Polymers – the Basics
• Polymers in Uses or Properties
• The power of combining answer sets
• Categorizing large answer sets
• Conclusions and more information
Polymers in CAS Registry

• CAS Registry has 65.5 Mio substances – **1.45 Mio** of them are Polymers

• CAS assigns a specific CAS Registry number for each polymer **preferably based on its monomers**

• Only if the monomers are not clearly defined in the patent or journal article, CAS will register the polymer (or parts of the polymer) based on the structural repeating unit (SRU)

• 549169 of the 1.45 Mio Polymers are registered with a SRU, but some of them are very common ones like PET, PEG or Nylon (where we only have a SRU)
Polymers in CAS Registry -

- Polymers with specified stereochemistry (tacticity) are registered separately.
- Block, graft or alternating polymers are registered separately (since 1986).
- No influence on registration:
  - The molecular weight (distribution)
  - Other physical characteristics
  - Number of repeating units
  - Component ratio
  - Initiators or catalysts used
  - Functionalization or reaction after the polymerization
Polymers in CAS Registry – Monomer based registration

Structure of the monomer with monomer CAS RN

Molecular Formula of the monomer based registration with (C5H8)X
Polymers in CAS Registry – SRU based registration

Molecular formula of the SRU with (C12H12O4)N

This SRU Structure is not searchable!
Polymers in CAS Registry – some monomers as SRU based registration

One component of the polymer is defined by an SRU.
Searching Polymers – the Basics

• The **first step** to find polymer information in SciFinder is to determine **the right CAS Registry Number**

• Never trust CAS RNs which you have found in the Internet, in catalogues or other sources. They might be wrong!

• **The basic search techniques are:**
  – Search by Structure
  – Search by Molecular Formula
  – Search by Name or CAS RN
  – Search with a Topic Search
Searching Polymers – by Structure

• This should be your first step: if you know one or more of the monomers of your polymer, just do a structure search on them!

• There are two very important limiters:
  – Single Component (if you mark it, you will retrieve as many components, as you have drawn)
  – Polymers (excludes organic substances)

• Sort the resulting Structure Answer Set with a new feature in SciFinder on the Web:
  – By „Number of References“

• Attention: You can search SRU based Polymers only by Substructure (more details in a special presentation)
Searching Polymers – by Structure

Please draw the monomers you know in the structure editor.

In this example we first choose the „Exact Search“
Please note: for sure also Substructure searches for polymers are possible!
Searching Polymers – by Structure

When you have drawn some monomers and you click OK, this warning will come up.

This is just a kind reminder 😊

You know what you want to do and it is correct - so just click „Continue“!!
When you mark „Single Component“ you will retrieve only polymers with exactly the 2 drawn monomers. If you leave it unchecked you will get all polymers, where these 2 monomers are present!

Please try it!

When you mark „Polymers“ here, you will exclude unwanted organic molecules.
This is a very valuable option: Sort by Number of References. It brings the most common substance to the top!

A block polymer ...

Just the unspecific ...
Searching Polymers – by Structure

• You can’t search SRU based registered Polymers by exact structure.
• It is however possible to search them with a substructure search.

• This will be explained in more detail in an additional presentation – keep in contact with me via E-Mail thaubenreich@cas.org
Searching Polymers – by Molecular Formula

• Searching by Molecular Formula is a very good tool to search (and find 😊) Polymers
• Please note that you will always get the Polymers with exactly the complete MF which you entered – no additional monomers!
• Indeed it is the only method in SciFinder to search specifically (exact) for SRU based Polymers!
• This is recommended especially for very simple SRU polymers.

• Important: if you don’t find a result --- always double check your molecular formula!
Searching Polymers – by Molecular Formula (monomer based registrations)

• For addition polymers and most condensation polymers put the molecular formula of the monomers, separated by dots, within brackets and close with an “X”

  – (C8H8)x for the styrene homopolymer
  – (C8H8 . C5H8)x for styrene-isoprene polymers
  – (C8 H4 Cl2 O2 . C2 H6 O2)x for a Polyester formed from terephthaloyl chloride with glycol

  Please note: you have to take the MF of the monomers, though in the final polymer, there is certainly no chlorine present!
Searching Polymers – by Molecular Formula (monomer based registrations)

Tip: If you have huge Molecular Formulas like:
(C15 H16 O2 . C8 H10 O4 . x (C8 H6 O4 . C2 H6 O2)x . x C5 H12 O2 . C3 H5 Cl O)x
perhaps better cut and paste them from a document 😊. Try this MF yourself!
Searching Polymers – by Molecular Formula (monomer based registrations) – also structure isomers!

Different Polymers with the same Molecular Formula are retrieved
Searching Polymers – by Molecular Formula (monomer based registrations) – remember „Sort by“ and „Refine“!

This is a very valuable option: Sort by Number of References. It brings the most common substance to the top!
Searching Polymers – by Molecular Formula (monomer based registrations) – „Refine“ by Structure!

Don’t forget: You can certainly refine with a structure!
We refine with the structure of isoprene...
Searching Polymers – by Molecular Formula (monomer based registrations) – „Refine“ by Structure!
Searching Polymers – by Molecular Formula (SRU based registrations)

• For structural repeating units of symmetric condensation polymers put the formula of the repeating unit within brackets and close with an “N”
  – (C14H12O4)n for polybutylene terephthalate
  – (C2H4O)nCH4O for α-methyl-ω-hydroxy Polyether
Remember to add the molecular formula of the end groups to one formula!
Here we add the α-methyl and the ω-hydroxy: CH$_3$ + OH = CH$_4$O
Searching Polymers – by Molecular Formula (SRU based registrations)

Here is our very basic polyether!
Searching Polymers – by Name

- Tradenames are a good start, don’t try complex chemical names! You can search Names also in the Substance Identifier search tool.
- Tip: Truncation is not possible in the Substance Identifier search.
- For ~200,000 manually registered Polymers, the tradename is the only way to get to the information. (this topic will be discussed further in the “Polymer Advanced” presentation!)
- Tip: if you want to look for more than one Polymer, you can enter up to 25 names in the „Substance Identifier“ (each name in a new line)
Searching Polymers – by Name

If you like you can search here more than one name (try synonyms or different spellings)

But you don’t have to ... 😊 Also one is very fine!
Searching Polymers – by Name

Dowlex 2517 – not much more known, but the name! Our editor only assumes, that it is a LLDPE

The famous PEG has 150000 references!

Only topped by Polypropylene...
Searching Polymers – by CAS RN

• For sure if you have a CAS Registry number from a catalogue you can search with that number in the Substance Identifier search tool
• Check the result! Many CAS numbers i.e. on the Internet are wrong or are not the specific ones.
• Tip: if you want to look for more than one Polymer, you can enter up to 25 CAS RN in the „Substance Identifier“ (each number in a new line)
Searching Polymers – by CAS RN

If you like you can search here more than one CAS RN (up to 25)

But you don't have to ...😊
Also one is very fine!
Searching Polymers – by CAS RN

Check out the results, whether you get the polymers that you want to have! If you get no result for a CAS Number you entered, this number was obviously wrong!

If you enter an old („deleted“) CAS RN you will retrieve the right entry with the right up to date CAS RN!

Polymers notoriously have many „deleted CAS RN“
Searching Polymers – with a Topic Search

• You can also search Polymers with a CAS Registry Number or a common Chemical Name directly in the **Topic Search** (by the way: this is the way, how most polymer chemists use SciFinder)

• This strategy has an advantage: you may retrieve brand new articles and patents, which are not yet indexed by CAS Editorial Staff. So these entries can’t be found with a structure or substance identifier search.

• **Tip**: best follow both strategies and combine the results!
We just enter the acronym LLDPE (linear low density polyethylene)
Searching Polymers – with a Topic Search

Take the 20008 results, where the intelligence of SciFinder is switched ON!
Searching Polymers – with a Topic Search

We just entered the acronym LLDPE – and synonyms are found too!
Polymers in Uses

- **Nobody** searches a Polymer just for fun 😊 !!!
- Typically everybody is interested in articles describing the Polymer in an application or with certain properties
- When you have found the right Polymer (**and its correct CAS Registry Number!**) you can combine these two pieces of information the a topic search
- Big Advantage: if you search like that you have the option to only retrieve the „**closely associated**“ answers which are typically the most relevant ones
Polymers in Uses

• You have determined the right CAS Registry number for a special polymer: 26023-30-3 (which is a nice organic polylactide)

• You are interested in Dental Materials using this Polymer

• Enter both concepts in the Topic Search, separated with „for“ (it is crucial to use prepositions between concepts, see a special presentation about Topic Search!)
You can take both answer sets but the "anywhere in the reference" answers include the first set anyway.
A mixture for the manufacture of medical implants

By: Stoch, Uwe; Stankowiak, Bernd

Abstract: Germany

Medical implants, esp. for periodontal and endodontic filling, and connection of bone defects are obtained polyurethane-based materials and fillers such as hydroxyapatite and/or poly(lactic acid). Thus, an endodontic filling material was obtained from methylene bis(cyclohexyl) diisocyanate, polytetramethylene oxide and ethylene glycol (in a molar ratio of 4:1:3) 70, thorium dioxide 25, and tetracycline 5 parts. The polymer matrix in this compo-showed a high crystallinity degree.

Reference Detail

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Nice hits and not too much information! But the right one.
Polymers in Uses – special properties

• In this example we are interested in the Young‘s modulus of Polyethylene
• In this case you don‘t need the CAS Registry Number first, as the name is very easy. SciFinder will search the CAS RN of Polyethylene automatically.
Polymers in Uses – special properties
There is certainly a lot of literature about a common polymer! We first choose the "closely associated" answers.
Polymers in Uses – special properties

We refine the big answer set by „Document Type“ to „Review“ first.

Analysis and Refine are the most important tools in SciFinder!
Polymers in Uses – special properties

9 nice reviews! Save your results in SciFinder for later use. And that you can combine them with other results!
The power of combining answer sets

- In SciFinder there are always several paths to your best results.
- Always **Save Answer sets**!
- You can creatively combine them to new results
The Power of Combine – Save Answer Sets!

When you save an Answer set in SciFinder give him a meaningful title (recommendation of the author, who always messes up his stored results ...
The power of combining answer sets

We combine the „Youngs Modulus Reviews“ with the results from „food packaging films“ to a new and pretty specific answer set!
A combined answer set

1. Use of delaminated waste laminated multi-ply cartons for liquid food as the fillers for polyethylene

2. Propylene resin compositions and films thereof with excellent rigidity, transparency, impact resistance, and heat-seal strength

3. Thermal, mechanical and permeation properties of gamma-irradiated multilayer food packaging films containing a buried layer of recycled low-density polyethylene

By Kovalsko, Ew; Rucnikos, Londra; Walczak, Zbigniew; Chorus, Marian
From Polymery (Warsaw, Poland) (2006), 51(7-8), 575-583 | Language: Polish, Database: CAplus

On the basis of literature data the possibilities of using waste multi-ply board packages for lip. food (e.g., milk or juice cartons) as the source of fibrous cellulose fibers for thermoplastic polymers composites is discussed. A novel method of delamination of such was developed and the delaminated products were used as fillers in polyethylene composites. The effects of polyethylene type (PE-HD, PE-LD, copolymer of PE-LD packaging film, PE-LD waste from cable production) and the content of cellulose fibers (up to 40 wt. %) what corresponds to 64.5 wt. % of waste boards) on the mechanical properties of the composites is presented. The obtained composites show significant stiffness and hardness, as well as good tensile and acoustic properties and esthetic surface. They can be applied to produce various objects of daily use (pots, buckets, trash cans, garden furniture etc.).

By Nizawa, Hiroshi

The compounds, useful for food packaging films, comprise (A) 83-95% propylene-copolymer consisting of propylene-based polymer parts and propylene-ethylene copolymer parts, satisfying 20%ylene-ol fraction (CXS) ≥ 2.10 and < 50% and intrinsic viscosity of CXS ([n]CS) ≥ 2.0 dl/g and (B) 5-17% ethylene-

By Cytryn, Stavroula; Sgouros, Antonios E.; Riganakos, Kyriakos A.; Kontominas, Michael G.
From Radiation Physics and Chemistry (2006), 75(5), 416-423 | Language: English, Database: CAplus

The effect of gamma radiation (doses 5-60 Gy) on the thermal, mechanical and permeation properties, as well as on IR-spectra of equally five-layer food packaging films were studied. Films contained a middle buried layer of recycled low-density polyethylene (LDPE) content 50.50% by wt. of the multilayer.
Categorizing large answer sets

- If you have a large answer set, CATEGORIZE can be able to help you in various ways.
- Play with the tool! It is impossible to show all combinations in a presentation.
- Categorize takes all Index Terms and assigned CAS RN out of an answer set and shows them in meaningful categories.
- In the example picture we categorize a set obtained by the topic search: „Polyethylene films as packaging material for food“
- One question: Which other polymers are dominant in this application?
You immediately see that Polypropylene and Polyesters are very important for food packaging films, too!

Please give Categorize a try and play with it a bit!
Conclusions and more information

• Please keep the 3 most important messages of this presentation in mind:

  • *Determine first the right CAS Registry Number for the Polymer you are looking for!*  
  • *Supplement this search, based on the CAS Registry Number, with an additional Topic Search* 
  • *Combine saved answer sets for more comprehensive or precise answer sets*
More Information

- There is a presentation „Finding Polymer Information – Part 2: Advanced“ available!
- Use the SciFinder Help for more technical questions, but also tips and tricks.
- Never give up! There is almost always a way in SciFinder to find your desired answers.
- Ask your local representative or describe your problem to our Help Desk:
  - help@cas.org
- Tip: save your history and attach it to your message to our Help Desk!
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Questions?
Comments?