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®
• Finding formulations in CAS REGISTRY℠
• Finding formulations in CAtplus℠
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
- CAB A
- 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® of multicomponent substances
    IT 179465-88-4, Y-ART-3 (pentagalloyl glucose, H sulfide, sodium)

• In REGISTRY, formulations are captured as multicomponent substances
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-(2,2-dichloroethenyl)-2,2-dimethyl-, (R)-cyano(3-phenoxyphenyl)methyl ester, (1S,3S)-rel
(CA INDEX NAME)
FS STEREOSEARCH
MF C22 H19 Cl2 N O3
CI COM
LC STN Files: AGRICOLA, ANABSTR, CASREACT, CBNB, CHEMCATS, CHEMLIST, CIN, CSNB, DDFU, DETHERM*, DRUGU, IFICDB, IFIPAT, IFIUDB, MSDS-OHS, PIRA, REAXYSFILE*, RTECS*, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL

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

- 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.
**REGISTRY record for multicomponent substance from US 20110256200**

- 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.

<table>
<thead>
<tr>
<th>RN</th>
<th>1246612-09-8 REGISTRY</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN</td>
<td>Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-trifluoro-1-propen-1-yl] -2,2-dimethyl-, (2-methyl[1,1'-biphenyl]-3-yl)methyl ester, (1R,3R)-rel-, mixt. with (3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate (CA INDEX NAME)</td>
</tr>
<tr>
<td>MF</td>
<td>C23 H22 Cl F3 O2 . C21 H20 Cl2 O3</td>
</tr>
<tr>
<td>CI</td>
<td>MXS</td>
</tr>
<tr>
<td>SR</td>
<td>CA</td>
</tr>
<tr>
<td>LC</td>
<td>STN Files: CA, CAPLUS, TOSCA</td>
</tr>
</tbody>
</table>

- CM 1
- CRN 82657-04-3
- CMF C23 H22 Cl F3 O2

- CM 2
- CRN 52645-53-1
- CMF C21 H20 Cl2 O3

Chemical structures of the components:
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

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
Select **Structure search > Family search** – Free sample

<table>
<thead>
<tr>
<th>L1</th>
<th>ANSWER 1 OF 1</th>
<th>REGISTRY</th>
</tr>
</thead>
<tbody>
<tr>
<td>RN</td>
<td>666741-24-8</td>
<td>REGISTRY</td>
</tr>
<tr>
<td>ED</td>
<td>Entered STN: 23 Mar 2004</td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>1,2-Benzenedicarboxamide, N1-triazol-1-yl-methylphenylmethylethyl-3-methylphenyl-5-(trifluoromethyl)-5-isoxazolyl-2-methylphenyl-3-iodo-N2-(1-methylethyl) (CA INDEX NAME)</td>
<td></td>
</tr>
<tr>
<td>MF</td>
<td>C24 H22 F3 I N6 O3</td>
<td></td>
</tr>
<tr>
<td>CI</td>
<td>COM</td>
<td></td>
</tr>
<tr>
<td>SR</td>
<td>CA</td>
<td></td>
</tr>
<tr>
<td>LC</td>
<td>STN Files: CA, CAPLUS, US</td>
<td></td>
</tr>
</tbody>
</table>

Click a hyperlinked RN to access the Search menu.
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
Select *Structure search* > *FAMILY search* – Full file

<table>
<thead>
<tr>
<th>L1</th>
<th>ANSWER 1 OF 1 REGISTRY</th>
</tr>
</thead>
<tbody>
<tr>
<td>RN</td>
<td>666741-24-8 REGISTRY</td>
</tr>
<tr>
<td>ED</td>
<td>Entered STN: 23 Mar 2004</td>
</tr>
<tr>
<td>CN</td>
<td>1,2-Benzenedicarboxamide, N1-triazol-1-yl-4-[4-(1-H-1,2,4-triazolyl)-5-(trifluoromethyl)-5-isoxazolyl]-2-methylphenyl-methylethyl-2</td>
</tr>
<tr>
<td>MF</td>
<td>C24 H22 F3 I N6 O3</td>
</tr>
<tr>
<td>CI</td>
<td>COM</td>
</tr>
<tr>
<td>SR</td>
<td>CA</td>
</tr>
<tr>
<td>LC</td>
<td>STN Files</td>
</tr>
</tbody>
</table>

![Molecule diagram]

Click the RN again to choose the Full file search from the displayed menu.
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
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)-, compd. 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

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

CM 2

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:

<table>
<thead>
<tr>
<th>PATENT NO.</th>
<th>KIND</th>
<th>DATE</th>
<th>APPLICATION NO.</th>
<th>DATE</th>
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<tbody>
<tr>
<td>JP 2005272443</td>
<td>A</td>
<td>20051006</td>
<td>JP 2005-38603</td>
<td>20050216</td>
</tr>
<tr>
<td>PRAI JP 2004-46912</td>
<td>A</td>
<td>20040223</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OS MARPAT 143:361659</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Many formulations are indexed as derivatives of a known compound.

<table>
<thead>
<tr>
<th>IT</th>
<th>188425-85-6D, Nicobifen, mixts. with benzanilides</th>
<th>189278-12-4D,</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>220899-03-6D, Metrafenone, mixts. with benzanilides</td>
<td>223580-51-6D,</td>
</tr>
<tr>
<td></td>
<td>Tiadinil, mixts. with benzanilides</td>
<td>229977-93-9D, Fluacrypyrim, mixts. with benzanilides</td>
</tr>
<tr>
<td></td>
<td>248593-16-0D, Orysastrobin, mixts. with benzanilides</td>
<td>283594-90-1D, Spiromesifen, mixts. with benzanilides</td>
</tr>
<tr>
<td></td>
<td>220899-03-6D, Metrafenone, mixts. with benzanilides</td>
<td>361377-29-9D, Fluacrypyrim, mixts. with benzanilides</td>
</tr>
<tr>
<td></td>
<td>223580-51-6D, Metrafenone, mixts. with benzanilides</td>
<td>380221-54-5D, Acypetacs zinc, mixts. with benzanilides</td>
</tr>
<tr>
<td></td>
<td>Tiadinil, mixts. with benzanilides</td>
<td>413615-35-7D, Benthiavalicarb, mixts. with benzanilides</td>
</tr>
<tr>
<td></td>
<td>666741-24-8D, mixts. containing</td>
<td>866187-83-9</td>
</tr>
<tr>
<td>RL:</td>
<td>AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(synergistic insecticides, acaricides, nematocides, fungicides, and antibacterial agents contg. benzanilide derivs.)</td>
<td></td>
</tr>
</tbody>
</table>

| 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-isoaxazolyl]-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

i-PrNH
Me
CF3
O

CH2-OEt
F3C
Br
NC
Cl
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)

```plaintext
=> 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

• 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 croscarmelose.

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
   ● ● ●
FS  STEREOSEARCH

Since tetrodotoxin has stereochemistry, run a Family structure search.
**Run a FAMILY structure search to find substances containing tetrodotoxin**

<table>
<thead>
<tr>
<th>L1</th>
<th>ANSWER 1 OF 1</th>
<th>REGISTRY</th>
</tr>
</thead>
<tbody>
<tr>
<td>RN</td>
<td>4368-28-9</td>
<td>REGISTRY</td>
</tr>
<tr>
<td>ED</td>
<td>Entered STN:</td>
<td>16 Nov 1984</td>
</tr>
<tr>
<td>CN</td>
<td>5,9:7,10,4,7,10,9,12 (hydroxymethyl)</td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>Tetrodotoxin</td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>(-)-Tetrodotoxin</td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>Araregai toxin</td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>Babylonia japonica toxin 1</td>
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</tr>
<tr>
<td>CN</td>
<td>BJT 1</td>
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</tr>
<tr>
<td>CN</td>
<td>Maculotoxin</td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>Spheroidine</td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>Tarichatoxin</td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>Tetrodotoxine</td>
<td></td>
</tr>
</tbody>
</table>

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 => D SCAN
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

Absolute stereochemistry.

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

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

=> FILE HCAPPLUS

=> 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:

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**.

Identify claim terms that are related to formulations.
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 croscarmelose.

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 CROSCARMELLOSE 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 CROSCARMELLOSE 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

<table>
<thead>
<tr>
<th>E#</th>
<th>FREQUENCY</th>
<th>AT</th>
<th>TERM</th>
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<tr>
<td>E1</td>
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<td>2</td>
<td>PHARMACEUTICAL ANALYSIS, SYNTHETIC ORGANIC COMPOUNDS/CC</td>
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<tr>
<td>E2</td>
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<td>PHARMACEUTICAL CHEMISTRY/CC</td>
</tr>
<tr>
<td>E3</td>
<td>683321</td>
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<td>PHARMACEUTICALS/CC</td>
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<tr>
<td>E4</td>
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<td>1</td>
<td>PHARMACEUTICALS (INCLUDING NUTRIENTS)/CC</td>
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=> 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.)

<table>
<thead>
<tr>
<th>Code</th>
<th>Number</th>
<th>BT1</th>
<th>Description</th>
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<tbody>
<tr>
<td>E17</td>
<td>7300818</td>
<td>BT1</td>
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<tr>
<td>E18</td>
<td>617986</td>
<td>--&gt;</td>
<td>63 PHARMACEUTICALS, 1967 TO PRESENT/CC</td>
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<tr>
<td>E21</td>
<td>52107</td>
<td>OLD</td>
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<td>E34</td>
<td>105987</td>
<td>NT1</td>
<td>64 PHARMACEUTICAL ANALYSIS, 1967 TO PRESENT/CC</td>
</tr>
</tbody>
</table>
Combine the formulation searches and refine with CA Section Codes

\[ \Rightarrow S\ L7-L9 \]

\[ L10 \quad 656 \ (L7 \ OR \ L8 \ OR \ L9) \]

\[ \Rightarrow S\ L10 \ AND \ (63 \ OR \ 64 \ OR \ PHARM?) /SC,SX \]

\[ L11 \quad 166 \ L10 \ AND \ (63 \ OR \ 64 \ OR \ PHARM?) /SC,SX \]

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 HCAPPLUS
TI Drug abstaining formulation and its
ST drug dependence abstinence formulation
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 HCAPPLUS
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
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.
**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