

CAS FORMULATIONS in STNext

Quick Start Guide

CASFORMULATIONS™ in STNext® is a new database from CAS. This database includes bibliographic, substance, and brand new formulation content. It is searchable with STNext power and control, and offers unparalleled content coverage.

CAS FORMULATIONS introduces many new search and display fields to STN®:

- Fields specific to Groups
- Fields specific to Components
- Fields specific to Targets
- CHEM display - essential formulation chemistry information, organized into Groups and Components
- PRODUCT display - detailed Product and Target information and Process notes
- Indented formats for these specialty displays are also available; ICHEM and IPRODUCT
- Consult the Database Summary Sheet and in-product HELP messages for further information, especially HELP SFIELDS, HELP DFIELDS and HELP FORMAT

Project Examples

Find IP citing Calcium Carbonate as an active ingredient, not as a filler or other role.

1. Using the (L) operator, search for the Registry Number linked with the desired function ("Active") in the formulation (Don't know the Registry Number? Check CAS REGISTRYSM).
2. Specify that the formulation description was taken from one or more of the Claims

The screenshot shows the STNNext search interface. At the top, the STNNext logo is on the left, and 'My Files' and a user profile icon are on the right. Below the header, the search title is 'Calcium Carbonate active'. The search results are displayed in a terminal-like window with the following content:

```
File: CASFORMULTNS
=> s 471-34-1/rn (1) (active ? or active)/cfu

    314 471-34-1/GRPRN
    49964 471-34-1/CMPRN
    0 471-34-1/SOLRN
    50075 471-34-1/RN
      (471-34-1/GRPRN, CMPRN, SOLRN)
    2921775 ACTIVE ?/CFU
    377743 ACTIVE/CFU
L1      6577 471-34-1/RN (L) (ACTIVE ? OR ACTIVE)/CFU

=> s 11 (1) (mandatory or "one or more")/cop

    4521512 MANDATORY/COP
    508287 "ONE OR MORE"/COP
L2      6457 L1 (L) (MANDATORY OR "ONE OR MORE")/COP

=> s 12 and claim/lcc

    1504428 CLAIM/LCC
L3      1249 L2 AND CLAIM/LCC

=>
=>
```

At the bottom of the interface, there is a command input field containing '=> enter command', a 'Submit' button, a 'Draw' button with a pencil icon, and a 'Scripts' button with a curly brace icon.

3. Review formulation chemistry in the CHEM format.

Note that hit highlighting is available (turn on Highlighting in STNext settings)

The screenshot displays the STNext web interface. At the top left is the STNext logo. To the right are icons for 'My Files' and a user profile. Below the header, a green bar indicates 'Transcript ON' and the title 'Calcium Carbonate active'. A file browser shows 'File CASFORMULTNS'. The main content area contains a transcript in CHEM format with highlighted terms. A decorative dashed line separates the transcript from the bottom navigation bar.

```
=> d 1 chem

L3 ANSWER 1 OF 1249 CASFORMULTNS COPYRIGHT 2019 ACS on STN

AN 2019:296438 CASFORMULTNS
LCC Claim
LCD claim 1

GROUP G1
GDS Additional ingredients
CMPS C1
GOP Mandatory

COMPONENT C1
RN 11098-84-3
CNM ammonium molybdate
CCN Ammonium molybdenum oxide (9CI, ACI)
CFU active agent
COP Mandatory

GROUP G6
GDS Additional ingredients
CMPS C6
GOP Mandatory

COMPONENT C6
RN 471-34-1
CNM calcium carbonate
CCN Carbonic acid calcium salt (1:1) (8CI, 9CI, ACI)
CFU active agent
COP Mandatory

GROUP G7
GDS Additional ingredients
CMPS C7
GOP Mandatory

COMPONENT C7
RN 9005-25-8
CNM starch
CCN Starch (8CI, 9CI, ACI)
CFU active agent
COP Mandatory

GROUP G8
```

Bottom navigation bar: **Submit** Draw Scripts

Locating patented herbicidal compositions against a particular target (Palmer Amaranth)

1. Search for Target organism by name(s) in the Target field
2. Restrict the result set to patents only
3. Use the SELECT command to determine the number of separate formulations that are in your results set.
4. Use the SELECT command and the CPAN (CA Accession Number) field to see how many unique patents are in the results set.

STNext My Files Profile

Transcript ON Palmer Amaranth

File CASFORMULTNS

```
=> s (amaranthus palmeri or palmer amaranth)/tgt

      4460 AMARANTHUS/TGT
        79 PALMERI/TGT
        79 AMARANTHUS PALMERI/TGT
          ((AMARANTHUS(W)PALMERI)/TGT)
        40 PALMER/TGT
        471 AMARANTH/TGT
        40 PALMER AMARANTH/TGT
          ((PALMER(W)AMARANTH)/TGT)
L1      119 (AMARANTHUS PALMERI OR PALMER AMARANTH)/TGT

=> s l1 and p/dt

      4098031 P/DT
L2      101 L1 AND P/DT

=> select an l2 1-

E1 THROUGH E101 ASSIGNED

=> select cpan l2 1-

E102 THROUGH E119 ASSIGNED
```

^ => enter command Submit Draw Scripts

5. Display the patent numbers for the 17 patent records. Each answer will display the CAPlus Accession Number for easy identification of the bibliographic record in CAPlus.

The screenshot shows the STNext interface with a terminal window. The terminal displays the command `=> d select e102-e119` and a list of 17 patent records. Each record consists of a patent number (E102-E119), a count, and a CAS accession number/CPAN.

Patent Number	Count	CAS Accession Number/CPAN
E102	29	2019:1098484/CPAN
E103	25	2018:1212923/CPAN
E104	9	2019:372852/CPAN
E105	8	2019:201824/CPAN
E106	7	2018:1215034/CPAN
E107	5	2017:1557956/CPAN
E108	4	2017:80903/CPAN
E109	2	2015:1207826/CPAN
E110	2	2018:1845897/CPAN
E111	2	2018:269259/CPAN
E112	1	2011:876749/CPAN
E113	1	2013:1384231/CPAN
E114	1	2013:604264/CPAN
E115	1	2014:354197/CPAN
E116	1	2014:788917/CPAN
E117	1	2018:158497/CPAN
E118	1	2019:171259/CPAN
E119	1	2019:372904/CPAN

6. Identify all formulations that CAS has indexed from these 17 patent records

The screenshot shows the STNext interface with a terminal window. The terminal displays the command `=> s e102-e119` and its output, which is a single line of text containing all the CAS accession numbers and CPAN values from the previous screenshot, enclosed in quotes and separated by OR operators.

```
L5      433 ("2019:1098484"/CPAN OR "2018:1212923"/CPAN OR "2019:372852"/CPAN OR "2019:201824"/CPAN OR "2018:1215034"/CPAN OR "2017:1557956"/CPAN OR "2017:80903"/CPAN OR "2015:1207826"/CPAN OR "2018:1845897"/CPAN OR "2018:269259"/CPAN OR "2011:876749"/CPAN OR "2013:1384231"/CPAN OR "2013:604264"/CPAN OR "2014:354197"/CPAN OR "2014:788917"/CPAN OR "2018:158497"/CPAN OR "2019:171259"/CPAN OR "2019:372904"/CPAN)
```

7. Identify all of the companies involved in Palmer Amaranth research

STNext My Files Profile

Transcript ON Palmer Amaranth

File CASFORMULTNS

```
L3      ANALYZE L2 1- PA :      13 TERMS

=> d 13 1- pa
L3      ANALYZE L2 1- PA :      13 TERMS

TERM #  # OCC  # DOC  % DOC PA
-----
  1     29   29  28.71 WEED OUT LTD.
  2     26   26  25.74 FMC CORPORATION
  3     10   10   9.90 BASF SE
  4     10   10   9.90 VALENT U.S.A. LLC
  5      7    7   6.93 FOSHAN BRIGHTMART CROP SCIENCE CO., LTD.
  6      5    5   4.95 BAYER CROPSCIENCE AKTIENGESELLSCHAFT
  7      4    4   3.96 VALENT U.S.A. CORPORATION
  8      3    3   2.97 MONSANTO TECHNOLOGY LLC
  9      2    2   1.98 UNIVERSITY OF KENTUCKY RESEARCH FOUNDATION
 10     1    1   0.99 EL PERTIGUERO, S.A.
 11     1    1   0.99 KUMIAI CHEMICAL INDUSTRY CO., LTD.
 12     1    1   0.99 SUMITOMO CHEMICAL COMPANY, LIMITED
 13     1    1   0.99 VALENT U.S.A., CORPORATION

***** END OF L3 *****
```

^ => enter command Submit Draw Scripts

8. Next, identify formulations that do not contain glyphosate, 2,4-D, and Dicamba, since Palmer Amaranth has developed resistance to these herbicides. You can supplement your chemical name search with CAS Registry Numbers to ensure that you capture records where brand names, etc. are used for these three herbicides.
9. Focus the results on active ingredients using the Component Function field

STNext My Files Profile

Transcript ON Palmer Amaranth

File CASFORMULTNS

```
=>
=> s 15 not ((glyphosate or 1071-83-6/rn) or (2,4-D or 94-75-7/rn) or (dicamba or 1918-00-9/rn))

22246 GLYPHOSATE
  1 GLYPHOSATES
22246 GLYPHOSATE
  (GLYPHOSATE OR GLYPHOSATES)
  9470 1071-83-6/RN
4250873 2
3754612 4
2336577 D
  7363 2,4-D
  (2(W)4(W)D)
3519 94-75-7/RN
5958 DICAMBA
3375 1918-00-9/RN
L6      67 L5 NOT ((GLYPHOSATE OR 1071-83-6/RN) OR (2,4-D OR 94-75-7/RN)
      OR (DICAMBA OR 1918-00-9/RN))

=> s active/cfu and L6

2955801 ACTIVE/CFU
L7      47 ACTIVE/CFU AND L6
```

^ => enter command Submit Draw Scripts

10. Display results using the CHEM format to see the names of the components, and their assigned function in the formulation

STNext My Files Profile

Transcript ON Palmer Amaranth X ✓

File CASFORMULTNS

L8 ANSWER 2 OF 41 CASFORMULTNS COPYRIGHT 2019 ACS on STN

AN 2019:180733 CASFORMULTNS
LCC Example
LCD example 2, table 2

GROUP G1
GDS Additional ingredients
CMPS C1
GOP Mandatory

COMPONENT C1
RN **77501-63-4**
CNM cobra herbicide
CCN Benzoic acid, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitro-, 2-ethoxy-1-methyl-2-oxoethyl ester (9CI, ACI)
CFU **active agent**; herbicides
CNO cobra® is a 24% lactofen formulation available from (and a registered trademark of) valent U.S.A. LLC.
COP Mandatory

GROUP G2
GDS C₁₆ to C₁₈ fatty acid methyl esters adjuvant system
GFU agrochemical adjuvants
CMPS C2; C3; C4; C5
GOP Mandatory

COMPONENT C2
CNM C₁₆ to C₁₈ fatty acid methyl esters mixture
CAM 88.3 % (w/w)
CFU agrochemical adjuvants
COP Mandatory

COMPONENT C3
CNM dodecylbenzene sulfonate salt in 2-ethyl hexanol/propylene glycol
CAM 6.2 % (w/w)
CFU agrochemical adjuvants
COP Mandatory

COMPONENT C4
RN **61791-12-6**
CNM Emulpon CO-550
CCN Castor oil, ethoxylated
CAM 2.9 % (w/w)
CFU agrochemical adjuvants
CNO Emulpon® CO-550 (available from Akzo Nobel N.V.) was used as the source of the POE(54) castor oil
COP Mandatory

COMPONENT C5
CNM POE(30) sorbitan mono tallate
CAM 2.6 % (w/w)
CFU agrochemical adjuvants
COP Mandatory

=>

^ => enter command Submit Draw Scripts

CAS FORMULATIONS in STNext FAQ

Who has access to CAS FORMULATIONS on STNext?

- All transactional customers
- GVP and SSVP customers who have added CAS FORMULATIONS to their contracts
- GVP and SSVP customers who have requested transactional CAS FORMULATIONS access. These customers will be invoiced for CAS FORMULATIONS usage in addition to the charges for their GVP and SSVP contracts.

What is the subject coverage of CASFORMULATIONS?

- The major areas of focus are agrochemical, pharmaceuticals and flavors/fragrances, with additional coverage in coatings, consumer goods, food, and materials.

Are SDIs available?

- Yes, for weekly, biweekly (default option) and monthly delivery.

How often is the database updated?

- The database is currently updated several times a week.

Other than drug product inserts, are there any records in CAS FORMULATIONS that do not have a counterpart in CPlusSM?

- No. We check daily to make sure that all CPANs and DNs in CAS FORMULATIONS link to records in CPlus.

Are trials available?

- Contact your Customer Success Specialist if you are interested in trial access of CAS Formulations to see how it can help your organization be more efficient.

Can I search CAS FORMULATIONS as part of a multi-file search?

- No, not at this time.

Is CAS FORMULATIONS part of any clusters?

- No, not at this time. Although there is a FORMULATIONS cluster, CAS FORMULATIONS is so different from the other databases in it that it does not make sense to include it there.

Is DUP IDE/DUP REMOVE available?

- No.

How do I know which CPlus records were selected for CAS FORMULATIONS indexing?

- The CPlus records that have content in CAS FORMULATIONS can be identified by looking at the OS (Other Sources) field, similar to our postings for MARPAT and CASREACT. Here's an example:
- OS CASFORMULTNS 2000:420972

- Note that the CASFORMULTNS link works differently than the OS links for CASREACT and MARPAT. Clicking the CASREACT or MARPAT link in the OS field displays the CASREACT or MARPAT record of interest. Clicking the CAS FORMULTNS link tells you how many formulations were indexed from the CAplus record, at least one but possibly as many as thousands.

How do I know if a Registry substance has ever been indexed in CAS FORMULATIONS?

- Look at the LC (Locator Code) field. Here's an example:
LC STN Files: CA, CAPLUS, CASFORMULTNS, CASREACT, CHEMCATS,
CHEMLIST, IFIALL, REAXYSFILE*, TOXCENTER, USPAT2, USPATFULL,
USPATOLD
(*File contains numerically searchable property data)

Other Sources: EINECS**

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

The information about the journals from which a formulation was indexed is limited to the source publication title. What if I need to know more?

- We supply the name of the journal in CASFORMULATIONS as a quality filter.
- To learn more about the journal article that supplied the formulations, copy the CPAN for the CAS FORMULATIONS record of interest, enter file CAplus, and search the CPAN (or the DN). Display in a format that includes bibliographic information, such as BIB.

The PI table in CAS FORMULATIONS is limited, and I need more information about the patent family. What do I do?

- Similar to the above.

What fields can I use in CAS FORMULATIONS for relevance checking?

- Both the Title and the Formulation Description fields can be displayed as a relevance check.

Is D SCAN available in CAS FORMULATIONS?

- No.

With a new database, there is bound to be some feedback including enhancement suggestions. How should I handle that?

- Send them to the CAS Help Desk at help@cas.org