

# STN<sup>®</sup>

## Strategies for Finding Compositions

## Compositions in patent claims

- **“Compositions of matter”** include compounds and mixtures
- **“Composition claims”** define a composition of matter invention based on component substance(s)
- Compositions can be made biologically, chemically or mechanically
- Focus on chemical mixture compositions - formulations

# Agenda

- Formulation information on STN<sup>®</sup>
- Finding formulations in CAS REGISTRY<sup>SM</sup>
- Finding formulations in CAplus<sup>SM</sup>

# The applications of formulation information are widespread

- Mix of non-reacting components according to a formula to create a product with the desired characteristics, e.g., improved effectiveness or safety
- Include adhesives, agricultural products, alloys, cosmetics, detergents, dyes, foods, fuels, lubricants, paints, and pharmaceuticals
- Allow for product life extension and market gains

# Formulations are covered in many STN databases

## Pharmaceuticals

- ADISINSIGHT
- BIOSIS®
- CAplus
- DRUGU
- Embase™
- MEDLINE
- REGISTRY
- USPAT files

## Chemical and Engineering

- AEROSPACE
- CABA
- CAplus
- COMPENDEX
- INSPEC®
- PASCAL
- REGISTRY
- SCISEARCH®

## How does CAS capture formulations?

- In CAplus, formulations are captured as text and as substances
  - Controlled Terminology text
    - IT Topical drug delivery systems  
(topical lotions; compns. comprising pentagalloyl glucopyranose)
  - Derivatives of known compounds
    - IT 14937-32-7D, 1,2,3,4,6-Penta-O-galloyl-.beta.-D-glucose, derivs.
  - CAS Registry Numbers<sup>®</sup> of multicomponent substances
    - IT 179465-88-4, Y-ART-3 (pentagalloyl glucose, H sulfide, sodium)
- In REGISTRY, formulations are captured as multicomponent substances

# CAplus record for a pesticide formulation

AN 2010:812403 CAPLUS [Full-text](#)

TI **Process and aqueous formulation for the impregnation of non-living-materials imparting a protective activity against pests**

IN Ishaque, Michael; Kraushaar, Arnold; Weinmueller, Egon

PA BASF SE, Germany

SO PCT Int. Appl., 25pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<a href="#">WO 2010072724</a>	A2	20100701	<a href="#">WO 2009-EP67663</a>	20091221
<a href="#">US 20110256200</a>	A1	20111020	<a href="#">US 2011-140960</a>	20110620

AB A process for the impregnation of nonliving-materials comprises the step of impregnating the nonliving material with an aqueous formulation free of organic solvents which comprises one or more pesticides and a polymeric binder comprising one or more fluorinated polyacrylates having a fluorine content (based on the solid content of the polymeric binder) of at least 10% by weight.

# Indexing from the CAplus record

IT [67375-30-8](#)

RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)

(process and aqueous formulation for impregnation of nonliving-materials imparting protective activity against pests)

IT [847137-26-2](#), Pluvioperl 9256 [1233839-73-0](#), Lurotex TX-R

[1233839-75-2](#), Lurotex TX-S [1233840-07-7](#), Evo Protect FCS

[1233840-12-4](#), Evo Gard FSU [1233840-24-8](#), Ruco-Guard AIR

RL: BUU (Biological use, unclassified); MOA (Modifier or additive use); PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); BIOL (Biological study); PROC (Process); USES (Uses) • • •

IT [52645-53-1D](#), Permethrin, mixts. containing [52918-63-5D](#),

Deltamethrin, mixts. containing [67375-30-8D](#), mixts. containing

[68359-37-5D](#), Cyfluthrin, mixts. containing [80844-07-1D](#),

Ethofenprox, mixts. containing [82657-04-3D](#), Bifenthrin, mixts.

containing RL: BUU (Biological use, unclassified); • • •

CAS will register:

- Individual substances
- Multicomponent mixtures

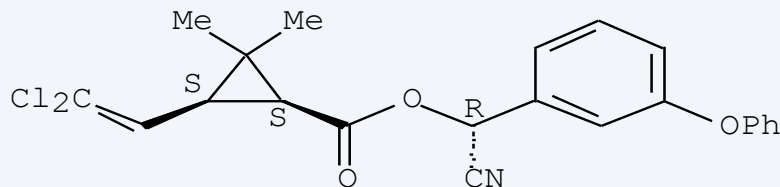


# REGISTRY record for single component substance from US 20110256200

RN 67375-30-8 REGISTRY ←  
 CN Cyclopropanecarboxylic acid, 3-(dimethyl-, (R)-cyano (3-phenoxyphenyl)- (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C22 H19 C12 N O3  
**CI COM**  
 LC STN Files: [AGRICOLA](#), [ANABSTR](#),

- Single component substance registrations have a Registry Number (RN) for the substance.
- The COM Class Identifier indicates that this substance is also found in a multicomponent registration.

[CASREACT](#), [CBNB](#), [CHEMCATS](#), [CHEMLIST](#), [CIN](#), [CSNB](#), [DDFU](#),  
[DETERM\\*](#), [DRUGU](#), [IFICDB](#), [IFIPAT](#), [IFIUDB](#), [MSDS-OHS](#), [PIRA](#),  
[REAXYSFILE\\*](#), [RTECS\\*](#), [TOXCENTER](#), [ULIDAT](#), [USAN](#), [USPAT2](#),  
[USPATFULL](#)



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

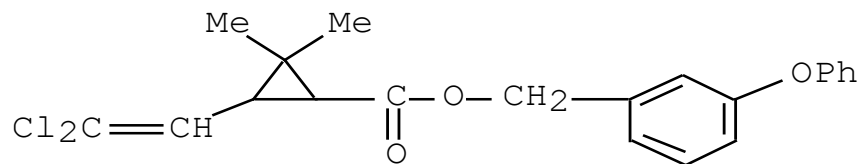
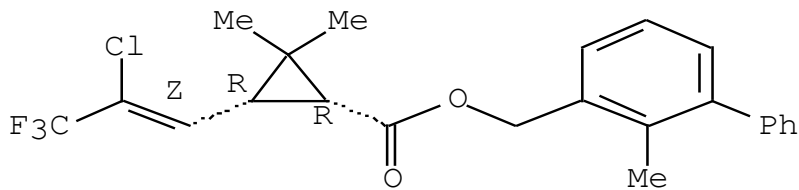
# REGISTRY record for multicomponent substance from US 20110256200

RN [1246612-09-8](#) REGISTRY  
 CN Cyclopropanecarboxylic acid, (2-methyl-3-(2,2-dichloroethyl)-2,2-dimethyl-1-phenyl)-2,2-dimethyl-, (2-methyl-3-(2,2-dichloroethyl)-2,2-dimethyl-1-phenyl)-2,2-dimethyl-, (1R,3R)-rel-, **mixt. with** (2-methyl-3-(2,2-dichloroethyl)-2,2-dimethyl-1-phenyl)-2,2-dimethyl-, (1R,3R)-rel-  
 MF C23 H22 Cl F3 O2 . C21 H20 O2  
**CI MXS**  
 SR CA  
 LC STN Files: CA, CAPLUS, T

- Multicomponent registrations have a Registry Number (RN) for the multicomponent substance.
- Each individual component is also represented with a RN in the Component Registry Number (CRN) field.

CM 1  
 CRN [82657-04-3](#)  
 CMF C23 H22 Cl F3 O2

CM 2  
 CRN [52645-53-1](#)  
 CMF C21 H20 Cl2 O3



# Options for searching formulation claims

1. “A composition comprising an optical isomer or racemic mixture of epinephrine.”
  - Search for epinephrine by chemical name and display the RN
  - Perform a Family structure search
2. “A composition comprising loratidine or pharmaceutically acceptable salts thereof.”
  - Search for loratidine by chemical name to find the RN
  - Search the RN as a Component Registry Number (CRN)
    - Only use CRN searches if no stereochemistry is possible
3. “A herbicidal composition comprising cyprosulfamide or derivatives thereof.”
  - Draw the chemical structure query, allowing for substitution
  - Perform a Substructure search

# Run a FAMILY structure search in REGISTRY to find formulations

- FAMILY structure search finds
  - Mixtures
  - Salts
  - Stereoisomers (optical isomers, +, -, R, S, L, D)
  - Isotopically labeled substances (radiolabelled, radionuclide, deuterated, tritiated)
  - Charged species (anion, cation, ion, +, -)
  - Hydrates
- Retrieves single component and multicomponent substances in a single step

## Search Example

Find references to formulations comprising the substance having CAS Registry Number 666741-24-8.

## FAMILY structure search in REGISTRY to find formulations of a substance

1. Find the substance of interest and display the REGISTRY record
2. Click the RN link and choose *Structure search > Family search – Free sample*
3. Review answers in **DISPLAY SCAN** mode
4. Click the RN link and choose *Structure search > Family search – Full file*
5. Review answers in **DISPLAY SCAN** mode

# Search the substance in REGISTRY and display the record

=> FILE REGISTRY

=> S 666741-24-8

L1 1 666741-24-8

=> D

RN 666741-24-8 REGISTRY

ED Entered STN: 23 Mar 2004

CN 1,2-Benzenedicarboxamide, N1-[4-[4,5-dihydro-3-(1H-1,2,4-triazol-1-yl)-5-(trifluoromethyl)-5-isoxazolyl]-2-methylphenyl]-3-iodo-N2-(1-methylethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

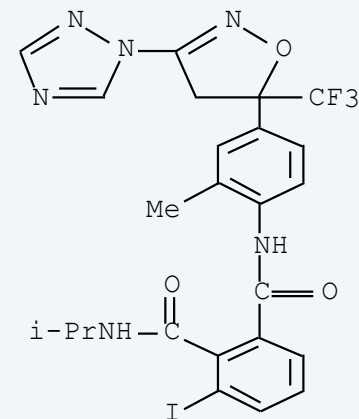
MF C24 H22 F3 I N6 O3

CI COM

SR CA

LC STN Files: [CA](#), [CAPLUS](#), [USPATFULL](#)

Hit RNs are highlighted in red and hyperlinked in the STN Express display.



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

# Select *Structure search* > *Family search* – *Free sample*

L1 ANSWER 1 OF 1 REGISTRY

RN 666741-24-8 REGISTRY

ED Entered S You have selected RN 666741-24-8

CN 1,2-Benzotriazol-1-yl

methylethyl

methylethyl

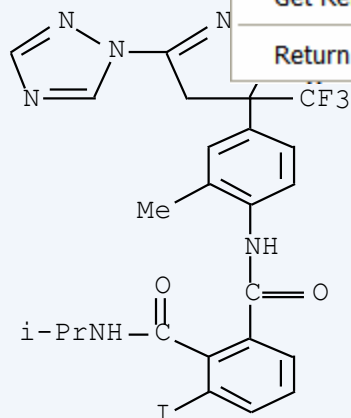
methylethyl

MF C24 H22 E

CI COM

SR CA

LC STN Files



- Get REGISTRY data ▶
- Get catalog data ▶
- Get regulatory data ▶
- Get MSDS data ▶
- Get spectra ▶
- Get property data ▶
- Structure search ▶**
- Get Related Polymers
- Get Related Sequences ▶
- Return to last file

Click a hyperlinked RN to  
access the Search menu.

- Exact search - Free sample
- Exact search - Full file
- Family search - Free sample**
- Family search - Full file



# STN Express executes a FAMILY SAMPLE search automatically

```
=> FILE REG
```

```
=> STR 666741-24-8
```

```
:END
```

```
L2 STRUCTURE CREATED
```

```
=> S L2 FAM SAM
```

```
SAMPLE SEARCH INITIATED 11:20:51
```

```
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE
```

```
100.0% PROCESSED 2 ITERATIONS 2 ANSWERS
```

```
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
```

```
L3 2 SEA FAM SAM L2
```

```
=> D SCAN
```

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

STN automatically:

- creates the structure
- runs the SAMPLE search
- enters the D SCAN command



# STN Express executes a FAMILY FULL file search

```
=> FILE REG
=> STR 666741-24-8
:END
L4 STRUCTURE CREATED
=> S L4 FAM FUL
FULL SEARCH INITIATED 11:24:12
FULL SCREEN SEARCH COMPLETED - 23 TO ITERATE
100.0% PROCESSED 23 ITERATIONS 23 ANSWERS
L5 23 SEA FAM FUL L4
=> D SCAN
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1): 1
```

STN automatically:

- creates the structure
- runs the FULL search
- enters the D SCAN command

# Continue to SCAN the answers

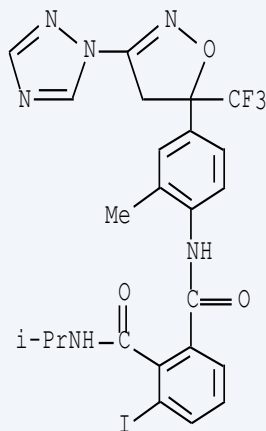
L5 23 ANSWERS REGISTRY

IN 1,2-Benzenedicarboxamide, N1-[4-[4,5-dihydro-3-(1H-1,2,4-triazol-1-yl)-5-(trifluoromethyl)-5-isoxazolyl]-2-methylphenyl]-3-iodo-N2-(1-methylethyl)-, comp. with N-[[[3,5-dichloro-4-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]phenyl]amino]carbonyl]-2,6-difluorobenzamide (1:1) (9CI)

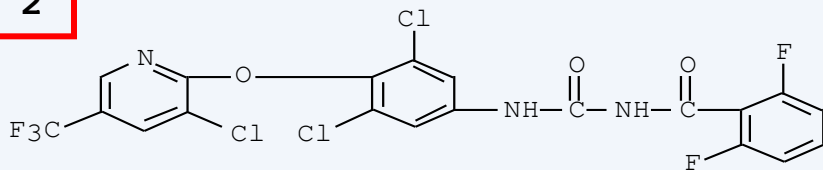
MF C24 H22 F3 I N6 O3 . C20 H9 Cl3 F5 N3 O3

CI MXS

CM 1



CM 2



The final answer set contains all substances in REGISTRY that contain the structure, including single component and multicomponent registrations.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):22

# Locate references in CAPLUS

=> FILE CAPLUS

=> S L5

L6                    3 L5

=> D IBIB ABS HITSTR 1-3

L6    ANSWER 2 OF 3    CAPLUS

ACCESSION NUMBER:            2005:1073977    CAPLUS    [Full-text](#)

DOCUMENT NUMBER:            143:361659

TITLE:                        Compositions containing benzanilides and  
their application as pesticides

INVENTOR(S) :                Takii, Shinji

PATENT ASSIGNEE(S) :        Nissan Chemical Industries, Ltd., Japan

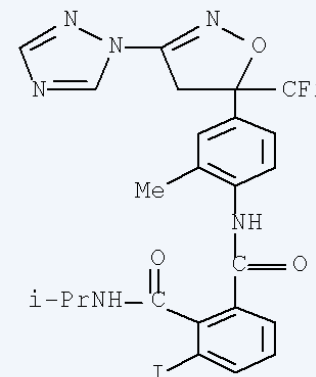
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
<a href="#">JP 2005272443</a>	A	20051006	<a href="#">JP 2005-38603</a>	20050216
PRAI <a href="#">JP 2004-46912</a>	A	20040223		
OS <a href="#">MARPAT 143:361659</a>				

# Many formulations are indexed as derivatives of a known compound

IT 188425-85-6D, Nicobifen, mixts. with benzanilides 189278-12-4D,  
 220899-03-6D, Metrafenone, mixts. with benzanilides 223580-51-6D,  
 Tiadinil, mixts. with benzanilides 229977-93-9D, Fluacrypyrim, mixts.  
 with benzanilides 248593-16-0D, Orysastrobin, mixts. with benzanilides  
 283594-90-1D, Spiromesifen, mixts. with benzanilides 361377-29-9D,  
 Fluoxastrobin, mixts. with benzanilides 380221-54-5D, Acypetacs zinc,  
 mixts. with benzanilides 413615-35-7D, Benthiavalicarb, mixts. with  
 benzanilides 666741-24-8D, mixts. containing 866187-83-9  
 RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL  
 (Biological study); USES (Uses)  
 (synergistic insecticides, acaricides, nematocides, fungicides, and  
 antibacterial agents contg. benzanilide derivs.)  
 RN 666741-24-8 CAPLUS  
 CN 1,2-Benzenedicarboxamide, N1-[4-[4,5-dihydro-3-  
 (1H-1,2,4-triazol-1-yl)-5-(trifluoromethyl)-5-isoxazolyl]  
 -2-methylphenyl]-3-iodo-N2-(1-methylethyl)- (CA INDEX NAME)

A Registry Number followed by the letter "D" indicates a derivative of the substance having the Registry Number.



# Many formulations are indexed as multicomponent substances

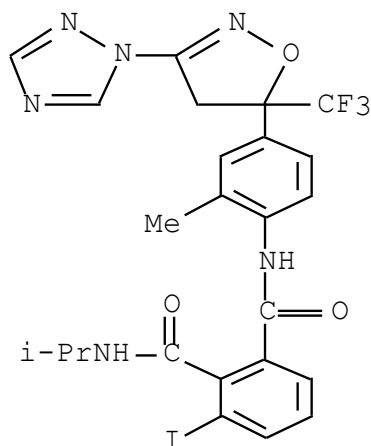
RN 866187-83-9 CAPLUS

CN 1,2-Benzenedicarboxamide, N1-[4-[4,5-dihydro-3-(1H-1,2,4-triazol-1-yl)-5-(trifluoromethyl)-5-isoxazolyl]-2-methylphenyl]-3-iodo-N2-(1-methylethyl)-, **compd. with** 4-bromo-2-(4-chlorophenyl)-1-(ethoxymethyl)-5-(trifluoromethyl)-1H-pyrrole-3-carbonitrile (1:1)  
(CA INDEX NAME)

CM 1

CRN 666741-24-8

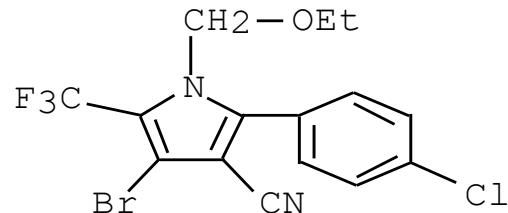
CMF C24 H22 F3 I N6 O3



CM 2

CRN 122453-73-0

CMF C15 H11 Br Cl F3 N2 O



# Search Component Registry Numbers (CRN) to find formulations

- A Component Registry Number is a RN assigned to each component of a multicomponent registration
- A CRN search retrieves multicomponent substances that contain the RN searched
- A CRN search does NOT retrieve single components, isomers, isotopically labeled, or charged species

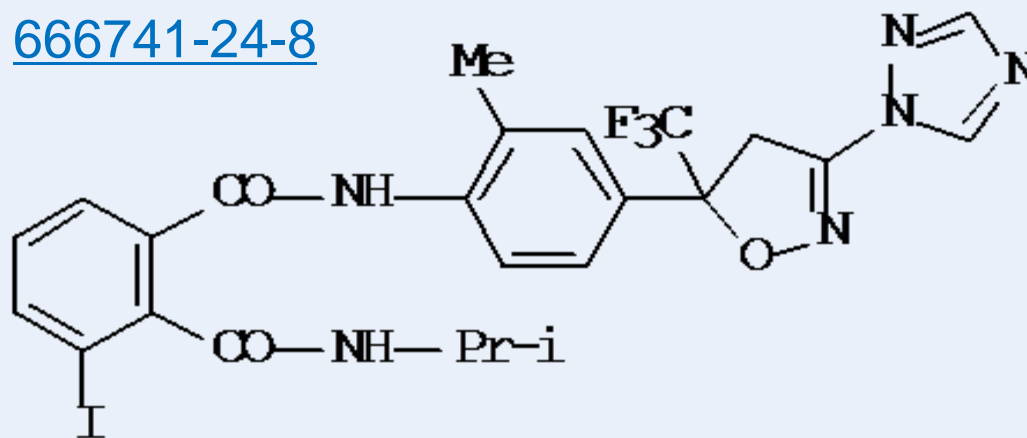


# Recall the question

## Search Example

Find references to formulations comprising the following compound:

RN [666741-24-8](#)



# Search strategy

1. Search the substance of interest and display the Registry Number (RN)
2. Search the Registry Number in the Component Registry Number (CRN) field
3. Review answers in **DISPLAY SCAN** mode

# Search the Registry Number in the Component Registry Number field (CRN)

=> FILE REG; S 666741-24-8/CRN

L1 22 666741-24-8/CRN

=> D SCAN

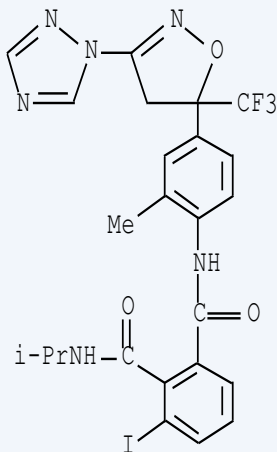
L1 22 ANSWERS REGISTRY

IN 5-Oxa-2,8-dithia-4,7,9-triazol-1-yl)-5-(trifluoromethyl)-5-isoxazolyl]-2-methylphenyl]-3-iodo-N2-(1-methylethyl)-1,2-benzenedicarboxamide (9CI)

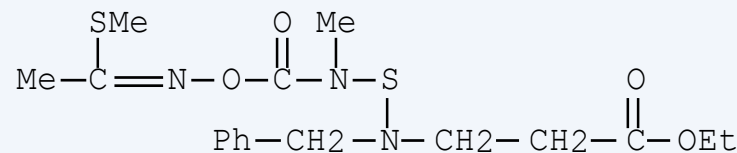
MF C24 H22 F3 I N6 O3 . C17 H25 N3 O4 S2

CI MXS

CM 1



CM 2



- The CRN search retrieves one less answer than the FAMILY structure search.
- The original substance is not retrieved.

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

# Comparison of REGISTRY options

## FAMILY Structure Search

- Retrieves salts, multicomponent registrations, and single components
- Retrieves stereoisomers, labeled, and charged species
- Broad search
- Can use STN Express Wizard
- Search any member of the family

## CRN Search

- Retrieves salts and multicomponent registrations
- Does not retrieve stereoisomers, isotopically labeled, or charged species
- Search is not as broad as FAM structure search
- Command line search
- Need to search the parent substance

## Search Example:

1. A pharmaceutical composition comprising tetrodotoxin in an outwardly solid form suitable for oral ingestion.
2. The pharmaceutical composition of claim 1, in which the tetrodotoxin is present in the form of a solvate.
3. The pharmaceutical composition of claim 1 that is a solid formulation.
4. The pharmaceutical composition of claim 1 in which the tetrodotoxin is in the form of a salt.
5. The pharmaceutical composition of claim 1 that is in the form of a tablet, a chewable tablet, a capsule, a drop or a dragee.
6. The pharmaceutical composition of any one of claims 1-5 that is formulated as an immediate release formulation.
7. The pharmaceutical composition of any one of claims 1-5 that is formulated as a controlled release formulation.

Tetrodotoxin, a neurotoxin, is the active ingredient in a Haitian witch doctor's potion for making a zombi.

## Search Example:

8. The pharmaceutical composition according to claim 1, further comprising lactose, or hydrates of lactose.
9. The pharmaceutical composition according to claim 1, further comprising croscarmellose.
10. The pharmaceutical composition of claim 9, further comprising a salt of an organic acid.
11. The pharmaceutical composition according to claim 1, further comprising a dibasic phosphate salt.
12. The pharmaceutical composition according to claim 1, further comprising microcrystalline cellulose.
13. The pharmaceutical composition according to claim 1, further comprising colloidal silicon dioxide.
14. The pharmaceutical composition according to claim 1, further comprising polyethylene glycol.

# CAplus formulation search strategy

1. Find the RN and synonyms for tetrodotoxin in REGISTRY
2. Run FAMILY structure search
3. Search tetrodotoxin synonyms and RNs in HCAplus
4. Refine with pharmaceutical section codes and keywords
5. Browse answers for relevancy
6. FOCUS answers
7. Display final results

# EXPAND and SEARCH in the chemical name field

```

=> FILE REG
=> E TETRODOTOXIN/CN; S TETRODOTOXIN/CN; D
L1          1 TETRODOTOXIN/CN

L1  ANSWER 1 OF 1  REGISTRY
RN  4368-28-9  REGISTRY
CN  5,9:7,10a-Dimethano-10aH-[1,3]dioxocino[6,5-d]pyrimidine-
    4,7,10,11,12-pentol, 2-amino-1,4,4a,5,9,10-hexahydro-12-
    (hydroxymethyl)-, (4R,4aR,5R,7S,9S,10S,10aR,11S,12S)- (CA
    INDEX NAME)
CN  Tetrodotoxin (8CI)
CN  (-)-Tetrodotoxin
● ● ●
CN  Araregai toxin
CN  Babylonia japonica toxin 1
CN  BJT 1
CN  Maculotoxin
CN  Spheroidine
CN  Tarichatoxin
● ● ●
ES  STEREOSEARCH

```

Since tetrodotoxin has stereochemistry, run a Family structure search.



# Run a FAMILY structure search to find substances containing tetrodotoxin

L1 ANSWER 1 OF 1 REGISTRY  
 RN [4368-28-9](#) REGISTRY  
 ED Entered You have selected RN 4368-28-9  
 CN 5,9:7,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100  
 (hydroxy) INDEX NA  
 CN **Tetrodo**  
 CN (-)-Tet  
 ● ● ●  
 CN Ararega  
 CN Babylon  
 CN BJT 1  
 CN Maculotoxin  
 CN Spheroidine  
 CN Tarichatoxin  
 CN Tetrodotoxin  
 CN  
 DR  
 MF  
 CI

Get REGISTRY data ▶  
 Get catalog data ▶  
 Get regulatory data ▶  
 Get MSDS data ▶  
 Get spectra ▶  
 Get property data ▶  
 Structure search ▶  
 Get Related Polymers  
 Get Related Sequences ▶  
 Return to last file

Exact search - Free sample  
 Exact search - Full file  
 Family search - Free sample  
 Family search - Full file

Click the RN link and run the FAMILY SAMPLE search first, and then run the FAMILY FULL file search.

Consider a Substructure search when a comprehensive search of analogs and derivatives of an active ingredient or other components in a formulation is required.

# STN Express runs a FAMILY full search

```
=> STR 4368-28-9
```

```
WARNING. STEREO DATA NOT INCLUDED IN MODEL (NOT SEARCHABLE)
```

```
:END
```

```
L4 STRUCTURE CREATED
```

```
=> S L4 FAM FUL
```

```
L5 158 SEA FAM FUL L4
```

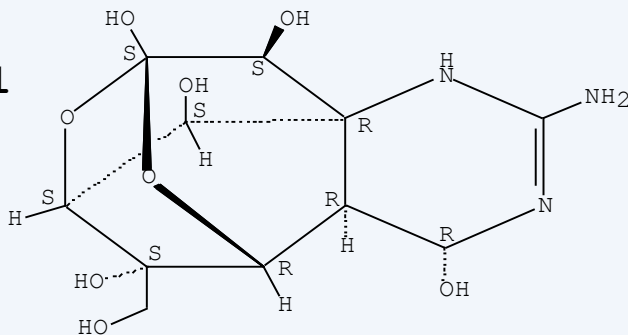
```
=> D SCAN
```

```
L5 158 ANSWERS REGISTRY
```

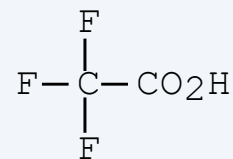
```
IN Tetrodotoxin, mono(trifluoroacetate) (9CI)
```

```
MF C11 H17 N3 O8 . C2 H F3 O2
```

```
CM 1
```



```
CM 2
```



```
Absolute stereochemistry.
```

The wizard runs the FAMILY search and displays results in **D SCAN** mode. 158 substances are found in REGISTRY.

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

# Crossover to HCAplus

```
=> FILE HCAPLUS
```

```
=> S L5 OR TETRODOTOXIN# OR ARAREGAI TOXIN OR BABYLONIA JAPONICA  
TOXIN 1 OR MACULOTOXIN OR SPHEROIDINE OR TARICHATOXIN
```

```
L6      14563 L5 OR TETRODOTOXIN# OR ARAREGAI TOXIN OR BABYLONIA  
        JAPONICA TOXIN 1 OR MACULOTOXIN OR SPHEROIDINE OR  
        TARICHATOXIN
```

A comprehensive search includes RNs from L5 as well as free-text terms. HCAplus is used because the strategy includes many search terms.

## Search Example:

Identify claim terms that are related to formulations.

1. A **pharmaceutical composition** comprising tetrodotoxin in an outwardly **solid form** suitable for **oral ingestion**.
2. The pharmaceutical composition of claim 1, in which the tetrodotoxin is present in the form of a **solvate**.
3. The pharmaceutical composition of claim 1 that is a **solid formulation**.
4. The pharmaceutical composition of claim 1 in which the tetrodotoxin is in the form of a **salt**.
5. The pharmaceutical composition of claim 1 that is in the form of a **tablet**, a **chewable tablet**, a **capsule**, a **drop** or a **dragee**.
6. The pharmaceutical composition of any one of claims 1-5 that is formulated as an **immediate release formulation**.
7. The pharmaceutical composition of any one of claims 1-5 that is formulated as a **controlled release formulation**.

## Search Example:

8. The pharmaceutical composition according to claim 1, further comprising **lactose**, or **hydrates of lactose**.
9. The pharmaceutical composition according to claim 1, further comprising **croscarmellose**.
10. The pharmaceutical composition of claim 9, further comprising a **salt of an organic acid**.
11. The pharmaceutical composition according to claim 1, further comprising a **dibasic phosphate salt**.
12. The pharmaceutical composition according to claim 1, further comprising **microcrystalline cellulose**.
13. The pharmaceutical composition according to claim 1, further comprising **colloidal silicon dioxide**.
14. The pharmaceutical composition according to claim 1, further comprising **polyethylene glycol**.

# Limit the tetrodotoxin search with “formulation” text terms

=> S L6 (L) (FORMULATION OR INGEST? OR ORAL? OR TABLET? OR CAPSULE? OR DROP? OR DRAGEE)

L7 304 L6 (L) (FORMULATION OR INGEST? OR ORAL? OR TABLET? OR CAPSULE? OR DROP? OR DRAGEE)

=> S L6 (L) ((CONTROL? OR SUSTAIN? OR IMMEDIATE?) (W) RELEASE? OR DELIVER? OR PHARMACEUTICAL (W) (PREP? OR COMPOSITION?))

L8 159 L6 (L) ((CONTROL? OR SUSTAIN? OR IMMEDIATE?) (W) RELEASE? OR DELIVER? OR PHARMACEUTICAL (W) (PREP? OR COMPOSITION?))

=> S L6 (L) (LACTOSE? OR 63-42-3 OR CELLULOSE OR 9004-34-6 OR CROSCARMELOSE OR CROSCARMELLOSE OR 74811-65-7 OR COLLOID? SILICON DIOXIDE OR 7631-86-9 OR POLYETHYLENE GLYCOL OR 25322-68-3 OR PHOSPHATE?)

L9 231 L6 (L) (LACTOSE OR 63-42-3 OR CELLULOSE OR 9004-34-6 OR CROSCARMELOSE OR CROSCARMELLOSE OR 74811-65-7 OR COLLOID?)

The LINK (L) operator searches terms that are within the same information unit, e.g., same title or same paragraph.

# Use the CA Section Code thesaurus to identify classifications for pharmaceuticals

```

=> E PHARMACEUTICALS/CC
E#    FREQUENCY    AT    TERM
--    -
E1          0      2    PHARMACEUTICAL ANALYSIS, SYNTHETIC ORGANIC
      COMPOUNDS/CC
E2          0      4    PHARMACEUTICAL CHEMISTRY/CC
E3    683321      4 --> PHARMACEUTICALS/CC
E4          0      1    PHARMACEUTICALS (INCLUDING NUTRIENTS)/CC
...

=> E E3+ALL
E13    683321      --> PHARMACEUTICALS/CC
E14    10175      USE  30 PHARMACEUTICALS, 1963-1966/CC
E15    3053       USE  39 PHARMACEUTICALS, 1962 ONLY/CC
E16    617986     USE  63 PHARMACEUTICALS, 1967 TO PRESENT/CC
***** END *****

```

The Classification Code (CC) field is used to open the thesaurus. Section Codes can be searched in the CC, SC (Section Code), and SX (Cross-reference section) fields.

# Use the CA Section Code thesaurus to identify classifications for pharmaceuticals (cont.)

=> E E16+ALL

E17 7300818 BT1 APPLIED/CC

E18 617986 --> 63 PHARMACEUTICALS, 1967 TO PRESENT/CC

NOTE THIS SECTION INCLUDES DRUG STANDARDS, PHARMACOPEIAS, PHARMACEUTICAL FORMULATIONS, BIOLOGICALS, COMMERCIAL PLANT-DRUG PREPARATIONS, PROSTHETIC MATERIALS, SURGICAL GOODS, LIFE-MAINTAINING DEVICES, RADIOPHARMACEUTICALS, AND PROPERTIES OF PHARMACEUTICALS SUCH AS DEGRADATION, SOLUBILITY, STABILITY, DISSOLUTION, AND BIOAVAILABILITY IN RELATION TO FORMULATION. PHARMACOLOGICAL, METABOLIC, AND STRUCTURE-ACTIVITY RELATIONSHIPS OF DRUGS ARE PLACED IN SECTION 1; ISOLATION OF PLANT CONSTITUENTS WITH NO COMMERCIAL DRUG USE IS COVERED IN SECTION 11; PREPARATION OF DRUGS BY FERMENTATION, IN SECTION 16; SYNTHESIS OF DRUGS, IN THE APPROPRIATE SYNTHETIC  
•••

HNTE SUBJECT WAS COVERED IN BROADER SECTIONS 30 PHARMACEUTICALS, 1963-1966, 39 PHARMACEUTICALS, 1962 ONLY, 17 PHARMACEUTICALS, COSMETICS, AND PERFUMES, 1936-1961, 17 PHARMACEUTICAL CHEMISTRY, 1911-1935, 18 PHARMACEUTICAL CHEMISTRY, 1910 ONLY, AND 17 PHARMACEUTICAL CHEMISTRY, 1906-1909. •••

E21 52107 OLD 17 PHARMACEUTICALS, COSMETICS, AND PERFUMES, 1936-1961/CC

E34 105987 NT1 64 PHARMACEUTICAL ANALYSIS, 1967 TO PRESENT/CC



# Combine the formulation searches and refine with CA Section Codes

```
=> S L7-L9
```

```
L10          656 (L7 OR L8 OR L9)
```

```
=> S L10 AND (63 OR 64 OR PHARM?)/SC,SX
```

```
L11          166 L10 AND (63 OR 64 OR PHARM?)/SC,SX
```

This further limitation to the pharmaceutical sections of CA is optional, but helps to focus the answer set, eliminating references that mention, but are not primarily directed to pharmaceutical formulations of tetrodotoxin.

# Scan answer titles and hit indexing

```
=> D L11 SCAN TI ST HITIND
```

```
L11 166 ANSWERS HCAPLUS
```

```
TI Drug abstaining formulation and its
```

```
ST drug dependence abstinence formulati
```

```
IT 4368-28-9, Tetrodotoxin
```

```
RL: PKT (Pharmacokinetics); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)
```

```
(drug abstaining formulation and its prepn.)
```

```
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5
```

```
L11 166 ANSWERS HCAPLUS
```

```
TI Solid orally ingestible formulations of tetrodotoxin
```

```
ST tetrodotoxin oral formulation tablet
```

```
IT 4368-28-9D, Tetrodotoxin, analogs
```

```
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(solid orally ingestible formulations of tetrodotoxin)
```

You can limit the **D SCAN** command to any field which could be included in the display, such as **TI, ST, IND.**

# Relevance rank answer set and display most relevant answers

=> FOCUS L11

L12 166 FOCUS L11 1-

=> D L12 BIB ABS HITIND 1-10

AN 2008:1494341 HCAPLUS

TI **Pharmaceutical composition**

from swellfish as anti-addictive and analgesic medicine

IN Wang, Kaiye

PA Shanghai Yinian Biotechnology Co., Ltd., Peop. Rep. China

SO Faming Zhuanli Shenqing, 26 pp. CODEN: CNXXEV

DT Patent

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
CN 101317846	A	20081210	CN 2008-10127045	20080618

CC **63-6 (Pharmaceuticals)**

Section cross-reference(s): 1

IT Freeze-dried drug **delivery** systems

**Pharmaceutical** injections

(freeze-dried injectable drug delivery systems;

**pharmaceutical composition** containing **tetrodotoxin**

**FOCUS** arranges the answers in relevance ranked order. The first answer is the patent application we searched, followed by other relevant references.

# D BIB ABS HITIND for the final results

AN 2003:950856 HCAPLUS  
 DN 140:19848  
 TI **Formulation** containing **tetrodotoxin** for abstinence and analgesic administered through respiratory tract  
 IN Pan, Xinfu; Liu, Zhuguo; Huang, Zhiqiang; Pan, Song  
 PA Peop. Rep. China

•••

PATENT NO.	KIND	DATE	APPL NO.	INT. CL. CLASS.
-----	----	-----	---	---
WO 2003099301	A1	20031204	WO 2003-CN370	20030520

All the identified names from the search recall records.

AB The present invention relates to **formulation** containing **tetrodotoxin** for abstinence and analgesic which is administered through respiratory tract, said **formulation** uses **tetrodotoxin** citrate or **tetrodotoxin** acetate as raw material, is made into aerosol, spray or gasoloid formulation by conventional process. The inventive **formulation** which is administered through ...

CC **63-6 (Pharmaceuticals)**

Section cross-reference(s): **64**

IT Drug **delivery** systems

(aerosols, inhalants; **formulation** containing **tetrodotoxin**)

# Summary

- Formulation compositions are registered as multicomponent substances in REGISTRY
- Search formulations in REGISTRY via
  - FAMILY structure search
  - Component Registry Number search
- Formulations are indexed in CAplus as
  - Derivatives of known substances
  - RNs of multicomponent substances
- Search formulations in CAplus via RN crossover and free text search