



Searching for  
Polymers & Formulations

STN User Days June 2008

# Agenda

- Overview
- Searching for Polymers & Surfactants – approaches to consider
- Pharmaceutical Formulations & Agrochemical formulations – special considerations
- Consider other industry-specific files

## There are three main ways for indexing polymers in CAplus

- A **CAS RN** represents the entire polymer
- A **CAS RN** is used for a known portion and a modification is described by text
- A **General Subject Heading** is used to describe the polymer

# Polymers are indexed by CAS RNs

- The entire polymer appears in REGISTRY and the CAS RN is the index term in the Caplus file:

**IT 9003-53-6, Polystyrene**

**RL: PEP (Physical, engineering or chemical process);  
PRP (Properties); TEM (Technical or engineered material  
use); PROC (Process); USES (Uses)  
(regeneration of polystyrene foam moldings by  
pulverization and compression and heating and cooling)**

# Text can be used to modify a CAS RN

- The RN for known portion is indexed
  - A “D” for Derivative is appended
  - Additional text describes modification in  
CAplus:

**IT 9003-53-6D, Polystyrene, sulfonated**  
RL: TEM (Technical or engineered material use);  
USES (Uses)  
(fiber, biconstituent, with polyethylene; chem.  
filters comprising ion-exchange fibers and  
activated carbon for adsorptive removal of  
ionic gases and org. gases)

# General subject index entries are used in some cases

- Previous CAS indexing policies
  - E.g., before 1987, certain rubbers and fibers were indexed only at a subject heading
- Incomplete description by an author

**IT Rubber, butadiene-styrene, uses**

**RL: USES (Uses) (thermoplastic, microballoon-filled, for heat and sound insulation)**

**IT Textiles**

**(nonwoven, thermoplastic SBR contg., for sound and thermal insulators)**

# Polymer registration in REGISTRY can have 2 approaches

- Primary registration is monomer-based
  - Each component has its own CAS RN
  - Each combination of components has an overall CAS RN
- A supplemental structural repeating unit (SRU) entry, having its own RN, may also be indexed

Some commonly occurring polymers  
are indexed using **ONLY SRU's**

- Nylon 6 (25038-54-4)
- Nylon 66 (32131-17-2)
- Polyethylene glycol (PEG) (25322-68-3)
- Polyethylene terephthalate (PET) (25038-59-9)
- Polypropylene glycol (PPG) (142901-89-1)

## Some factors affect polymer registration

- Different stereochemistry (Tacticity )
  - Atactic polypropylene (NS) 9003-07-0
  - Isotactic polypropylene 25085-53-4
  - Syndiotactic polypropylene 26063-22-9
- Presence of end-groups (SRU only)
- Different architectures
  - Block, graft, alternating polymer forms

**STN** Only since 1987 (12CI)

# 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 Registry Number
- Number of repeating units in the polymer backbone
- Head-to-head versus head-to-tail arrangements
- Most post-treatment reactions
- Polymer Blends

## Tips for locating polymers when name information is known

- CAS RNs for polymers may be obtained by using
  - The names of the monomer components
  - The name of the final polymer
  - A trade name or acronym
- Names work best with
  - Homopolymers
  - Simple copolymers

Tip: Verify name with EXPAND in CN index  
Alternatively, consider a FAMILY structure search based on known component

Polymers may be located using the names of the component monomers

**Search Question:** Find the copolymer of terephthalic acid and 1,4-butylene glycol.

## Search Strategy

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

# Search each component name separately to find Component RN

```
=> FILE REGISTRY
=> E TEREPHTHALIC ACID/CN
E1      1      TEREPHTHALHYDROXIMOYL CHLORIDE/CN
E2      1      TEREPHTHALHYDROXYAMOYL CHLORIDE-4,4'...
E3      1  --> THIOL POLYMER/CN
          TEREPHTHALIC ACID/CN
•••
=> S E3;D
L1      1 "TEREPHTHALIC ACID"/CN

L1      ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
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:
CN      1,4-Dicarboxybenzene
CN      4-Carboxybenzoic acid
•••
```

# Search the RN for each component and limit number of components (/NC)

```
=> E 1, 4 - BUTYLENE GLYCOL /CN
•••
=> S E3;D
L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 110-63-4 REGISTRY
CN 1,4-Butanediol (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1, 4 -Butylene glycol
CN 1, 4 -Dihydroxybutane
=> SET EXPAND CONTINUOUS
=> SELECT RN L1;SEL RN L2
=> S E1/CRN AND E2/CRN
=> S L3 AND 2/NC
L4 1 L3 AND 2/NC
```

SELECT extracts the CAS RN for each component. Search the resulting E-numbers in the Component Registry Number (/CRN) field.

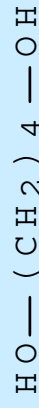
# Records with related polymer registrations are flagged

=> D

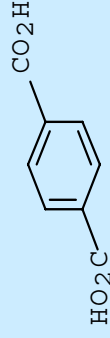
CN 1,4-Benzenedicarboxylic acid, polymer with 1,4  
butanediol (9CI)  
MF (C8 H6 O4 . C4 H10 O2) x  
CI PMS, COM

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

CM 1  
CRN 110-63-4  
CMF C4 H10 O2



CM 2  
CRN 100-21-0  
CMF C8 H6 O4



Every polymer record  
having at least one  
additional linked polymer  
is flagged.

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

- POLYLINK may be used on:
  - Individual CAS RNs
  - E-numbers containing a RN
  - REGISTRY answer sets
  - ANALYZE L-numbers containing RNs
- POLYLINK creates a new answer set with
  - All of the RNs in the original set
  - All polymer RNs that have been linked to the original set

# POLYLINK retrieves additional relevant polymer records

=> POLYLINK L4

POLYLINK retrieves 15 additional CAS RNs.

L5 **16** POLYLINK L4

=> **D SCAN**

L5 16 ANSWERS REGISTRY 2004 ACS on STN

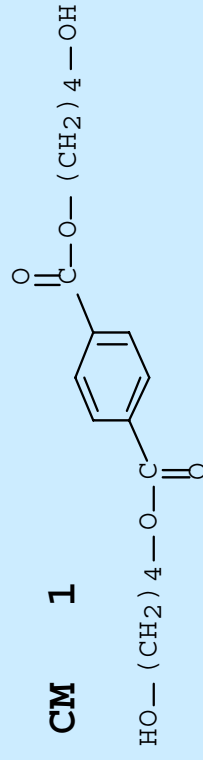
IN 1,4-Benzenedicarboxylic acid, polymer with bis(4-hydroxybutyl) 1,4-benzenedicarboxylate (9CI)

MF (C16 H22 O6 · C8 H6 O4)x

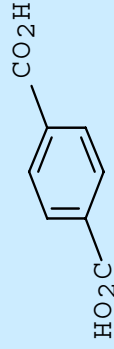
CI PMS

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

CM 1



CM 2



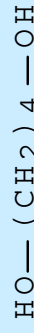
# POLYLINK retrieves additional monomer-based records...

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

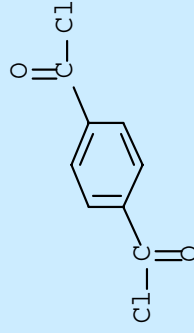
L5 16 ANSWERS REGISTRY 2004 ACS on STN  
IN 1,4-Benzenedicarbonyl dichloride, polymer with 1,4-  
butanediol (9CI)  
MF (C8 H4 Cl2 O2 . C4 H10 O2)x  
CI PMS, COM

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

CM 1



CM 2

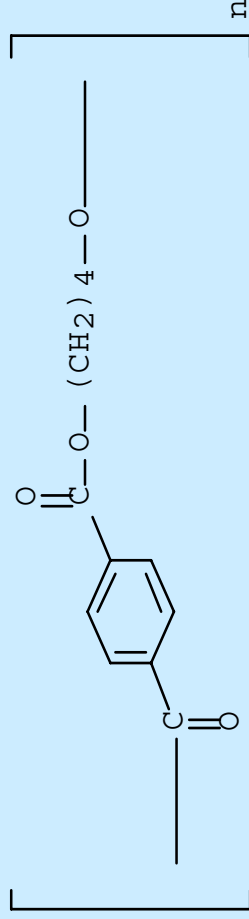


Dicarbonyl dichloride  
copolymer...

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

L5 16 ANSWERS REGISTRY 2004 ACS on STN  
IN Poly(oxy-1,4-butanediyl)oxycarbonyl-1,4-  
phenylenecarbonyl) (9CI)  
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT  
MF (C12 H12 O4)<sub>n</sub>  
CI PMS, COM

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



SRU entry.

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

# Polymer Class Terms (PCTs) describe broad classes of polymers

- PCTs are searchable
- Each term represents the structural characteristics of the polymer backbone
  - The types of linkages formed in the polymerization process
  - Linkages already present within the monomer backbone
  - Linkages present in structural repeating unit (SRU) backbones

# Drug Formulations

- An important part of pharmaceutical R&D
- Significant scientific and marketing gains
  - Therapeutic or safety profile
  - Pharmacokinetic profile
  - Ease of drug administration
  - Cost of drug compounding
  - Patient compliance
  - Drug combinations

# Identifying Drug Combinations

- Component Registry Number search in the REGISTRY File and limit by number of components (/INC)
- EXPAND known chemical names and use **SELECT CHEM** to create additional search terms (**useful for searching in other files**)
- FAMILY structure search in the REGISTRY File

# Identifying Formulations

- Online Thesauri
  - [CA Lexicon](#) in the CAPlus File
  - MESH in Medline
  - Identify specific and broad formulation terms
  - Develop free-text query
- Formulations cluster
  - Use [INDEX](#) to identify files

# Search Question

***Claritin, (Loratadine) is a drug which is used by millions of people around the world. Over the years, new offerings have been provided by the drug maker to provide more effective alleviation of allergy symptoms. Retrieve literature describing the various formulations as well as combination products and uses of Claritin .***

# Search Strategy

- Identify CAS RNs for combinations
- Develop file-specific queries
  - Identify terminology for drug names
  - Identify terminology for formulations
  - Combine concepts
  - Save answer set

## Optionally

- Merge results, remove duplicates, display records
  - Retrieve formulations from a patent file
  - Retrieve formulations from pipeline files

# CAS RNs for Combinations

- Salt forms  
Each have a unique CAS RN
- Actual combinations  
CAS RN for each component (/CRN) as well as overall mixture

# CAS RNs for Combinations

- Identify substances containing known name
- Extract CAS RNs
- Re-search CAS RNs as component registry numbers

**Note:** a FAMILY structure search provides an alternative approach. This will broaden query to include stereoisomers and radiolabeled products.

# Identify chemical moieties containing Claritin

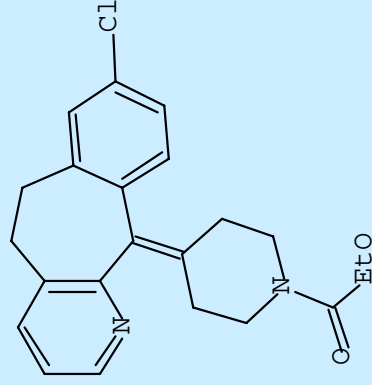
=> FILE REGISTRY

L1 STRUCTURE UPLOADED

=> D L1

L1 HAS NO ANSWERS

L1 STR



# Identify chemical moieties containing Claritin

=> S L1 FAM SAM

SAMPLE SCREEN SEARCH COMPLETED - 6 TO ITERATE

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 6 TO 266

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA FAM SAM L1

=> S L1 FAM FULL

FULL SEARCH INITIATED 14:55:18

L3 113 SEA FAM FUL L1 EXTEND

CANDIDATE STRUCTURE SEARCH COMPLETED - 113 TO ITERATE

100.0% PROCESSED 113 ITERATIONS

L4 13 SEA FAM FUL L1

# Identify chemical names containing Claritin

## => FILE REGISTRY

|      |             |                                      |
|------|-------------|--------------------------------------|
| => E | CLARITIN/CN |                                      |
| E1   | 1           | CLARITHROMYCIN-OMEPRAZOLE MIXT./CN   |
| E2   | 1           | CLARITHROMYCIN-PANTOPRAZOLE MIXT./CN |
| E3   | 1 -->       | CLARITIN/CN                          |
| E4   | 1           | CLARITIN EXTRA/CN                    |
| E5   | 1           | CLARITIN-D/CN                        |
| E6   | 1           | CLARITINE/CN                         |
| E7   | 1           | CLARITONE/CN                         |
| E8   | 1           | CLARITY/CN                           |
| E9   | 1           | CLARITYN/CN                          |
| E10  | 1           | CLARITYNE/CN                         |
| E11  | 1           | CLARITYNE D/CN                       |
| E12  | 1           | CLARITYNE D REPETABS/CN              |

*An Expand on the known product name may identify some salts or combinations, but only if the name is based on the known product name.*

# Identify chemical names containing Claritin

=> S CLARITIN

L5

2 CLARITIN

The search could have been just as easily performed with E3 instead of the full compound name

# Look for Additional Names:

=> D L5

L5 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 79794-75-5 REGISTRY  
CN 1-Piperidinecarboxylic acid, 4-(8-chloro-5,6-dihydro-11H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-ylidene)-, ethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 11H-Benzo[5,6]cyclohepta[1,2-b]pyridine, 1-piperidinecarboxylic acid deriv.

OTHER NAMES:

CN Alavert  
CN Anhissen  
CN Bonalerg  
CN Civeran  
CN Claratyne  
CN Claritin  
CN Claritine  
CN Clarityn  
CN Clarityne



# Look for Additional Names:

```
CN Lowadina
CN Optimin
CN Polaratyne
CN Pylor
CN Restamine
CN Sch 29851
CN Sensibit
CN Sohotin
CN Tadine
CN Velodan
CN Zeos
```

```
=> S E3-E6, E9-E12
```

```
L6 2 (CLARITIN/CN OR "CLARITIN EXTRA"/CN OR CLARITIN-D/CN OR
CLARITINE/CN OR CLARITYN/CN OR CLARITYNE/CN OR "CLARITYNE
D"/CN OR "CLARITYNE D REPETABS"/
```

```
=> SELECT CHEM L6 1-
E86 THROUGH E140 ASSIGNED
```

*We can quickly see that a number of other names exist in addition to Claritin. We can select the names and Registry numbers very easily by use of the **SELECT CHEM** command.*

*We search on the E-numbers which have drug names that we see from a display. Searching E7-E8 would provide numerous false drops as they are not synonyms for Claritin.*

**SELECT CHEM** selects Registry numbers, drug codes and Names.

# Extract CAS RNs

=> SEL RN L6 1-  
E141 THROUGH E142 ASSIGNED

=> S E141-E142/CRN

L7 11 (156098-07-6/CRN OR 79794-75-5/CRN)

=> S L4 OR L6 OR L7

L8 13 L4 OR L6 or L7

*SELECT RN selects Registry numbers.*

*Searching as a /CRN will find the drug as a component of a mixture.*

*The Family search was able to find all the variations for Claritin. In searching other drug formulations, this may not be the case.*

## CAplus - Specific Query

- CA Lexicon is useful for identifying controlled terminology
- Search CT terms directly
- Develop a free-text query based on indexing terms

**HINT: HELP messages for CA Lexicon**

**=> HELP LEXICON**

**=> HELP THESAURUS**

**=> HELP RCODES**

# CAplus - Specific Query

```
=> FILE ZCAPLUS  
=> SET EXPAND CONT
```

**To NOT overwrite earlier E-numbers, set EXPAND to CONT.**

# CAplus - Formulations

=> E FORMULATIONS/CT

| E#   | FREQUENCY | AT | TERM                                 |
|------|-----------|----|--------------------------------------|
| --   | -----     | -- | ----                                 |
| E143 | 0         | 1  | FORMULATED/CT                        |
| E144 | 0         | 2  | FORMULATED FLAVORING<br>MATERIALS/CT |
| E145 | 0         | 1  | --> FORMULATIONS/CT                  |
| E146 | 62        | 2  | FORMVAR/CT                           |
| E147 | 0         | 2  | FORMVAR 12/85/CT                     |



*The controlled term "formulations" appears to be reserved for agrochemical applications*

*The relationship code of KT show those controlled terms containing the key word "formulations"*

# CAplus – KT Formulations

```
=> E E145+KT
E155      0  --> Formulations/CT
E156    2554  KT  Agrochemical formulations/CT
E157      KT  Agrochemical formulations (L) adjuvants/CT
E158      KT  Agrochemical formulations (L) controlled-
              release/CT
E159      KT  Agrochemical formulations (L) dispersions/CT
E160      KT  Agrochemical formulations (L) emulsions/CT
E161      KT  Agrochemical formulations (L) granules/CT
E162      KT  Agrochemical formulations (L) microcapsules/CT
●●●
E178      KT  Pesticide formulations (L) adjuvants/CT
E179      KT  Pesticide formulations (L) dispersions/CT
E180      0  KT  Suspensions agrochem. formulations/CT
E181      0  KT  Sustained-release agrochem. formulations/CT
E182      0  KT  Wettable powders agrochem. formulations/CT
***** END *****
```

# CAplus - Formulations

=> E DRUG DOSAGE FORM/CT 7

| E#   | FREQUENCY | AT  | TERM                    |
|------|-----------|-----|-------------------------|
| --   | -----     | --  | ----                    |
| E183 | 10194     | 23  | DRUG DESIGN/CT          |
| E184 | 1767      | 11  | DRUG DISCOVERY/CT       |
| E185 | 0         | --> | DRUG DOSAGE FORM/CT     |
| E186 | 0         | 2   | DRUG GELS/CT            |
| E187 | 0         | 2   | DRUG HABITUATION/CT     |
| E188 | 0         | 2   | DRUG INCOMPATIBILITY/CT |
| E189 | 0         | 2   | DRUG INTERACTION/CT     |

*Still we see that Drug dosage form is not in the system as an indexing term.*

# CAplus – Lexicon

=> E DRUG/CT

| E#   | FREQUENCY | AT    | TERM                                     |
|------|-----------|-------|--|
| --   | -----     | --    | ----                                     |
| E195 | 1         |       | DRUDE THEORY/CT                          |
| E196 | 0         | 1     | DRUENTIUS/CT                             |
| E197 | 1         | 2 --> | DRUG/CT                                  |
| E198 | 0         | 2     | DRUG ABUSE/CT                            |
| E199 | 23        | 2     | DRUG ADDICTION/CT                        |
| •    |           |       |  |
| •    |           |       |  |
| •    |           |       |  |
| E208 | 0         | 2     | DRUG CARRIERS/CT                         |
| E209 | 0         | 2     | DRUG CARRIERS (DRUG DELIVERY SYSTEMS)/CT |
| E210 | 0         | 2     | DRUG DELIVERY CARRIER/CT                 |
| E211 | 0         | 2     | DRUG DELIVERY IMPLANTS/CT                |
| E212 | 0         | 2     | DRUG DELIVERY MICELLES/CT                |
| E213 | 120509    | 352   | DRUG DELIVERY SYSTEMS/CT                 |

# CAplus – Lexicon

=> E E213+ALL

|      |        |     |   |
|------|--------|-----|---|
| E219 | 1348   | BT1 | Health products/CT                                      |
| E220 | 120509 | --> | Drug delivery systems/CT                                |
|      |        |     | HNTE Valid heading during volume 126 (1997) to present. |
| E221 | 2071   | OLD | Drug targeting/CT                                       |
| E222 | 48095  | OLD | Pharmaceutical dosage forms/CT                          |
| E223 | 4391   | OLD | Pharmaceutical preparations/CT                          |
| E224 |        | UF  | Delivery systems (pharmaceutical)/CT                    |
| E225 |        | UF  | Dosage forms (pharmaceutical)/CT                        |
| ●    |        |     |   |
| E563 | 623    | NT1 | Tinctures/CT  |
| E564 |        | NT1 | Toxins (L) immuno-/CT                                   |
| E565 | 17909  | RT  | Drug bioavailability/CT                                 |
| E566 | 10194  | RT  | Drug design/CT  |
| E567 | 3863   | RT  | Drug metabolism/CT                                      |
| E568 | 19823  | RT  | Drugs/CT  |
| E569 | 21205  | RT  | Genetic vectors/CT                                      |
| E570 | 24170  | RT  | Nanoparticles/CT  |

# CAplus Formulation Concept

- Terms identified in the CA Lexicon may be searched in the CT index = precision
- A free-text query may be developed = comprehension
- Thesaurus relationship codes may also be used for searching

- +PFT

- +NT

# HCAplus – Formulations Concept

=> FILE HCAPLUS

FILE 'HCAPLUS' ENTERED AT 13:22:47 ON 10 MAY 2005

=> S E220+PFT,NT

L9 188153 "DRUG DELIVERY SYSTEMS"+PFT,NT/CT (345 TERMS)

**Note:** It is most cost-effective to search many terms in the HCAplus File

# Search compounds and Names found in Registry

=> S E86-E140

L10 901(AIRET/BI OR ALAVERT/BI OR ANHISSEN/BI OR  
"BONALERG

D"/BI OR "SCH 29851"/BI OR 156098-07-6/BI OR...)

=> S L8

L11 747 L8

=> S L10 OR L11

L12 902 L10 OR L11

# Combine results and Utilize Specific CA query

=> S L12 AND L9

L13            277 L12 AND L9

=> S L13 AND (63 OR 64) /CC, SX

323262 63/CC

138427 63/SX

65999 64/CC

13416 64/SX

L14            251 L13 AND (63 OR 64) /CC, SX

*To provide additional precision a search may be limited to CA sections (CC) or a cross-referenced section (SX).*

*Adding section codes for the pharmaceuticals sections of CPlus have little effect for this controlled term search. One of the two non-pharmaceuticals records deals with synthesis.*

# Review answers

=> D L14 2-3 BIB ABS

L14 ANSWER 2 OF 251 HCAPLUS COPYRIGHT 2005 ACS on STN  
AN 2005:325504 HCAPLUS [Full-text](#)  
DN 142:379390  
TI Pharmaceutical formulations comprising microparticles with improved  
dispersibility, suspendability or wettability  
IN Chickering, Donald E.; Reese, Shaina; Narasimhan, Sridhar; Straub,  
Julie A.; Bernstein, Howard; Altreuter, David; Huang, Eric K.;  
Brito, Luis A.; Jain, Rajeev A.  
PA USA  
SO U.S. Pat. Appl. Publ., 26 pp., Cont.-in-part of U.S. Ser. No.  
324,550. CODEN: USXXCO  
DT Patent  
LA English  
FAN.CNT 2  
●●●

# Review answers

| PATENT NO.          | KIND | DATE     | APPLICATION NO. | DATE     |
|---------------------|------|----------|-----------------|----------|
| PI US 2005079138    | A1   | 20050414 | US 2004-955261  | 20040930 |
| US 2004121003       | A1   | 20040624 | US 2002-324558  | 20021219 |
| PRAI US 2002-324558 | A2   | 20021219 |                 |          |

AB Methods are provided for making a dry powder blend pharmaceutical formulation, comprising the steps of: (a) providing microparticles which comprise a pharmaceutical agent; (b) blending the microparticles with at least one excipient in the form of particles to form a powder blend; and (c) jet milling the powder blend to form a dry powder blend pharmaceutical formulation having improved dispersibility, suspendability, or wettability as compared to the microparticles of step (a) or the powder blend of step (b). The method can further include dispersing the dry powder blend pharmaceutical formulation in a liquid pharmaceutically acceptable vehicle to make an formulation suitable for injection. Alternatively, the method can further include processing the dry powder blend pharmaceutical formulation into a solid oral dosage form. In one embodiment, the microparticles of step (a) are formed by a solvent precipitation or crystallization process. PLGA microspheres containing mannitol and Tween 80 having number average particle size of 1.96  $\mu\text{m}$ , and volume average particle size of 4.04  $\mu\text{m}$  were prepared. The jet milling provided significant particle deagglomeration.

## CAS Indexing Policies for Agrochemical Formulations

- The Controlled Term "Pesticide formulations" is indexed when the novelty of the paper/patent is in the compounding and formulation of the agrochemical.
- The active component is indexed as specifically as possible.
- Often more than one active component is present; when these are deliberately admixed and remain discrete in the medium, the mixture is indexed.
- Substances designated as herbicide synergists are included as mixture components.

- Additives such as stabilizers which are regarded as inactive are not routinely indexed as mixture components but may be indexed separately if significant.
- Adjuvants are indexed when there are data demonstrating that such substances improve properties of the formulation.
- If a large formulation has more than 9 active ingredients, and it does not have a trade name, the components are indexed separately in **CAplus** (with the phrase "mixtures containing" in the beginning of the text modification) rather than as a single mixture registration.

# Tools for Searching Agrochemical Formulations in REGISTRY

- **CAS REGISTRY** number of the synergistic mixture  
to find formulation entries in REGISTRY and records in CAplus
- **Derivative REGISTRY number (“D”)** (**caution!**)  
to find records for synergistic combinations (mixtures) in CAplus
- **Component REGISTRY number (/CRN)** or chemical  
name segments (/CNS)  
to find the RN for formulations and mixtures which are indexed in  
Registry
- **Family search with one component** (**very useful**)  
to find the RN for formulations and mixtures which are indexed in  
Registry (isomers, enantiomers and isotopes are retrieved as well)

# Tools for Searching Agrochemical Formulations in REGISTRY

- **Number of components (/NC)**  
To refine your search in Registry
- **SELECT CHEM (very useful)**  
To retrieve all chemical names (including trade names) for a single compound or/and for a mixture (RNs are also retrieved with Select Chem)
- **Class Identifier (MXS/CI; com/CI)**
  - To see if a single substance is also indexed as part of a multi-component system (com/CI)
  - To see if the multi-component system is indexed as a mixture (MXS/CI)

(caution: agrochem. formulations indexed in Registry only get MXS/CI when they are described as mixtures in the original document)

# Tools for Searching Agrochemical Formulations in CAPlus

- **CAS Role: AGR**

To refine your answer set (very broad). There is a thesaurus for roles in the CA file (=> e agr/rl).

- **Section Code: Agrochemical bioregulators/CC**

(1982-), the old sections can be searched using the +old relationshipcode with the e-number for agrochemical bioregulators (very broad)

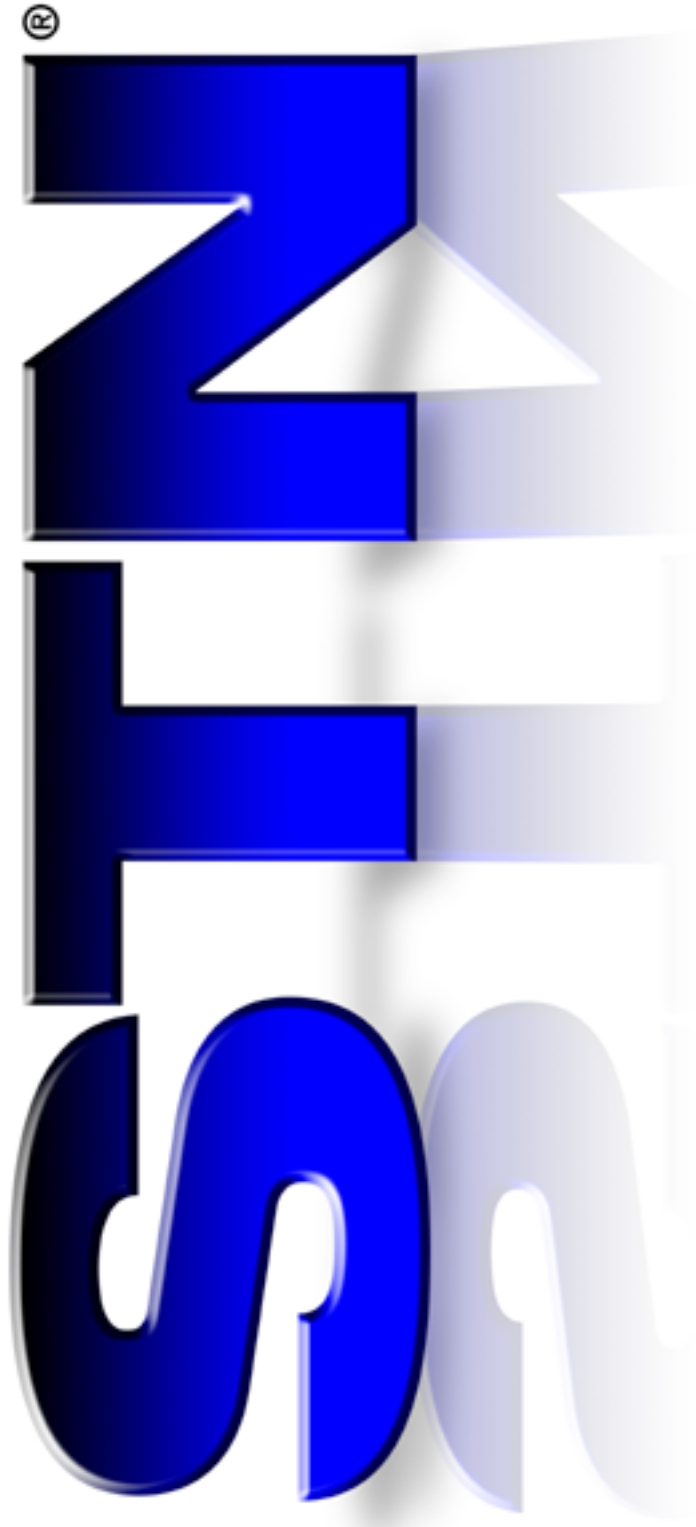
- **CAS Thesaurus (Controlled terms): Pesticides, Fungicides, Herbicides, Agrochemical formulations, Pesticide formulations, Weed control**

Use Agrochemical formulations (1992-), Pesticide formulations(1998-)  
when you are looking for formulations

Use Pesticides/CT, Fungicides/CT, Herbicides, weed control/IT when you  
are also looking for synergistic mixtures. Expand on Pesticides+LT,KT /CT  
or on Formulations+LT,KT/CT to determine more specific terminology

# Summary

- Searching for Polymers & Surfactants – approaches to consider
- Pharmaceutical Formulations & Agrochemical formulations – special considerations
- Consider other industry-specific files



Searching for  
Polymers & Formulations