



CAS Formulations

Agenda

- Introduction
- Indexing and Retrieval Aspects
- Formulation Search Example



CAS FORMULATIONS facilitates precise searches for formulations

- Searchable with STNnext® power and control for database subscribers
- Hybrid of bibliographic, substance, and brand-new formulation content
- Humanly curated formulation data designed for precision searching
- Weekly updates

Most complete and comprehensive formulation source

Includes patents, journals and product inserts

Focus: Pharma, Agrochemistry, Cosmetics

Based on English, French, German, Japanese, Chinese and Korean publications

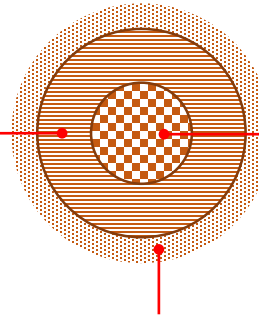
20+
years of back file coverage

CAS FORMULATIONS defines the components of a formulation

- Three main document types in the database
 - Patents (P/DT), Journal articles (J/DT) and Product Inserts (I/DT)
- Each record in CASFORM describes a single formulation
 - Generally **multiple** CASFORM records are extracted out of **one** publication
- Every CASFORM record has the following sections
 - Bibliographic details, location, groups with their components, product descriptions, target definition, process notes and experimental data

Formulation chemistry is broken down into **groups** and **components**

Bilayered tablet with optional coating



Drug layer 2 (Group G2)

GROUP G2

GDS tramadol layer
GLO second layer
CMPS C7; C8; C9; C10; C11

...

COMPONENT C7

RN 36282-47-0
CNM tramadol hydrochloride
CVO Formulation active agents;
Active agents;
CAM 4-11 % (w/w)
CFU active agent; analgesics

...

Optional coating (Group G3)

GROUP G3

GDS pharmaceutical excipients
GFU coating materials
GLO coating
CMPS C12; C13; C14; C15; C16; C17
GOP Optional
GVO Pharmaceutical excipients...

COMPONENT C12

RN 9002-89-5
CNM polyvinyl alcohol

...

Drug layer 1 (Group G1)

GROUP G1

GDS ketorolac layer
GFU active agent
GLO first layer
CMPS C1; C2; C3; C4; C5; C6

...

COMPONENT C1

RN 74103-07-4
CNM ketorolac tromethamine
CVO Formulation active agents;
Active agents; Formulation active
agent;
CAM 1-6 % (w/w)
CFU active agent; analgesics

...

Product-related information (product insert)

PRODUCT PA1

PUP **sunscreens**

FEA net content: 100 mL/3.4 FL OZ in 1 bottle

net content: 200 mL/6.7 FL OZ in 1 bottle

Broad Spectrum SPF: 50

PF Desc: cosmetic lotions

DR topical

ANTE package description: NDC: 72645-003-02, 200
combination product.

TGR decreases

TGD risk caused by the sun

TGT **skin neoplasm**

PV0 Topical drug delivery systems; Topical pharmaceuticals; Topical medicaments; Pharmaceutical topicals; Topical drugs; Topical; Topical oils; Skin preparations; Topical oil; Topical drug; Topical medicament; Topical pharmaceutical; Topical ointment; Topical drug delivery system; Topical drug preparations; Topical drug preparation; Topicals; Topical ointments; Sunscreens; Skin sunscreens; Suntan lotions; Sun block; Sunscreen; Suntan lotion; Sunscreen cream; Sunscreen lotions; Sunscreen creams; Sun blocks; Sunscreen gels; Stick sunscreens; Sunscreen sticks; UV filters; UV filter; UV-absorbing sunscreens; UV absorbers, sunscreens; UV sunscreens; UV-absorbent sunscreens; UV absorber sunscreens; UV sunscreen; UV absorbent sunscreen; UV blockers; Sunscreen gel; Sunblock gel; Sunblock gels; Sunscreening agents; Sunscreening agent; Sunscreen agent; Sunscreen agents; Inorganic sunscreen agent; Sunscreens agents; Sun protection agents; Sun protection agent; Organic sunscreen agents; Organic sunscreen agent; Sunscreen active agent; Sunscreen active agents; Cosmetic lotions; Aftershave lotion; Lotion cosmetics; Cosmetic lotion; Moisturizing lotions; Hair setting lotions; Wave-setting hair lotions; Hair wave-setting lotions; Hair lotions; Aftershave lotio

Product vocabulary

Names and functions - Original versus standardized terminology

COMPONENT C11
RN 25086-89-9

CNM copovidone

CVO Wetting agents; Detergents, wetting agents; Wettening agents; Wetting, agents; Wetting agent; Wettening agent; Wetness agents; Wetness agent; Acceptable wetting agents; Levigating agent; Levigating agents; Moistening agent; Moistening agents; Moisturizing agents; Wettability agent; Wettability agents; Binders; Bonding agents; Sticking agents; Binder materials; Binding agents; Binding material; Bonding materials; Binder; Bonding agent; Binding elements; Bonders; Bonder; Binding agent

CCN Acetic acid ethenyl ester, polymer with 1-ethenyl-2-pyrrolidinone (9CI, ACI)

CCN 2-Pyrrolidinone, 1-ethenyl-, polymer with ethenyl acetate (9CI); 2-Pyrrolidinone, 1-vinyl-, polymer with vinyl acetate (8CI); Acetic acid vinyl ester, polymer with 1-vinyl-2-pyrrolidinone (8CI)

CCN 1-Vinyl-2-Pyrrolidinone-vinyl acetate copolymer; 1-Vinyl-2-pyrrolidone-vinyl acetate copolymer; Agrimer VA 03E; Agrimer VA 05E; Agrimer VA 07E; Agrimer VA 3; Agrimer VA 31; Agrimer VA 3E; Agrimer VA 5; Agrimer VA 5I; Agrimer VA 6; Agrimer VA 64; Agrimer VA 6W; Agrimer VA 7W; Akon KS; Akon M; Akorn KS; Copolyvidon; Copolyvidonum; Copovidon; Copovidone; Copovidone K 28; Copovidone VA 64; DimaFIX; E 335; E 335 (polymer); E 535; E 635; E 635 (polymer); E 735; Eukaline 480; GAF-E 735; GAF-S 630; Ganex E 535; Gantron PVP; Gantron S 630; Gantron S 860; I 335; I 535; I 635; I 735; Kolima 10; Kolima 35; Kolima 75; Kollidon 64

CAM 15-25 pbw

CFU binder; wetting agent

COP Mandatory

CNM is the original name from the publication

CVO is component-related vocabulary added by CAS to ease retrieval

The CN field in CASFORM reflects the chemical names from CAS Registry.
(!) CN in CASFORM is **limited to the first 50 chemical names** from a Registry entry.

CFU shows the function as mentioned in the source document

CA Index Name

Other CA Index Names

Other Names

The group and component information unit

GROUP G5
GDS extended release coating
GFU pharmaceutical coatings
CMPS C8-C10
GOP Optional
GAM 93 mg

COMPONENT C8
RN 9004-57-3
CNM Aquacoat ECD 30
CCN Cellulose, ethyl ether (8CI, 9CI, ACI)
CAM 67 mg
CFU pharmaceutical coatings
CNO 14.3 w/w %; ethylcellulose dispersion;
water-insoluble
film-forming polymer.
COP Mandatory

These specific fields or their words in the Basic Index can be linked together using (L) proximity

GAM/FA
GFU/FA
GVO/FA

RN/FA
CNM/FA
CN/FA
CAM/FA
CFU/FA
CVO/FA

Words describing the groups and components can be found in the Basic Index

- The (L) operator can be used to link fields within a group/component unit
 - Link a component to its function
 - Link a component to the group description
 - Link the amount availability to a function
 - Link a component to its component or group optionality
- For example:
 - S 9063-38-1 (L) (DISINTEGRA? OR SUPERDISINTEGRA?)
 - S ?PARABEN?/CNS (L) EXCLUDE/COP,GOP

Compound searching strategies

=> **FILE REG**

=> S HYALURON?

L7 5202 HYALURON?

=> S HYALURON? AND CASFORM?/LC

 2779278 CASFORM?/LC

L9 264 HYALURON? AND CASFORM?/LC

=> S ?HYALURON?/ENTE AND CASFORM?/LC

L11 39 ?HYALURON?/ENTE AND CASFORM?/LC

=> **FILE CASFORM**

264 substance entries appear in the formulations database, that's 5% of all Hyaluron? entries.

39 Hyaluron product registrations are indexed in CASFORM

Compound searching strategies

```
=> S L9 OR L11
      60829 L9
      382 L11
L12   61142 L9 OR L11
```

```
=> S ?HYALURON? (P) CNM/FA (NOTL) RN/FA
      79443 ?HYALURON?
      5021148 CNM/FA
      4896482 RN/FA
L13   7958 ?HYALURON? (P) CNM/FA (NOTL) RN/FA
```

```
CNM  hyaluronic acid-L-alanine-chitosan oligosaccharide lactate nanoconjugate
CNM  non-crosslinked hyaluronic acid
CNM  hyaluron sun HA-Q
CNM  sodium acetylated hyaluronate
CNM  aqueous sodium hyaluronate
```

Combining the Registry BI and ENTE search approaches.

Separate search for Hyaluron formulations which have an original name (CNM), but which don't have a Registry Number (RN) assigned.

About 8k formulations are related to Hyaluron but not indexed with a Registry number.

Substances without any CAplus references can have references in CASFORM

RN 8001-21-6 REGISTRY *

* Use of this CAS Registry Number alone as a search term in other STN files may result in incomplete search results. For additional information, enter HELP RN* at an online arrow prompt (=>).

ED Entered STN: 16 Nov 1984

CN Sunflower oil (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Oils, sunflower

OTHER NAMES:

CN Agri-Pure AP 65

CN AP 80

CN Captex 20539 Agripure 80

CN Collageneer

CN Cotebar A

CN Florasun 90

CN Gina

CN Gina (glyceride)

CN Haioru 75B

...

LC STN Files: ADISNEWS, ANABSTR, BIOSIS, BIOTECHNO, CABA, CASFORMULTNS, CHEMCATS, CHEMLIST, CIN, EMBASE, IPA, TOXCENTER, USPAT2, USPATFULL

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

Entered CASFORMULTNS 12

L21 20274 S 8001-21-6

The Registry number of Sunflower oil finds more than 20k formulations

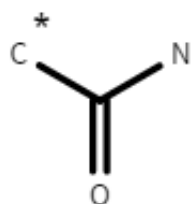
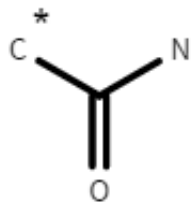
Use case: Agrochemical formulation

Formulations comprising a **diamide insecticide**, a **fungicide** and **one additional insecticide**

- Requirements
 - Diamide compound with 1-6 rings
 - Diamide compound should have a defined amount
 - Fungicide as a mandatory function for a group or component
 - Insecticide as a mandatory or preferred component except when it overlaps with the diamide compounds

Structure search of compounds with two amide groups

=> FILE REG



Structure search for two fragments in CAS Registry

L1 STRUCTURE UPLOADED

=> S L1 SSS FUL

FULL SEARCH INITIATED 03:40:12

100.0% PROCESSED 13564849 ITERATIONS 10142402 ANSWERS

SEARCH TIME: 00.00.07

L2 10142402 SEA SSS FUL L1

Refining the structure answers

L2 10142402 SEA SSS FUL L1

=> S L2 NOT (POLYMER/CI,CCI OR PROTEIN/FS)

L3 6187938 L2 NOT (POLYMER/CI,CCI OR PROTEIN/FS)

Exclude polymers and proteins

=> S L3 AND 1-6/NR

L4 5781521 L3 AND 1-6/NR

Require the presence of 1-6 rings

=> S L4 AND CASFORM?/LC

 2764210 CASFORM?/LC

L5 100414 L4 AND CASFORM?/LC

Require compounds are indexed in
CASFORMULTNS

Cross-over from REGISTRY to CASFORMULTNS

L5 100414 L4 AND CASFORM?/LC (Registry)

=> **FILE CASFORM**

=> S L5

L6 102203 L5

The 100K CAS RNs in L5 resulted in 102K formulations in L6

=> S L6(L)(MANDATORY OR PREFERRED)/COP,GOP

L7 97733 L6(L)(MANDATORY OR PREFERRED)/COP,GOP

Refining to only mandatory compounds

=> S L7 AND FUNGICID?(L)CNM/FA

L8 6470 L7 AND FUNGICID?(L)CNM/FA

Adding a fungicide component in the formulation

Adding further requirements

- The formulation already includes a diamide insecticide plus a fungicide
- If we just combine with INSECTICIDE? (L) CNM/FA, this will overlap with the components in L6 which have the diamides
- By using (NOTL) L6 the retrieved insecticide should be different from the ones defined in L6
- Leaving out many answers with a large range of optional alternative insecticide the second one should also be mandatory

Adding another insecticide that doesn't match the list of diamide compounds

L8 6470 L7 AND FUNGICID?(L)CNM/FA

=> S L8 AND INSECTICID?(L)CNM/FA (L) (MANDATORY OR PREFERRED)/COP (NOTL) L6

L9 1184 ...

(NOTL) L6 makes sure this 2nd insecticide search does not overlap with our diamide insecticide

=> S L6(L)CAM/FA

L11 28881 L6(L)CAM/FA

Adding the requirement to the insecticide that the amount should be specified

=> S L11 AND L9

L12 426 L11 AND L9

This is the final set of positives

Since there are multiple formulations from each publication FSORT is used to group these together

=> **FSORT L12**

```
L13          426 FSO L12

          32 Multi-record Families    Answers 1-408
            Family 1                  Answers 1-9
            Family 2                  Answers 10-17
            Family 3                  Answers 18-32
            Family 4                  Answers 33-35
            Family 5                  Answers 36-39
            Family 6                  Answers 40-92
            Family 7                  Answers 93-98
    o o o o
            Family 30                 Answers 236-402
            Family 31                 Answers 403-405
            Family 32                 Answers 406-408
    18 Individual Records    Answers 409-426
    0 Non-patent Records
```

Option: SELECT CPAN would limit to the number of corresponding CPlus records

The source information

L13 ANSWER 33 OF 426 CASFORMULTNS COPYRIGHT 2020 ACS on STN

AN 2019:370504 CASFORMULTNS

CPAN 2019:1750028

TI Treatment agent of radix astragali root disease and its application in
treatment of radix astragali root disease

AU Qi, Yonghong; Chen, Aichang; Cao, Sufang

PA Institute of Plant Protection, Gausu Academy of Agricultural Sciences

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
CN 110226602	A	20190913	CN 2019-10583782	20190701

FN Form 2

FD Astragalus Root Disease Treating Composition

GRPS G1-G6

LCC Example

LCD Example 1, 3, Table 1, 2

Component 1 is the diamide insecticide

GROUP G1

GDS Additional ingredients

CMPS C1

GOP **Mandatory**

COMPONENT C1

RN **736994-63-1**

CNM cyantraniliprole

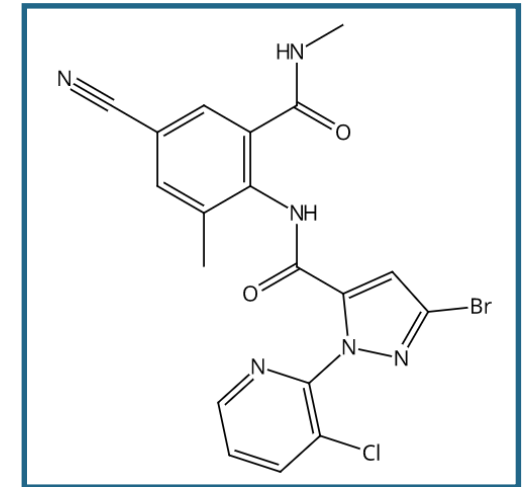
CCN 1H-Pyrazole-5-carboxamide, 3-bromo-1-(3-chloro-2-pyridinyl)-N-[4-cyano-2-methyl-6-[(methylamino)carbonyl]phenyl]- (9CI, ACI)

CAM **10 mL**

CFU seed treating agent; insecticide

CNO the cyantraniliprole accounts for 20% of the total mass; selected from Syngenta (china) investment Co., Ltd.

COP **Mandatory**



Component 2 is the second insecticide

GROUP G2

GDS Additional ingredients

CMPS C2

GOP Mandatory

COMPONENT C2

RN 153719-23-4

CNM **thiamethoxam**

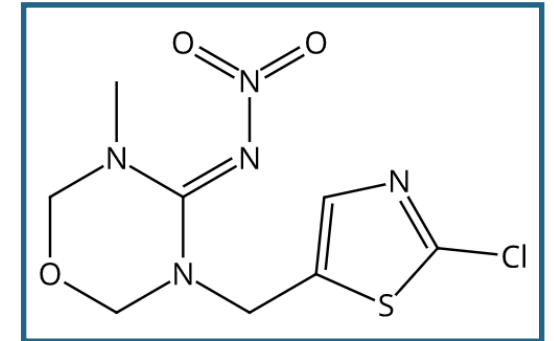
CCN 4H-1,3,5-Oxadiazin-4-imine, 3-[(2-chloro-5-thiazolyl)methyl]tetrahydro-5-methyl-N-nitro- (9CI, ACI)

CAM 10 mL

CFU seed treating agent; insecticide

CNO the thiamethoxam accounts for 20% of the total mass; selected from Syngenta (china) investment Co., Ltd.

COP **Mandatory**



Component 4 is the fungicide

GROUP G4

GDS Additional ingredients

CMPS C4

GOP Mandatory

COMPONENT C4

RN 57837-19-1

CNM **metalaxyl**

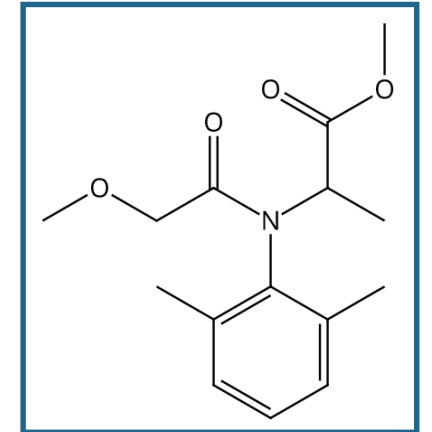
CCN Alanine, N-(2,6-dimethylphenyl)-N-(2-methoxyacetyl)-, methyl ester (ACI)

CAM 0.5 mL

CFU seed treating agent; **antifungal agent**

CNO the metalaxyl accounts for 2% of the total mass; selected from Syngenta (china) investment Co., Ltd.

COP Mandatory



The records doesn't highlight "fungicide",
but it is relevant

How would this search work without CASFORM?

- It would require a broader retrieval of hits that would have to be reviewed manually for relevance
 - CAplus retrieves 1005 hits on the compounds refined by both fungicide and insecticide terms
 - This includes 780 patent families versus 50 patent families in CASFORM
 - There are 211 patent families in CAplus that do not have CASFORM indexing
 - Out of the 50 families in CASFORM, 31 were not retrieved in the 780 families from CAplus
- CASFORM provides a **higher quality result** and **saves 65% of the post-retrieval relevance work** compared to a CAplus search

CAS FORMULATIONS provides high precision searching

- CAS FORMULATIONS will save a lot of valuable time and effort in evaluating the relevant hits for formulation searches
 - CASFORMULTNS/OS field in CAplus helps to exclude content that was already searched in more detail for to-up searches
- First response from IP search professionals is very positive
 - Finding unique answers not found in other searches
 - Quickly find highly relevant results to get first IP insight
 - Product Inserts add very useful information to patents and journals
- CAS FORMULATIONS is only available on STNext

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