

STN[®]

Searching in DWPI Chemistry Resource (DCR)

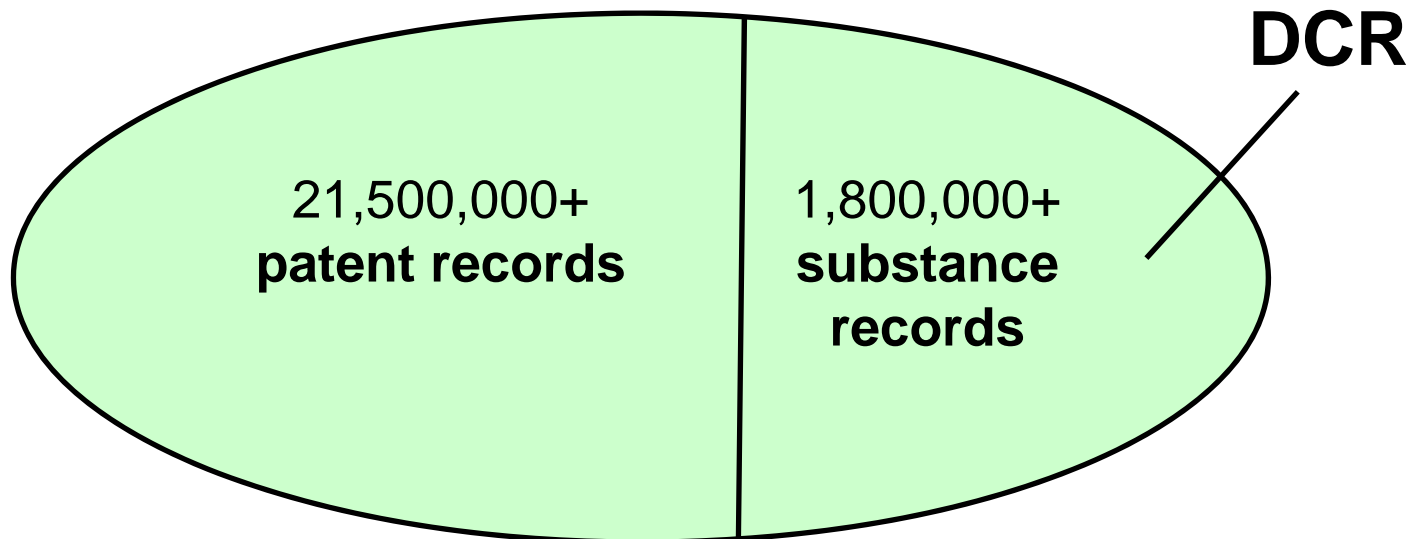
Robert Austin – FIZ Karlsruhe

Agenda

- What is the Derwent World Patents Index[®] (DWPISM) Chemistry Resource (DCR)?
- How to search DCR
- How to refine DCR searches
- How to run a multiframe structure search including DWPI/DCR and CAS files

What is DWPI Chemistry Resource?

- DCR is a chemical structure database covering specific chemical structures indexed in DWPI bibliographic patent records
- An integral part of DWPI on STN since 1999
- Available to all users of DWPI



DWPI Chemistry Resource (DCR)

- For each specific chemical substance a DCR record is created with a unique DCR number
 - Basic compound
 - Salts, isotopes, mixtures, isomers
- Substance records include structure diagrams and substance data, e.g.
 - IUPAC-name, synonyms
 - Molecular formula, molecular weight
- DCR numbers (/DCR) form the connection to DWPI patent records

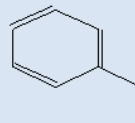
DWPI provides bibliographic patent records and chemical substance records

Bibliographic record

L1 ANSWER 1 OF 1 WPIINDEX COPYRIGHT 2012 THOMSON REUTERS on STN
AN 2005-217884 [23] WPIINDEX
TI Recovery of solvent and styrene from polystyrene solution involves recovering solvent by evaporation and recovering styrene from polystyrene thermally decomposed by solvent
DC A13; A35; E14; J01
IN KANG E; KYO Y; OGURA A
PA (TOSH-N) TOSHIBA PLANT KENSETSU KK
PI JP 2005060471 A 20050310 (200523)* JA 10[2] C08J0011-12
ADT JP 2005060471 A JP 2003-290004 20030808
PRAI JP 2003-290004 20030808
IPCR B01D0001-22 [I,A]; B01D0001-22 [I,C]; B01D0003-00 [I,A]; B01D0003-00
AB JP 2005060471 A UPAB: 20050708
NOVELTY - Solvent from a polystyrene solution obtained by dissolving polystyrene in a solvent is evaporated and the solvent is recovered. The solvent thermally decomposes the separated polystyrene and styrene is recovered.
DETAILED DESCRIPTION - An INDEPENDENT CLAIM is included for equipment for recovering solvent and styrene from a polystyrene solution.
USE - Used for recovering solvent and styrene from a polystyrene solution.
ADVANTAGE - The solvent and styrene are recovered efficiently from the polystyrene solution. The styrene monomer of high purity is obtained with high yield.
DESCRIPTION OF DRAWINGS - The figure shows the thermal decomposition portion of the apparatus used for solvent and styrene recovery. (Drawing includes non-English language text).
Storage tank (1)
Transfer pump (2)
Solvent evaporator (3)
Piping (4)
Condenser (5)
TECH ORGANIC CHEMISTRY - Preferred Process: The cracked gas obtained by thermally decomposing polystyrene is condensed. The oil component is distilled and styrene of high purity is recovered.
FS CPI
MC CPI: A04-C02D; A10-E05C; A10-G01A; E10-J02A1; E10-J02B2; E11-Q01A; J01-A01
IT UPIT 20050708
2113-DIS 2113-PRD; 368-CL 368-PRD

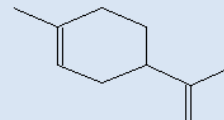
Substance record (DCR)

L2 ANSWER 1 OF 2 WPIINDEX COPYRIGHT 2012 THOMSON REUTERS on STN
ACCESSION NUMBER: DCR-368
DERWENT CHEM.RES.NO.: 368-0-0-0
PREF. CHEMICAL NAME: STYRENE
SYSTEMATIC NAME: Vinyl-benzene
SYNONYM: POLYSTYRENE (MONOMER); STYRENE



MOLECULAR FORMULA: C₈ H₈
MOLECULAR WEIGHT: 104.1512
DERWENT COMPOUND NO.: R00708
DERWENT REGISTRY NO.: 0708

L2 ANSWER 2 OF 2 WPIINDEX COPYRIGHT 2012 THOMSON REUTERS on STN
ACCESSION NUMBER: DCR-2113
DERWENT CHEM.RES.NO.: 2113-0-0-0
PREF. CHEMICAL NAME: LIMONENE
SYSTEMATIC NAME: 4-Isopropenyl-1-methyl-cyclohexene
SYNONYM: (+)-LIMONENE; 1,8-P-MENTHADIENE; CAJEPUTENE; CINENE; DIPENTENE; DL-LIMONENE; EULIMEN; KAUTSCHIN; LIMONENE; MENTHADIENE, 1,8-P-; REFCHOLE

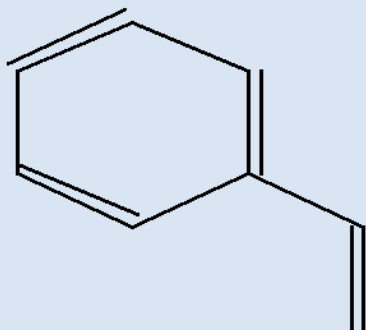


MOLECULAR FORMULA: C₁₀ H₁₆
MOLECULAR WEIGHT: 136.239
DERWENT COMPOUND NO.: R01119
DERWENT REGISTRY NO.: 1119

DCR substance record

L1 ANSWER 1 OF 1 WPINDEX COPYRIGHT 2012 THOMSON REUTERS on STN
ACCESSION NUMBER: **DCR-368**
DERWENT CHEM.RES.NO.: 368-0-0-0
PREF. CHEMICAL NAME: STYRENE
SYSTEMATIC NAME: Vinyl-benzene
SYNONYM: POLYSTYRENE (MONOMER); STYRENE

DCR numbers form the connection to DWPI patent records.



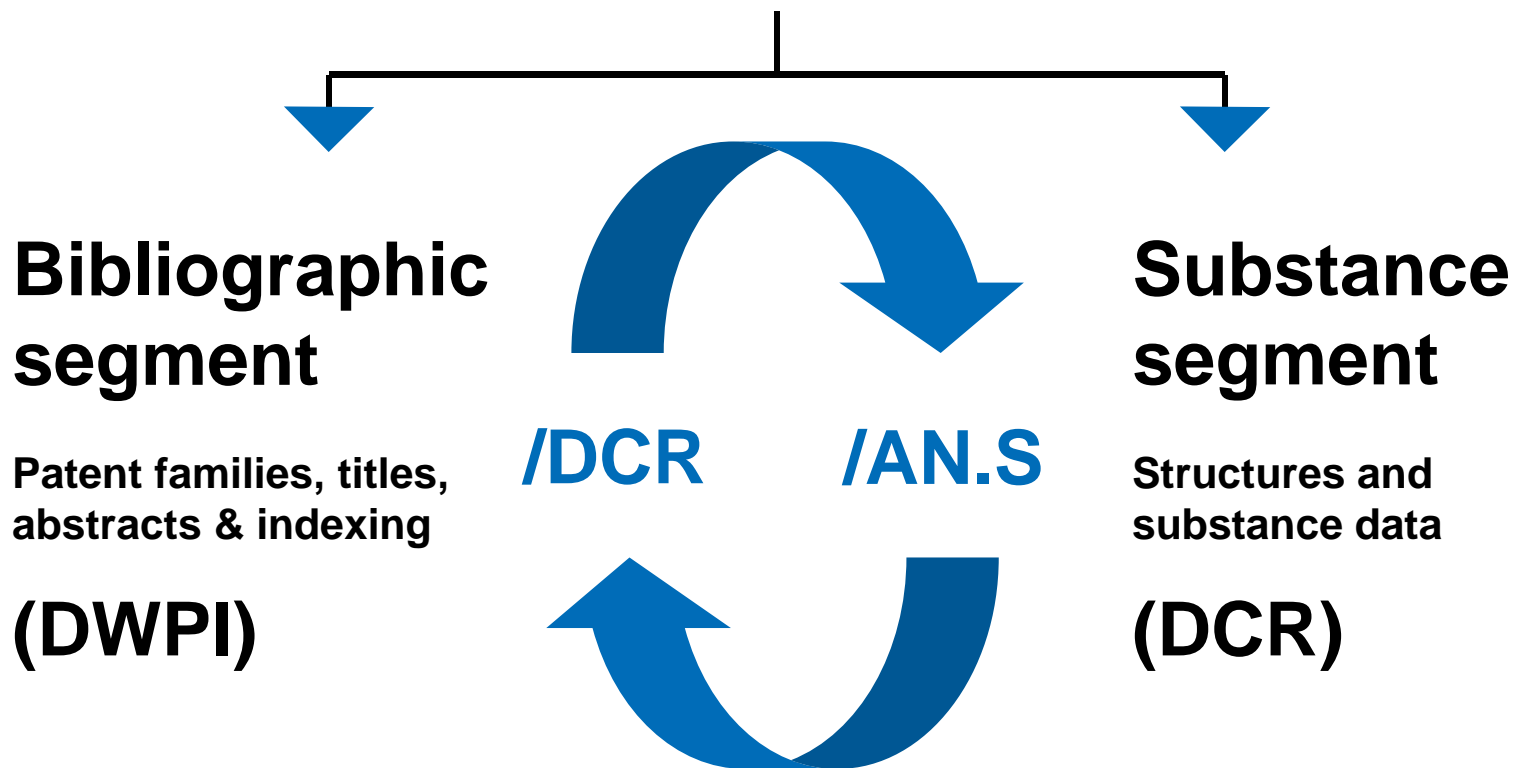
Chemical structures are searchable in the STN standard format.

CROSS REFERENCE: 104475 : SEE ALSO104481 : SEE ALSO
MOLECULAR FORMULA: C8 H8
STANDARD MOL. FORMULA: C8 H8 *1; TOTAL *1; TYPE *1
MOLECULAR WEIGHT: 104.15
DERWENT COMPOUND NO.: R00708
DERWENT REGISTRY NO.: 0708

Substance records may include older numbering systems: DCN and DRN.

DCR numbers form the connection between substance and patent records

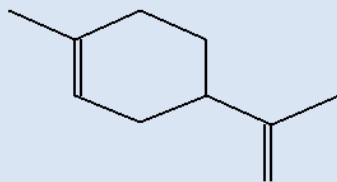
WPINDEX/WPIDS/WPIX



DCR numbers form the connection between substance and patent records (cont.)

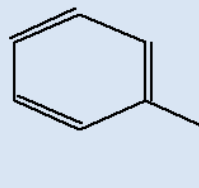
L1 ANSWER 1 OF 1 WPINDEX COPYRIGHT 2012 THOMSON REUTERS on STN
AN 2005-217884 [23] WPINDEX
TI Recovery of solvent and styrene from polystyrene solution involves recovering solvent by evaporation and recovering styrene from polystyrene thermally decomposed by solvent
. . . .
IT UPIT 20050708
2113-DIS 2113-PRD; 368-CL 368-PRD

AN.S DCR-**2113**
DCSE 2113-0-0-0
CN.P LIMONENE
CN.S 4-Isopropenyl-1-methyl-cyclohexene
SY (+)-LIMONENE; 1,8-P-MENTHADIENE;...



MF C10 H16

AN.S DCR-**368**
DCSE 368-0-0-0
CN.P STYRENE
CN.S Vinyl-benzene
SY POLYSTYRENE (MONOMER); STYRENE



MF C8 H8

Searching DCR numbers

- Use the field **/AN.S** to retrieve substance records

=> **S DCR-368/AN.S**

L1 1 DCR-368/AN.S

- Use the field **/DCR** to retrieve patent records

=> **S DCR-368/DCR**

L1 119347 DCR-368/DCR

DCR-368 is the DCR number for styrene.

DCR coverage

- Specific chemical compounds indexed by Thomson Reuters from basic patents in DWPI
- DWPI patents classified in Pharmaceutical (B), agrochemical (C) and/or general chemical (E)
- Comprehensive coverage began in 4/1999*
- Selective coverage for approximately
 - 20,000 substances from 1/1987 to date
 - 2,100 substances from 7/1981 to date

* Except Japanese patents which are covered from 9/2000 onwards.

Which compound types are in DCR?

- Organic and inorganic specific compounds
- Specific peptides up to 15 amino acid residues
- Oligomers up to 8 repeat units
- Natural products including enzymes and proteins
- Chemically modified polysaccharides
- 'Standard' polymers (for chemical indexing)

Note: peptides are searchable in the DCR comment (/CMT) field, using three-letter amino acid symbols.
For example: => [S ALA PHE ARG HIS/CMT](#).

Which compounds are selected for DCR?

- Novel chemical compounds from the claims
- Known chemical compounds from the claims
- The main examples and other representative examples from the description
- Up to 99 chemical compounds are indexed from the DWPI basic patent (system limit)

See also: DWPI CPI Chemical Indexing Guidelines:

http://ip-science.thomsonreuters.com/m/pdfs/mgr/chemical_index_guidelines.pdf

The DWPI ALLSTR display format

- All specific chemical structures indexed for a given DWPI record, may be displayed in one step using the “all structure” (**ALLSTR**) display format
- ALLSTR combines all DCR structures associated with a DWPI record into a single unified display
- Additional text data relating to the structures are displayed as well, including the DCR numbers, and any DCR preferred or systematic chemical names
- ALLSTR is a free-of-charge format for DWPI on STN

Example: ALLSTR format

=> S WO2010028012/PN

L1 1 WO2010028012/PN

=> D AN TI ALLSTR

L1 ANSWER 1 OF 1 WPINDEX COPYRIGHT 2012 THOMSON REUTERS on STN

AN 2010-C71770 [201021] WPINDEX

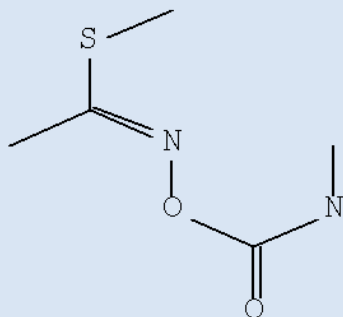
TI Protection of plant from phytophagous nematode for reducing crop production losses comprises applying nematocide mixture consisting of methomyl and neonicotinoids to plant, seed or growing medium

AN.S DCR-72275

CN.P METHOMYL

SDCN R01993

SDRN 1993



...

The ALLSTR display can be combined with any standard DWPI bibliographic displays, e.g., the Thomson Reuters enhanced title (TI).

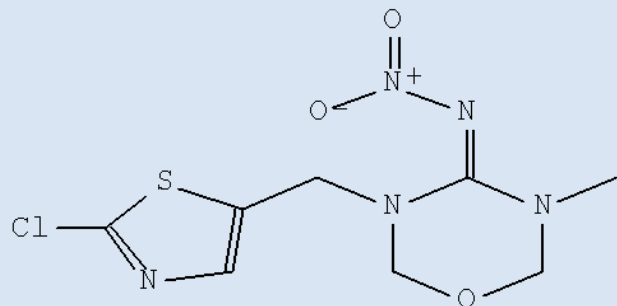
Example: ALLSTR format (cont.)

AN.S DCR-200552

CN.P THIAMETHOXAM

CN.S 3-(2-chloro-1,3-thiazol-5-ylmethyl)-5-methyl-1,3,5-oxadiazinan-4-ylidene(nitro)amine; 3-[(2-chloro-5-thiazolyl)methyl]tetrahydro-5-methyl-N-nitro-4H-1,3,5-oxadiazin-4-imine

SDCN RA0I7Q



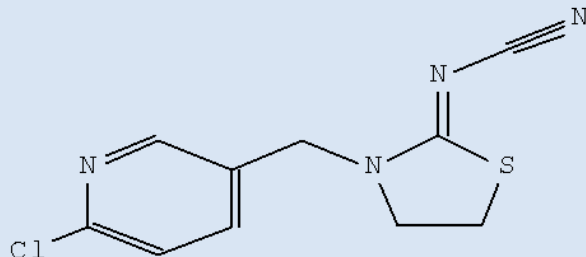
ALLSTR combines all of the DWPI Chemistry Resource (DCR) structures associated with a DWPI bibliographic record, into a single display.

AN.S DCR-226531

CN.P THIACTOPRID

CN.S 3-(6-Chloro-pyridin-3-ylmethyl)-thiazolidin-2-ylidene-cyanamide

SDCN RA0JU9



Agenda

- What is the Derwent World Patents Index (DWPI) Chemistry Resource (DCR)?
- **How to search DCR**
- How to refine DCR searches
- How to run a multiframe structure search including DWPI/DCR and CAS files

Important search options for DCR searching

- Chemical names /CN
- Chemical name segments /CNS
- Molecular formula /MF
- Element information /ELS
- Structure searching
- Classification codes /CC
-

General strategy for searching specific chemical compounds in DWPI

1. Search for substance records in DCR (**Lx**)
2. Display DCR-records in a free format
=> **D SCAN** or => **D TRIAL**
3. Retrieve DWPI patent records (**Ly**)
=> **S Lx/DCR**
4. Display patent records and hit structures with
=> **D Ly FULL HITSTR**

Note: **HITSTR** is a free-of-charge display format in DWPI on STN.

DCR provides several chemical name search and display fields

- A Preferred Name (/CN.P) may be chosen by Thomson, e.g. a generic drug name
- Synonyms (/SY) may be selected for inclusion by Thomson, e.g. trivial names, trade names
- Chemical Name (/CN) field provides one step search/display of all names in CN.P and SY
- A Systematic Chemical Name (/CN.S) may also be available, generated using AutoNom software
- Chemical name segment (/CNS) provides name fragment searching for all CN and CN.S names

Chemical Name Searching (/CN)

Search for the drug pantoprazole

=> FILE WPINDEX

=> E PANTOPRAZOLE/CN 15

```
E1          1      PANTOPENIL/CN
E2          2      PANTOPON/CN
E3          1  --> PANTOPRAZOLE/CN
E4          1      PANTOPRAZOLE HYDROXY SESQUIHYDRATE/CN
E5          1      PANTOPRAZOLE HYDROXY TETRAHYDRATE/CN
E6          1      PANTOPRAZOLE LITHIUM/CN
E7          1      PANTOPRAZOLE MAGNESIUM DIHYDRATE/CN
E8          1      PANTOPRAZOLE MAGNESIUM DIMETHANOLATE/CN
E9          1      PANTOPRAZOLE MAGNESIUM HEMIPENTAHYDRATE/CN
E10         1      PANTOPRAZOLE MAGNESIUM TETRAHYDRATE/CN
E11         1      PANTOPRAZOLE POTASSIUM/CN
E12         1      PANTOPRAZOLE SODIUM/CN
E13         1      PANTOPRAZOLE ZINC/CN
E14         1      PANTOPRIM/CN
E15         1      PANTOS/CN
```

=> S E3-E13

```
L1          11 (PANTOPRAZOLE/CN OR "PANTOPRAZOLE HYDROXY . . . . .")
```

=> D TRIAL 1-11

.

Use EXPAND in the CN field to see which names are indexed.

11 substance records are retrieved for *pantoprazole* and salts (L1).

Review the DCR records in the free-of-charge TRIAL format.

Chemical Name Searching (/CN)

Search for the drug pantoprazole (cont.)

L1 ANSWER 10 OF 11 WPINDEX COPYRIGHT 2010

THOMSON REUTERS on STN

CN.P PANTOPRAZOLE SODIUM

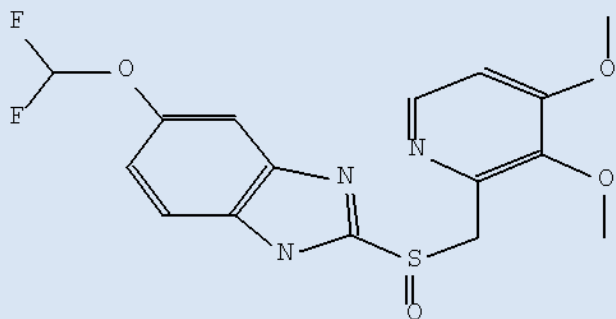
MF C16 H15 F2 N3 O4 S . Na

CM 1

Na

CM 2

The 11 substance records (L1) include both the parent compound and its salts.



L1 ANSWER 11 OF 11 WPINDEX COPYRIGHT 2010

THOMSON REUTERS on STN

CN.P PANTOPRAZOLE

CN.S 5-Difluoromethoxy-2-(3,4-dimethoxy-pyridin-2-ylmethanesulfinyl)-1H-benzoimidazole

MF C16 H15 F2 N3 O4 S

.....

Chemical Name Searching (/CN) (cont.)

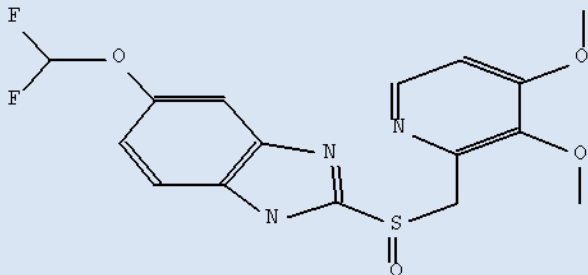
=> S L1/DCR

L2 540 L1/DCR

The 11 pantoprazole substance records (L1) retrieve 540 patent records (L2).

=> D BIB HITSTR

L2 ANSWER 1 OF 540 WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN
AN 2010-G95503 [201043] WPINDEX Full-text
TI Composition useful for treating diabetes, preferably type II diabetes
or reducing hemoglobin Alc in mammal, comprises proton pump inhibitor
and insulin secretagogue
DC A96; B04; B05
IN MEFFORD I N
PA (MEFF-N) MEFFORD SCI LLC
CYC 124
PIA WO 2010068907 A2 20100617 (201043)* EN 79[11]
ADT WO 2010068907 A2 WO 2009-US67733 20091211
PRAI US 2008-121748P 20081211
US 2008-121760P 20081211
AN.S DCR-111250
CN.P PANTOPRAZOLE
CN.S 5-Difluoromethoxy-2-(3,4-dimethoxy-pyridin-2-ylmethanesulfinyl)-1H-
benzoimidazole
SDCN R22667



The hit structure (HITSTR) display is useful for reviewing in-context results following a DCR search.

DCR is a useful source for synonyms

Search for the drug cetirizine

=> **E CETIRIZINE/CN 5**

```
E1          2      CETIPRIN/CN
E2          2      CETIPRIN-NOVUM/CN
E3          1 -->  CETIRIZINE/CN
E4          1      CETIRIZINE DIHYDROCHLORIDE/CN
E5          1      CETIRIZINE HYDROCHLORIDE/CN
```

1. EXPAND on compound name.

=> **S E3**

```
L1          1      CETIRIZINE/CN
```

2. Search for compound name.

=> **SEL CN**

```
E1 THROUGH E8 ASSIGNED
```

3. Select synonym names.

=> **D SEL**

```
E1          2      CETIRIZINE/CN
E2          1      ALERLISIN/CN
E3          1      CIRRUS/CN
E4          1      P-071/CN
E5          1      REACTINE/CN
E6          1      SM-12800/CN
E7          1      VIRLIX/CN
E8          1      ZYRTEC/CN
```

4. Display selected synonyms.

DCR is a useful source for synonyms

Search for the drug cetirizine (cont.)

L1 ANSWER 1 OF 1 WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN

AN.S DCR-90453

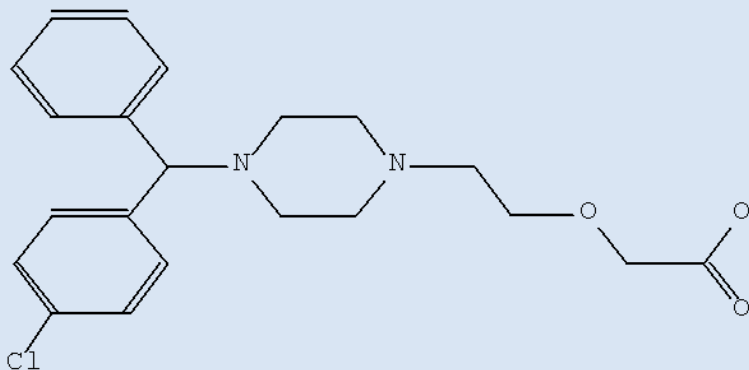
DCSE 90453-0-0-0

CN.P CETIRIZINE

CN.S (2-{4-[(4-Chloro-phenyl)-phenyl-methyl]-piperazin-1-yl}-ethoxy)-acetic acid

SY ALERLISIN; CETIRIZINE; CIRBUS; P-071; REACTINE; SM-12800; VIRLIX; ZYRTEC

ALL display format.



There are eight synonyms (SY) recorded in the DCR record for cetirizine.

MF C21 H25 Cl N2 O3

SMF C21 H25 Cl N2 O3 *1; TOTAL *1; TYPE *1

MW 388.89

SDCN R14937; R16291

DCR is a useful source for synonyms

Search for the drug cetirizine (cont.)

=> S E1-E8/BI

L2 569 (CETIRIZINE/BI OR ALERLISIN/BI OR CIRBUS/BI OR P-071/BI OR
REACTINE/BI OR SM-12800/BI OR VIRLIX/BI OR ZYRTEC/BI)

5. Search the selected synonyms in the Basic Index (/BI) of the target STN database, e.g. DWPI.

=> S CETIRIZIN? OR ALERLISIN OR CIRBUS OR P(W)071 OR P071 OR
REACTINE OR SM(W)12800 OR SM12800 OR VIRLIX OR VIRLEX OR
ZYRTEC OR ZIRTEC

L3 574 CETIRIZIN? OR ALERLISIN OR CIRBUS OR P-071 OR P071 OR
REACTINE OR SM 12800 OR SM12800 OR VIRLIX OR VIRLEX OR
ZYRTEC OR ZIRTEC

Option: create a customized keyword query from the selected synonyms, incorporating truncation and spelling variation.

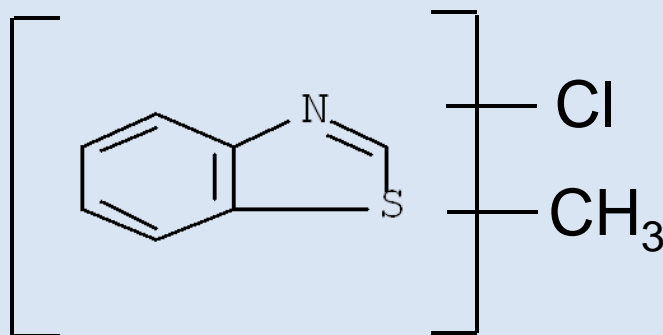
DCR provides several molecular formula (MF) search and display fields

- Molecular Formula (MF)
 - E.g.: C6 H11 Br O2 . Na
- Element Symbol (/ELS)
 - E.g.: => S BR/ELS
- Element Symbol Count (/ELS.CNT)
 - E.g.: => S O 2-3/ELS.CNT

Example: combining name segment (/CNS) and molecular formula (/MF) searching

Search Question:

Search for patent references to benzothiazole substituted with chlorine and methyl



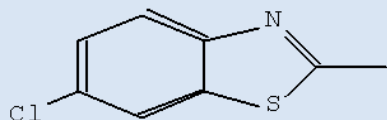
Example: combining name segment (CNS) and molecular formula (MF) searching (cont.)

```
=> S (BENZOTHAZOLE AND METHYL AND CHLORO)/CNS AND C8 H6 CL N S/MF  
L1          3 (BENZOTHAZOLE AND METHYL AND CHLORO)/CNS AND C8 H6 CL N S/MF
```

```
=> D TRIAL 1-3
```

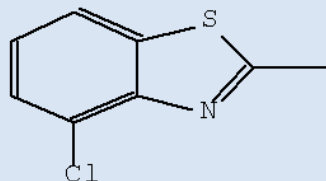
```
L1 ANSWER 1 OF 3 WPINDEX COPYRIGHT 2010  
CN.S 6-Chloro-2-methyl-benzothiazole  
MF C8 H6 Cl N S
```

This search retrieves methyl substituted benzothiazole, with a chloro-substituent at any position.



```
L1 ANSWER 2 OF 3 WPINDEX COPYRIGHT 2010  
CN.S 4-Chloro-2-methyl-benzothiazole  
MF C8 H6 Cl N S
```

THOMSON REUTERS on STN



```
L1 ANSWER 3 OF 3 WPINDEX COPYRIGHT 2010  
CN.S 5-Chloro-2-methyl-benzothiazole  
MF C8 H6 Cl N S . . . .
```

THOMSON REUTERS on STN

DWPI standard structure search options

- Exact search (**EXA**)
 - Retrieves specific compounds and isotopes
- Family search (**FAM**)
 - Retrieves specific compounds, isotopes, salts and mixtures
- Closed Substructure Search (**CSS**)
 - Allows for substitution at defined positions
- Substructure Search (**SSS**)
 - Allows for substitution at any position
- Sample search (**SAM**)
 - Free-of-charge pre-search
- Subset search (**SUBSET**)
 - Structure search on a database subset
- Batch search (**BATCH**)
 - For broad structure queries which may reach system limits

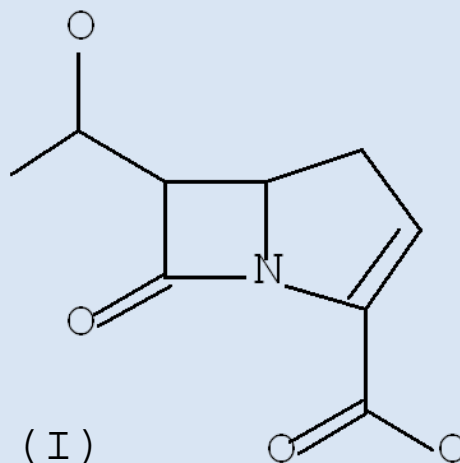
How to run a DWPI structure search

1. Draw & save the structure query in standard format with STN Express (or STN on the Web)
2. Upload the structure query to DWPI on STN
3. Run the structure search, e.g.:
 - a. Sample search => **S L1 SSS SAM**
 - b. Full search => **S L1 SSS FULL**
4. Retrieve DWPI patent records
E.g.: => **S L2/DCR**
5. Display DWPI patent records with DCR hit structures (HITSTR) in-context
E.g.: => **D L3 1- FULLG HITSTR**

DWPI structure search example

Search Question:

Search for DWPI patent references to specific carbapenem derivatives of substructure (I)



Learn more about the basics of structure searching:
<http://www.cas.org/support/stngen/stndoc/structure.html>.

Draw & save the structure query in standard format with STN Express

The image displays two windows from the STN Express software. The top window, titled "STN Express", has a menu bar with "File", "Logon", "Query", "Results", "Setup", "Web", and "Help". The toolbar contains various icons, with the "Prepare Query" icon (a hexagon with a pencil) circled in red. A red arrow points from this icon to the "Structure Drawing" window below. The "Structure Drawing" window is titled "Structure Drawing - [CARBAPENEM.str *Standard*]" and has a menu bar with "File", "Edit", "Draw", "Template!", "QueryDef", "Display", "Preferences!", "Window", and "Help". Its toolbar includes a "Save" icon (a floppy disk) also circled in red. The main drawing area shows the chemical structure of Carbapenem, a bicyclic beta-lactam antibiotic. The structure consists of a fused bicyclic core with a penam nucleus and a dihydrothiazine ring, substituted with a methyl group, a propyl group, and a propionic acid side chain. The bottom of the window features a chemical element palette with buttons for C, H, O, S, N, P, Cl, Br, F, Si, I, and a bond type selector.

Upload the structure query to DWPI on STN

The screenshot shows the STN Online and Results interface. The main window displays the text: `FILE 'WPINDEX' ENTERED AT 15:47`, `COPYRIGHT (C) 2010 THOMSON REUT`, `FILE LAST UPDATED: 15 JUL 2010`, `MOST RECENT UPDATE: 201045`, `DERWENT WORLD PATENTS INDEX, COVERS 1963`, `>>> Now containing more than 1.6 million`, `>>> IPC, ECLA, US National Classification and FI-Terms have been updated with r end of March 2010.`, `No update date (UP) has been created documents, but they can be identified specific update codes (see HELP CLA 1`, `>>> FOR THE LATEST DERWENT WORLD PATENTS STN USER DOCUMENTATION, PLEASE VISIT: http://www.stn-international.com/stn`, `>>> HELP for European Patent Classificati`, `>>> For changes in DWPI see HELP CHANGE`, `>>> New display format ALLSTR available`, `>>> US National Patent Classification the`, and `=>`.

A blue box highlights the 'Q' button in the toolbar, with the text: **Upload the query with the 'Q' button.**

A 'Structure File:' dialog box is open, showing the file name 'CARBAPENEM' and the file type 'Query Files (*.str)'. The 'Open' button is circled in red. The dialog also displays the chemical structure of Carbapenem: CC1(C)NC(=O)C2=C1N(C)C(=O)C2=O.

The status bar at the bottom shows: `Discover! Transcript WPINDEX INS Hold Off Print Off Online 00:09:35`.

Run a sample structure search

```
=>
Uploading C:\. . . .\My Documents\STN Express 8.4\Queries\CARBAPENEM.str
```

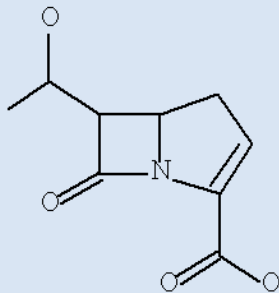
```
L1      STRUCTURE UPLOADED
```

The uploaded structure query (L1).

```
=> D
```

```
L1 HAS NO ANSWERS
```

```
L1      STR
```



Option: display the query (L1), to verify that the Upload was successful.

Structure attributes must be viewed using STN Express query preparation.

```
=> S L1 SSS SAM
```

```
SAMPLE SEARCH INITIATED 15:54:25 FILE '1
SAMPLE SCREEN SEARCH COMPLETED -
```

Run a substructure (SSS) sample (SAM) search using the query (L1).

```
100.0% PROCESSED
```

```
152 ITERATIONS
```

```
50 ANSWERS
```

```
. . . .
```

```
L2      50 SEA SSS SAM L1
```

50 compounds are retrieved (L2).

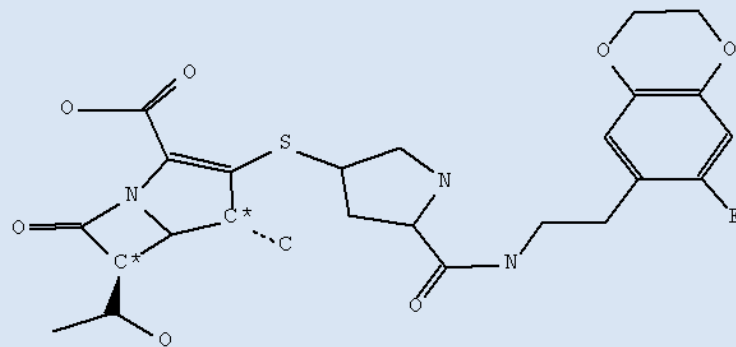
Review some answers using D SCAN

=> D SCAN

L2 50 ANSWERS WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN

CN.S 3-{5-[2-(7-Fluoro-2,3-dihydro-benzo[1,4]dioxin-6-yl)-ethylcarbamoyl]-pyrrolidin-3-ylsulfanyl}-6-(1-hydroxy-ethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid

MF C25 H30 F N3 O7 S



The effectiveness of the query (L1) may be assessed by reviewing some records (L2), e.g. using the free-of-charge SCAN format.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L2 50 ANSWERS WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN

CN.S 3-{5-[2-(7-Fluoro-2,3-dihydro-benzo[1,4]dioxin-6-yl)-ethylcarbamoyl]-pyrrolidin-3-ylsulfanyl}-6-(1-hydroxy-ethyl)-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid

MF C25 H30 F N3 O7 S

. . . .

Run a full structure search

=> S L1 SSS FUL

FULL SEARCH INITIATED 15:55:45 FILE 'WP
FULL SCREEN SEARCH COMPLETED - 1413

Run a substructure (SSS) full-file (FUL) search using the query (L1).

100.0% PROCESSED 1413 ITERATIONS
SEARCH TIME: 00.00.02

1184 ANSWERS

L3 1184 SEA SSS FUL L1

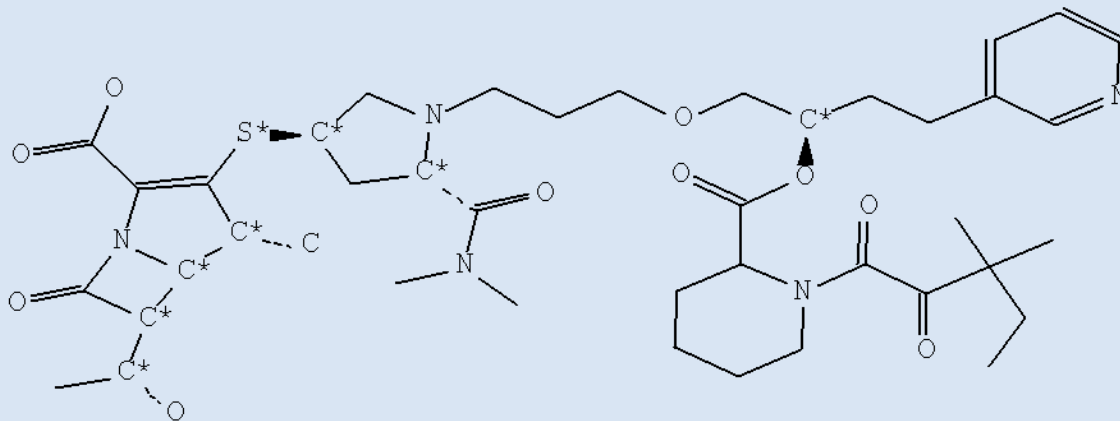
1184 compounds are retrieved (L3).

=> D TRIAL 1-30

...

L3 ANSWER 20 OF 1184 WPINDEX COPYRIGHT 2010
MF C42 H61 N5 O10 S

THOMSON REUTERS on STN



...

Option: review the DCR records retrieved (L3) using, e.g. the free-of-charge TRIAL format.

Retrieve and display DWPI patent records

=> S L3/DCR

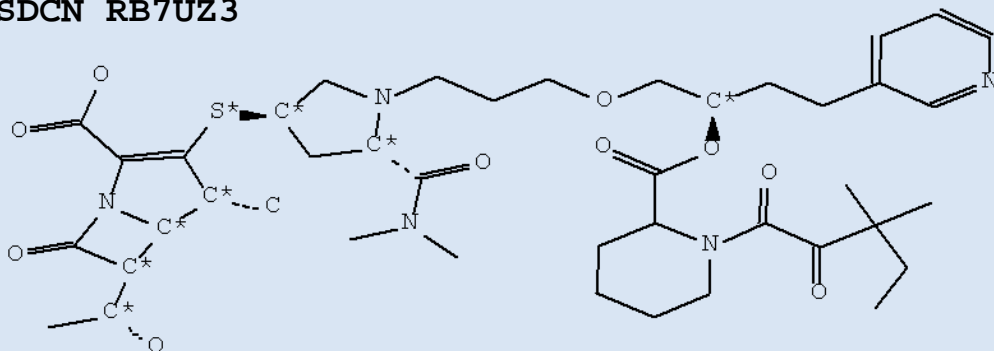
L4 602 L3/DCR

602 DWPI patent records are retrieved (L4).

=> D BIB HITSTR

L4 ANSWER 1 OF 602 WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN
AN 2010-G49777 [201043] WPINDEX
TI New 3-(pyrrolidin-3-yl-sulfanyl)-1-aza-bicyclo(3.2.0)hept-2-ene-2-carboxylic acid compounds useful for treating microbial, preferably bacterial, fungal and/or viral infections, where the bacteria is e.g. *Listeria* and *Enterococcus*
DC B02; C02
IN AUNGST R A; BARR K J; MAKARA G; MUTZ M
PA (AMPL-N) AMPLYX PHARM INC
CYC 124
PIA WO 2010065110 A2 20100610 (201043)* EN 140[3]
ADT WO 2010065110 A2 WO 2009-US6343 20091201
PRAI US 2009-171279P 20090421
US 2008-200694P 20081201
AN.S DCR-2303617
SDCN RB7UZ3

Display the DWPI patent records with in-context hit structures (HITSTR).



Agenda

- What is the Derwent World Patents Index (DWPI) Chemistry Resource (DCR)?
- How to search DCR
- **How to refine DCR searches**
- How to run a multiframe-structure-search including DWPI/DCR and CAS files

DCR searches can be refined using a series of roles

- “Roles” in DWPI describe the function of a compound in the patent, e.g.
 - Compound is prepared, purified or part of a mixture
 - Compound is claimed or from the examples
- DCR compounds can have two types of roles assigned
 - 2-3-letter codes from the IT-field (DCR Roles)
 - Single-letter codes from the chemical code field CMC (DCN Roles)
- Both types of roles can be linked to DCR numbers via the (T)-proximity operator

There are two distinct groups of DCR Number Roles available for searching

```
L1 ANSWER 1 OF 1 WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN
AN 2005-217884 [23] WPINDEX
TI Recovery of solvent and styrene from polystyrene solution involves
recovering solvent by evaporation and recovering styrene from
polystyrene thermally decomposed by solvent
. . . .
IT UPIT 20050708
2113-DIS 2113-PRD; 368-CL 368-PRD
CMC UPB 20050708
DRN: 0708-P 0708-U 1119-P 1119-U

M3 *01* G035 G562 H7 H721 M210 M211 M213 M232 M240 M282 M320 M415
M424 M510 M520 M530 M541 M610 M720 M740 N163 N480 N513 Q431
M905 M904 M910
DCN: R01119-K R01119-P
DCR: 130846-P 130846-U 2113-K 2113-P 2113-U

M3 *02* G010 G100 H7 H715 H721 M210 M212 M240 M281 M320 M414 M424
M510 M520 M531 M540 M610 M720 M740 N163 N480 N513 Q110 Q431
M905 M904 M910
DCN: R00708-K R00708-P
DCR: 368-K 368-P 368-U
```

The index term field (IT) includes the DCR roles.

The chemical code field (CMC) includes the DCN roles.

HELP ROLES provides all roles which can be used with DCR-numbers

DCR Roles		DCN Roles	
CL	Claim	A	Analyzed/Detected
EX	Example	C	Catalyst
DIS	Disclosure	D	Detecting agent
NEW	New	R	Purifying agent
PRD	Produced	S	Reactant
USE	Use	X	Substance removed
DET	Detected	N	New compound
RCT	Reactant	P	Produced
RGT	Reagent	Q	Product
PUR	Purified	M	Mixture
CMP	Mixture	U	Use
TES	Tested		
.....		

Example of DCR role searching: Preparation

```
=> S L3/DCR (T) (PRD OR P OR NEW OR N)/DCR  
L5          254 L3/DCR (T) (PRD OR P OR NEW OR N)/I
```

Use (T)-operator to link DCR numbers with roles.

```
=> D BIB HIT HITSTR 3
```

```
L5 ANSWER 1 OF 254 WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN  
AN 2010-G49777 [201043] WPINDEX  
TI New 3-(pyrrolidin-3-yl-sulfanyl)-1-aza-bicyclo[2.2.1]heptane-2-carboxylic acid compounds useful for treating
```

L3 – carbapenem structure search (see slide 36).

```
DC B02; C02  
IN AUNGST R A; BARR K J; MAKARA G; MUTZ M  
PA (AMPL-N) AMPLYX PHARM INC
```

```
CYC 124  
PIA WO 2010065110 A2 20100610 (201043)*
```

```
ADT WO 2010065110 A2 WO 2009-US6343 200912
```

```
PRAI US 2009-171279P 20090421  
US 2008-200694P 20081201
```

```
IT UPIT 20100712
```

```
. . . ; 2303617-DIS 2303617-NEW; 2303618-DIS 2303618-NEW; . . . .
```

```
CMC UPB 20100712
```

```
M2 *03* D011 D013 D014 D016 D030 D690 F011 F012 F013 F014 . . . .
```

```
DCN: RB7UZ3-N
```

```
DCR: 2303617-N
```

```
AN.S DCR-2303617
```

```
SDCN RB7UZ3
```

```
. . . .
```

Display the DWPI patent records with in-context hit structures (HITSTR).

Example of DCR role searching: Use

```
=> S L3/DCR (T) (USE OR U OR CMP OR M)/DCR
L6          368 L3/DCR (T) (USE OR U OR CMP OR M)/I
```

Use (T)-operator to link DCR numbers with roles.

```
=> D BIB HIT HITSTR
```

```
L6 ANSWER 1 OF 368 WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN
```

```
AN 2010-G49214 [201039] WPINDEX Full-text
```

```
TI Pharmaceutical composition useful for infec
```

L3 – carbapenem structure search (see slide 33).

```
DC B02; B03; B07
```

```
IN KASIVISWANATHAN K
```

```
PA (GLAD-N) GLADE ORGANICS PRIVATE LTD
```

```
CYC 124
```

```
PIA WO 2010064261 A1 20100610 (201039)* EN 30[8
```

USE, U – use roles.
CMP,M – mixture roles.

```
ADT WO 2010064261 A1 WO 2009-IN698 20091201
```

```
PRAI IN 2008-MU2510 20081201
```

```
IT UPIT 20100621
```

```
88192-CL 88192-USE; 100514-CL 100514-USE; 402340-CL 402340-USE; . . .
```

```
CMC UPB 20100621
```

```
M2 *02* D013 D014 D690 F012 F014 F423 H4 H401 H481 H5 H592 . . . .
```

```
DCN: R23271-K R23271-M
```

```
DCR: 100514-K 100514-M
```

```
AN.S DCR-100514
```

```
CN.P MEROPENEM
```

```
CN.S 3-(5-Dimethylcarbamoyl-pyrrolidin-2-yl)-6-methyl-7-oxo-1-aza-bicyclo[3.2.1]octane-2-carboxylic acid
```

Display the DWPI patent records with in-context hit structures (HITSTR).

```
SDCN R23271
```

```
. . . .
```

DCR searches may also be refined using chemical fragmentation codes (CMC)

```
=> S TAURINE/CN
L1          1 TAURINE/CN

=> S L1/DCR(P)Q25#/M0,M2,M3,M4
L2          164 L1/DCR(P)Q25!/M0,M2,M3,M4
```

WPIDS/WPIX-users can link DCR numbers with fragmentation codes via the (P)-proximity operator.

```
=> D AN TI HIT
```

M0,M2,M3,M4 = fragmentation code search fields.

Q25# = cosmetic applications.

```
L2 ANSWER 1 OF 164 WPIX COPYRIGHT 2010
AN 2010-H51057 [201046] WPIX
```

```
TI Cosmetic use of an active agent or active agent mixture, obtained from
e.g. Clintonia borealis or Punica granatum, for preventing and/or
inhibiting the effect (i.e. non-pathological effect) of
psychoemotional stress on the hair
```

```
CMC UPB 20100721
```

(P)

```
M2 *12* H1 H100 H181 K0 K4 K431 M280 M312 M321 M332 M342 M383 M391
M416 M620 M750 N102 Q254 M905 M904 M910
DCN: R00828-A R00828-K
DCR: 73384-A 73384-K
```

DCR-73384: Taurine.

Agenda

- What is the Derwent World Patents Index (DWPI) Chemistry Resource (DCR)?
- How to search DCR
- How to refine DCR searches
- How to run a multiframe-structure-search including DWPI/DCR and CAS files

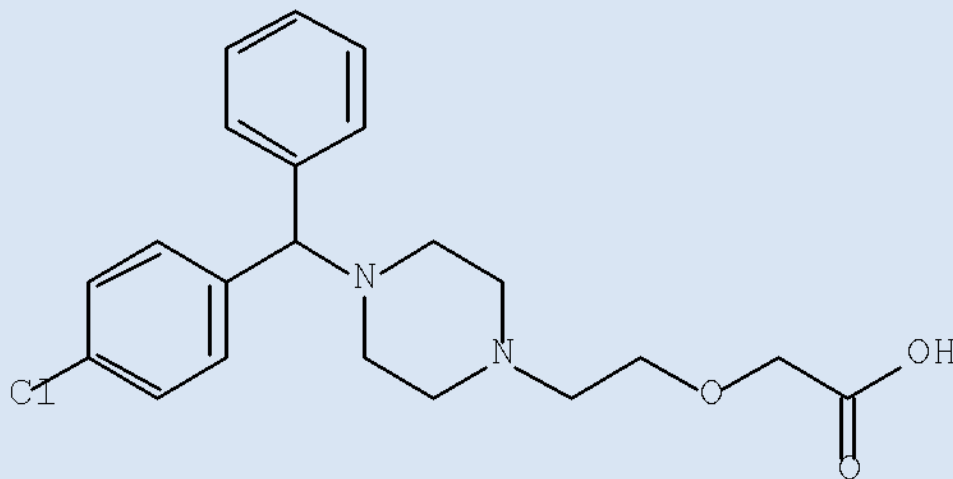
Multifile structure searching using DWPI/DCR and CAS files

1. Prepare a suitable standard structure query for REGISTRY/MARPAT and DWPI
2. Run the search in CAplus/REGISTRY and display records
3. Run the search in MARPAT, remove duplicates between CAplus and MARPAT and display additional MARPAT records
4. Run the search in DWPI/DCR
5. Remove duplicates between CAplus/MARPAT and DWPI, display additional DWPI records

Multifile structure search example: DWPI/DCR and CAS files

Search Question:

Search for all patent references of cetirizine, including salts and mixtures



Multifile search: REGISTRY

=> FILE REGISTRY

=>

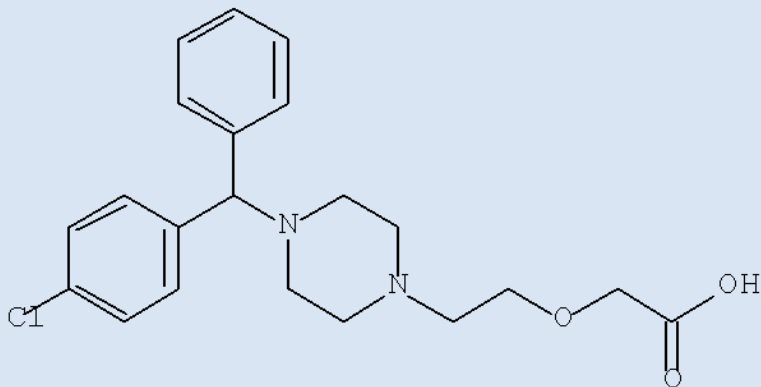
Uploading C:\. . . .\My Documents\STN Express 8.4\Queries\cetirizine.str

L1 STRUCTURE UPLOADED

=> D

L1 HAS NO ANSWERS

L1 STR



Upload the structure query to STN (L1).

Display the query to verify that the upload was successful.

Structure attributes must be viewed using STN Express query preparation.

Multifile search: REGISTRY

=> S L1 FAM SAM

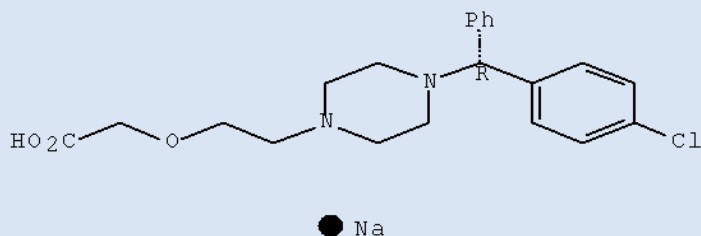
. . . .

L2 3 SEA FAM SAM L1

=> D SCAN

L2 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Acetic acid, 2-[2-[4-[(R)-(4-chlorophenyl)phenylmethyl]-1-piperazinyl]ethoxy]-, sodium salt (1:1)
MF C21 H25 Cl N2 O3 . Na

Absolute stereochemistry.



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

=> S L1 FAM FULL

. . . .

L3 77 SEA FAM FUL L1

Run a free sample search (L2), and review some answers with D SCAN to confirm the query is ok.

The full file structure search retrieves 77 REGISTRY records (L3).

Multifile search: CAplus

=> FILE CAPLUS

=> S L3 AND P/DT

L4 691 L3 AND P/DT

=> D BIB HITSTR

L4 ANSWER 1 OF 691 CAPLUS COPYRIGHT 2010 ACS on STN
AN 2010:833680 CAPLUS
TI Method for determining cetirizine concentration in urine
IN Cao, Cuizhen
PA Peop. Rep. China
SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 6pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CN 101762645	A	20100630	CN 2008-10154880	20081027
PRAI	CN 2008-10154880		20081027		
IT	INDEXING IN PROGRESS				
IT	83881-51-0, Cetirizine				
	RL: ANT (Analyte); ANST (Analytical study)				
	(method for detg. cetirizine concn. in urin				
RN	83881-51-0 CAPLUS				
CN	Acetic acid, 2-[2-[4-[(4-chlorophenyl)phenylme				
	piperazinyl]ethoxy]- (CA INDEX NAME)				

The full file structure search (L3) retrieves 691 patent records (P/DT) in CAplus (L4).

Display CAplus patent records with in-context hit structures (HITSTR).

Multifile search: MARPAT

=> FILE MARPAT

=> S L3 CSS SAM

...

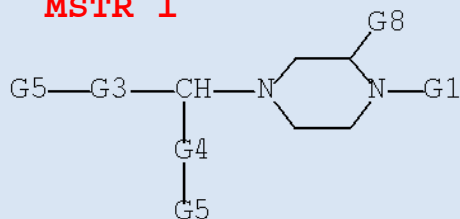
L5 1 SEA CSS SAM L1

=> D SCAN

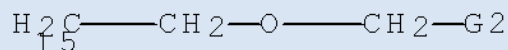
L5 1 ANSWERS MARPAT COPYRIGHT 2010 ACS on STN

...

MSTR 1



G1 = 15



G2 = CO₂H

G3 = phenylene

G4 = phenylene

G5 = Cl

Patent location: claim 1

...

Use the REGISTRY answer set (L3) for the MARPAT search.

In MARPAT there is no family search option, so we use CSS instead.

Run a free sample search (L5), and review answers with D SCAN.

Multifile search: MARPAT

=> S L3 CSS FUL

. . . .

L6 25 SEA CSS FUL L1

The MARPAT search retrieves 25 patent records (L6).

=> S L6 NOT L4

L7 6 L6 NOT L4

The MARPAT search retrieves 6 additional CAS patent records (L7).

=> D BIB FQHIT

L7 ANSWER 1 OF 6 MARPAT COPYRIGHT 2010 ACS on STN
AN 146:386929 MARPAT
TI Pharmaceuticals for treating viral infections
IN Chakraborty, Atrina Nath; Dastidar, Sujatha Ghosh
PA India
SO Indian Pat. Appl., 29pp.
CODEN: INXXBQ
DT Patent
LA English
FAN.CNT 1

Display MARPAT answers, e.g. in BIB FQHIT format.

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	IN 1998CA01961	A	20050805	IN 1998-CA1961	19980831
PRAI	IN 1998-CA1961	19980831			

MSTR 1

. . . .

For information on display formats in MARPAT enter **HELP FORMAT** at the STN prompt (=>).

Multifile search: DWPI/DCR

=> FILE WPINDEX

=> S L1 FAM SAM

. . . .

L8 5 SEA FAM SAM L1

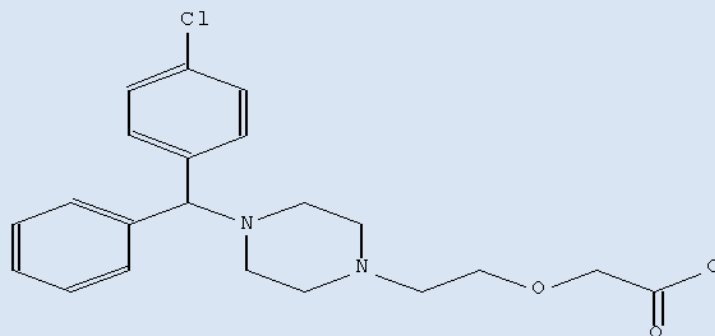
=> D SCAN

L8 5 ANSWERS WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN
CN.S (2-{4-[(4-Chloro-phenyl)-phenyl-methyl]-piperazin-1-yl}-ethoxy)-acetic
acid; monohydrochloride
MF C21 H25 Cl N2 O3 . H Cl

CM 1

Cl

CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

Repeat the structure search in DWPI.

Run a free sample search (L8), and review answers with D SCAN.

Multifile search: DWPI/DCR

=> S L1 FAM FUL

. . . .

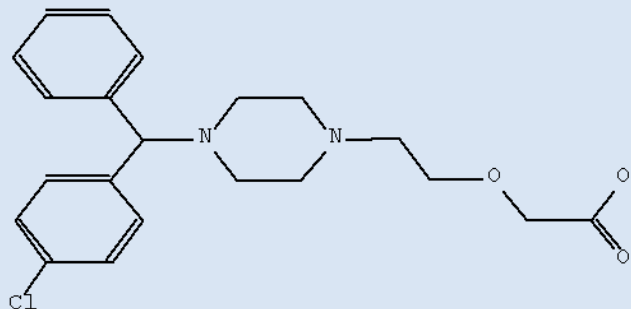
L9 44 SEA FAM FUL L1

=> S L9/DCR

L10 550 L9/DCR

=> D AN TI HITSTR

L10 ANSWER 1 OF 550 WPINDEX COPYRIGHT 2010 THOMSON REUTERS on STN
AN 2010-G97573 [201046] WPINDEX
TI Medicine preparation used for treating cold and influenza comprises
pholcodine, antipyretic analgesics, and decongestant
AN.S DCR-90453
CN.P CETIRIZINE
CN.S (2-{4-[(4-Chloro-phenyl)-phenyl-methyl]-piperazin-1-yl}-ethoxy)-acetic
acid
SDCN R14937; R16291



The full file structure search retrieves 44 DCR records (L9).

The 44 DCR records (L9) retrieve 550 patent records (L10).

Review the results, e.g. using the DWPI enhanced title (TI) and DCR hit structure (HITSTR).

Multifile search: duplicate removal

=> DUP IDE L4 L7

FILE 'CAPLUS' ENTERED
FILE 'MARPAT' ENTERED

Tip: Use DUPLICATE IDENTIFY to merge the CAPLUS (L4) and MARPAT (L7) answer sets together (L11).

L11 697 DUP IDE L4 L7 (INCLUDES 0 SETS OF DUPLICATES)

=> FILE WPINDEX

Re-enter WPINDEX.

=> TRANSFER L11 PN 1-

L12 TRANSFER L11 1- PN :
L13 846 L12

Use TRANSFER to bring the patent numbers from the CAS results (L11) into WPINDEX (L13).

=> S L10 NOT L13

L14 103 L10 NOT L13

The DWPI/DCR search (L10) adds 103 unique inventions (L14) to the CAS database search results (L11).

Multifile search: DWPI display

=> D AN TI 1-50

Review additional records
from the DWPI/DCR search.

L14 ANSWER 1 OF 103 WPINDEX COPYRIGHT 2010

AN 2010-F66310 [201037] WPINDEX

TI Making levocetirizine involves resolving pair of diastereomer of piperazine compound into single diastereomer, and converting single diastereomer of piperazine compound with 1-((4-chloro-phenyl)-phenyl-methyl)-piperazine into levocetirizine

. . .

L14 ANSWER 3 OF 103 WPINDEX COPYRIGHT 2010

THOMSON REUTERS on STN

AN 2010-F34949 [201037] WPINDEX

TI Adjustable neonatal airway stent for protecting the mucosal layer of an airway in a neonate from denudation due to mechanical ventilation, comprises a flexible mesh member having a cylindrical shape and size, and locking projections

. . .

L14 ANSWER 19 OF 103 WPINDEX COPYRIGHT 2010

THOMSON REUTERS on STN

AN 2009-L77524 [200949] WPINDEX

TI Pharmaceutical compositions for treatment of allergic rhinitis contain hepatoprotective, anti-inflammatory, anti-histaminic and decongestant with stimulant

. . .

L14 ANSWER 24 OF 103 WPINDEX COPYRIGHT 2010

THOMSON REUTERS on STN

AN 2009-J67366 [200936] WPINDEX

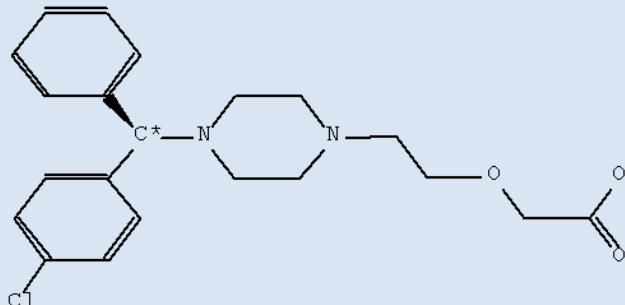
TI Orally disintegrating tablet useful for delivering main ingredient e.g. cetirizine hydrochloride for treating allergy, comprises main ingredient having specified water solubility and does not contain binder

Multifile search: DWPI display (cont.)

=> D BIB HITSTR

L14 ANSWER 1 OF 103 WPINDEX COPYRIGHT 2010
AN 2010-F66310 [201037] WPINDEX
TI Making levocetirizine involves resolving pair of diastereomer of piperazine compound into single diastereomer, and converting single diastereomer of piperazine compound with 1-((4-chloro-phenyl)-phenyl-methyl)-piperazine into levocetirizine
DC B03; B05
IN FIRET J J; ZHU J
PA (SYNT-N) SYNTHON BV
PIA WO 2010057515 A1 20100527 (201037)* EN 35[0]
ADT WO 2010057515 A1 WO 2008-EP9977 20081121
PRAI WO 2008-EP9977 20081121
AN.S DCR-174423
CN.P LEVOCETIRIZINE
CN.S (2-{4-[(4-Chloro-phenyl)-phenyl-methyl]-piperazin-1-yl}-ethoxy)-acetic acid
SDCN RA0WVA

Display additional records
from the DWPI/DCR search.



What is unique to DWPI/DCR?*

• Preparations	1
• Preparation of intermediate	1
• Highly relevant formulations	23
• Other formulations	57
• Methods of disease treatment	13
• Delivery devices	8
	<hr/>
	103 unique

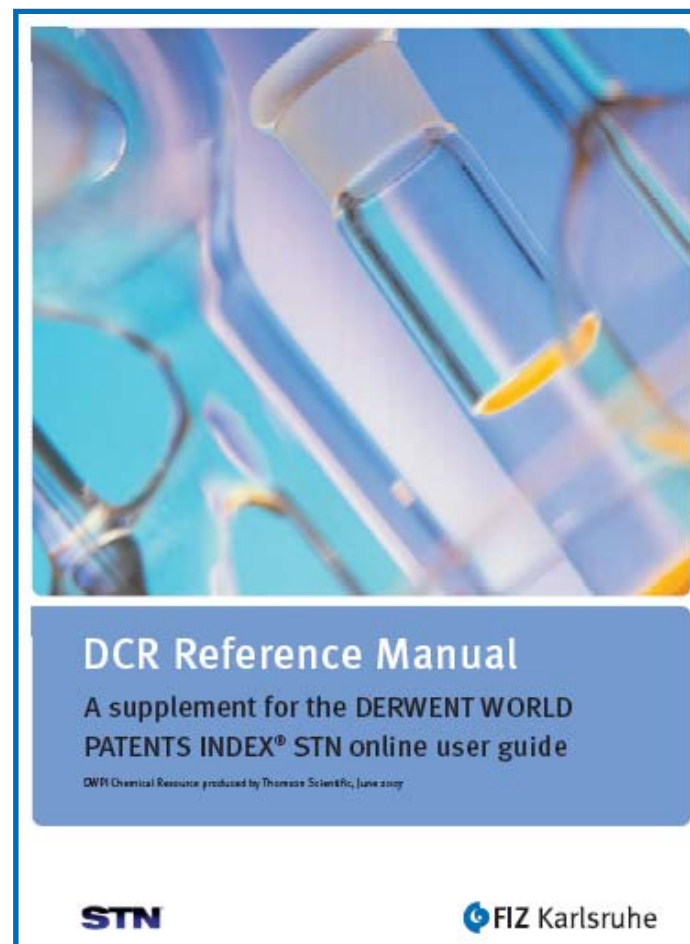
* 22nd of July 2010

Why are both the CAS files and Derwent World Patents Index required for comprehensiveness?

- CAS and Thomson apply different indexing guidelines to chemical patent publications
 - Different compounds are selected from the claims and the description for substance specific indexing
- Patent authority, document type and historical coverage varies between CAplus and DWPI
- Timeliness of coverage and indexing
- For a particular invention CAS and Thomson index the basic patent publication
 - The basic patent may vary for CAplus and DWPI
 - The patent content is dependent on the family member

DCR Reference Manual

- A supplement for the Derwent World Patents Index STN Online User Guide
- Provides extra detail on DCR coverage & features – including search examples



http://www.stn-international.com/dcr_reference_manual.html

Summary

- DWPI Chemistry Resource (DCR) is an important resource for specific compounds in patents
- DCR can be searched with standard STN structure queries used in REGISTRY or ReaxysFile
- DCR-records are a very useful source of synonyms for chemical compounds
- DCR provides various options to search using other substance-specific information
- DCR searches can be refined using roles and fragmentation codes

Resources

- DWPI on STN User Documentation
 - http://www.stn-international.com/stn_dwpi.html
 - DWPI on STN Reference Manual
 - DCR Reference Manual
 - DWPI Classification (DC) guide
 - Summary table of member level data coverage
 - Global Patent Sources – DWPI coverage in detail
 - Chemistry, Engineering and Polymer User Guides
- DWPI on STN database summary sheet
 - <http://www.stn-international.com/wpindex.html>

STN[®]

For more information ...

CAS

E-mail: help@cas.org

Support and Training:

www.cas.org

FIZ Karlsruhe

helpdesk@fiz-karlsruhe.de

Support and Training:

www.stn-international.de