

**STN<sup>®</sup>**

**Searching in DWPI Chemistry  
Resource (DCR)**

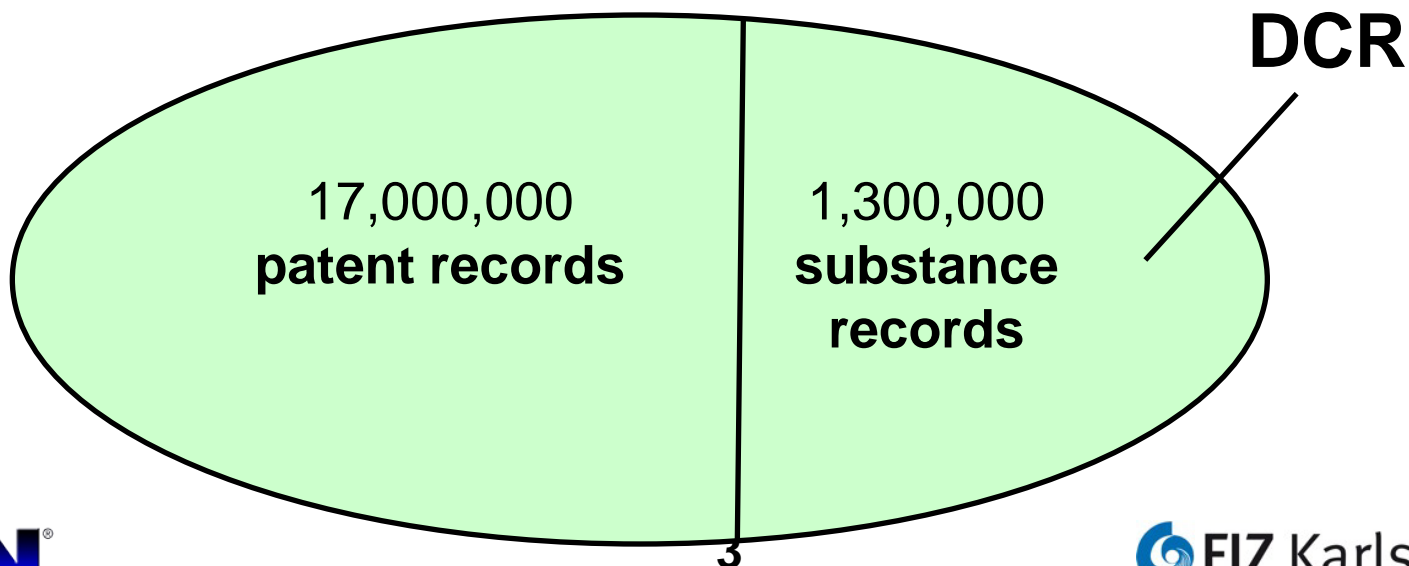
FIZ Karlsruhe

# Agenda

- What is DWPI Chemistry Resource?
- How to search DCR
- How to refine DCR searches
- How to run a multiframe-structure-search including DWPI/DCR and the CAS files

# What is DWPI Chemistry Resource?

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



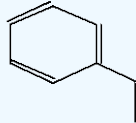
# DWPI provides bibliographic and chemical substance records

## bibliographic record

L1 ANSWER 1 OF 1 WPIINDEX COPYRIGHT 2007 THE THOMSON CORP 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

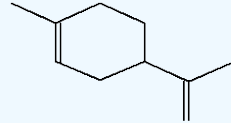
## substance record (DCR)

L2 ANSWER 1 OF 2 WPIINDEX COPYRIGHT 2007 THE THOMSON CORP 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 2007 THE THOMSON CORP 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

# DWPI Chemistry Resource (DCR)

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

# Substance Record from DCR

L1 ANSWER 1 OF 1 WPINDEX COPYRIGHT 2005 THOMSON CORP on STN

ACCESSION NUMBER: **DCR-368**

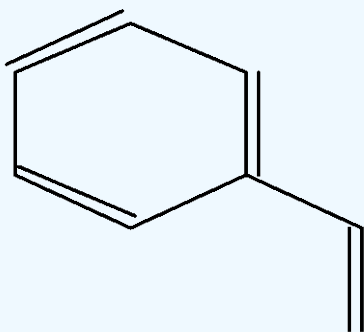
DCR numbers form the connection  
to DWPI patent records

DERWENT CHEM.RES.NO.: 368-0-0-0

PREF. CHEMICAL NAME: STYRENE

SYSTEMATIC NAME: Vinyl-benzene

SYNONYM: POLYSTYRENE (MONOMER); STYRENE



Chemical structures are searchable in  
the STN standard format

MOLECULAR FORMULA: C8 H8

STANDARD MOL. FORMULA: C8 H8 \*1; TOTAL \*1; TYPE \*1

MOLECULAR WEIGHT: 104.1512

DERWENT COMPOUND NO.: R00708

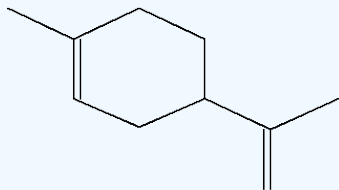
Substance records can  
include older numbering  
systems: DCN number

DERWENT REGISTRY NO.: 0708

# DCR-Numbers form the connection between substance records and DWPI patent records

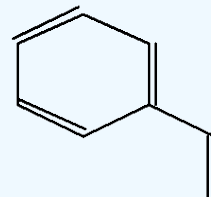
L1 ANSWER 1 OF 1 WPINDEX COPYRIGHT 2007 THE THOMSON CORP on STN  
AN 2005-217884 [23] WPINDEX  
TI Recovery of solvent and styrene from polystyrene solution involves recovering solvent by evaporation and recovering styrene from polystyrene thermally decomposed by solvent  
. . . .  
IT UPIT 20050708  
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

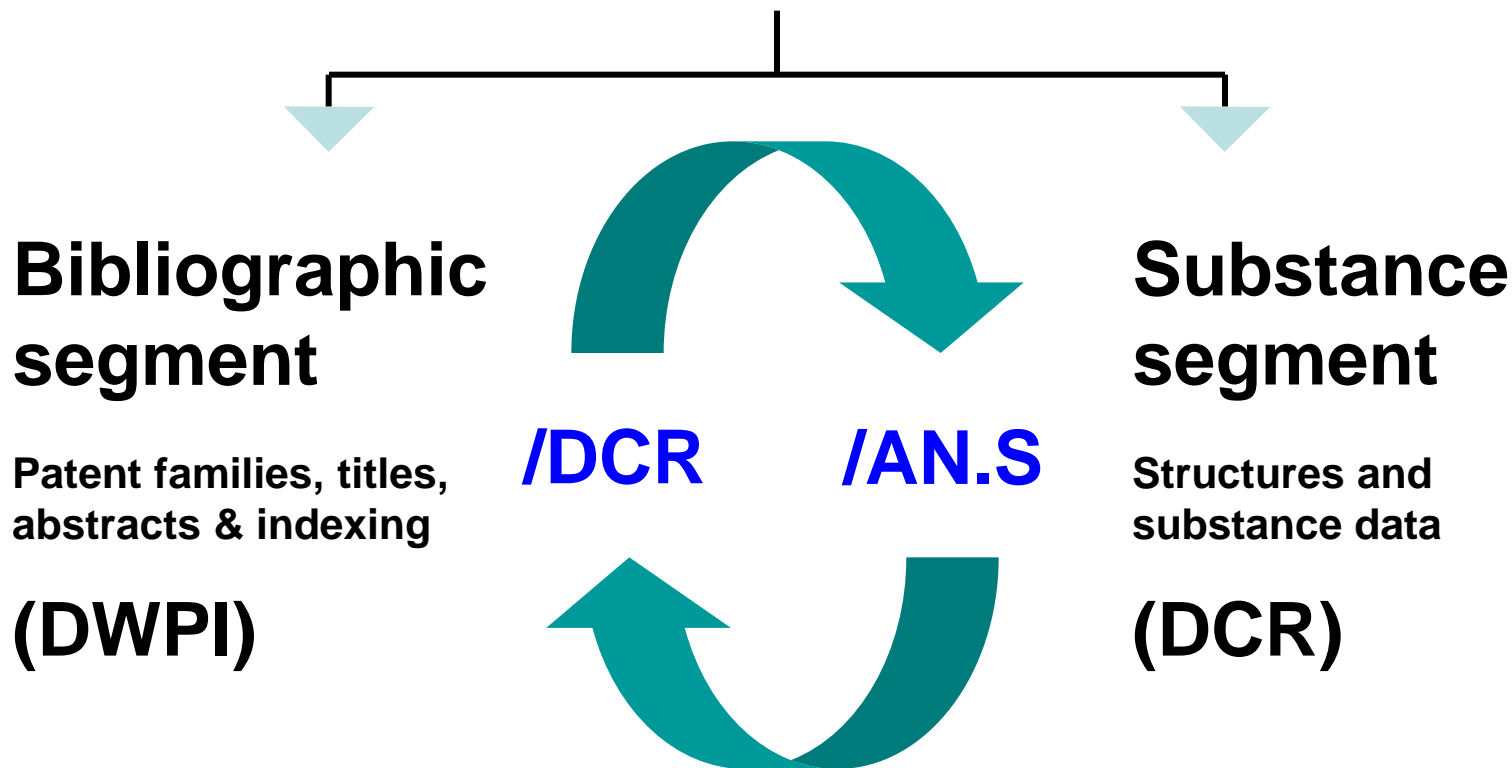
AN.S DCR-368  
DCSE 368-0-0-0  
CN.P STYRENE  
CN.S Vinyl-benzene  
SY POLYSTYRENE (MONOMER); STYRENE



MF C8 H8

DCR-Numbers form the connection between substance records and DWPI patent records

**WPINDEX/WPIDS/WPIX**



# Searching DCR-Numbers

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

=> S DCR-111250/AN.S

L1 1 DCR-111250/AN.S

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

=> S DCR-111250/DCR

L1 317 DCR-111250/DCR

# DWPI Chemistry Resource Coverage

- Pharmaceutical (B), agrochemical (C) and general chemical (E) patent records
- Comprehensive coverage from 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 kind of compounds are covered in DCR?

- specific organic compounds
- specific inorganic compounds
- specific peptides up to 15 amino acid residues
- oligomers up to 8 repeat units
- modified polysaccharides
- natural products including enzymes and proteins

# Which compounds are selected for DCR?

- all **novel** specific chemical compounds from the claims
- all known compounds from the claims
- the main examples and other representative examples from the description
- up to **99** compounds are indexed from the **basic patent** (system limit)

# Agenda

- What is DWPI Chemistry Resource?
- How to search DCR
- How to refine DCR searches
- How to run a multiframe-structure-search including DWPI/DCR and the CAS files

# Important search options for DCR-searching

- chemical names /CN
- chemical name segments /CNS
- molecular formula /MF
- structure searching
- element information /ELS
- classification codes /CC
- ....

# General strategy for searching specific chemical compounds in DWPI

1. Search for substance records in DCR ( $L_x$ )
2. Display DCR-records in a free format  
 $\Rightarrow$  D SCAN or  $\Rightarrow$  D TRIAL
3. Retrieve DWPI patent records with  
 $\Rightarrow$  S  $L_x$ /DCR
4. Display patent records and hit structures with  
 $\Rightarrow$  D  $L_y$  FULL HITSTR

HITSTR – free-of-charge display format

# Chemical Name Searching /CN

## *Search for the drug pantoprazole*

=> E PANTOPRAZOLE/CN

E#	FILE	FREQUENCY	TERM
--	----	-----	----
E1	WPIX	1	PANTOPENIL/CN
E2	WPIX	2	PANTOPON/CN
E3	WPIX	1 -->	PANTOPRAZOLE/CN
E4	WPIX	1	PANTOPRAZOLE HYDROXY SESQUIHYDRATE/CN
E5	WPIX	1	PANTOPRAZOLE HYDROXY TETRAHYDRATE/CN
E6	WPIX	1	PANTOPRAZOLE LITHIUM/CN
.....			
E11	WPIX	1	PANTOPRAZOLE POTASSIUM/CN
E12	WPIX	1	PANTOPRAZOLE SODIUM/CN
E13	WPIX	1	PANTO
E14	WPIX	1	PANTO

use EXPAND for the CN-field to see which names are indexed

=> S E3-13

L1 11 (PANTOPRAZOLE/CN OR "PANTOPRAZOLE HYD

11 substance records are retrieved for *pantoprazole* and salts

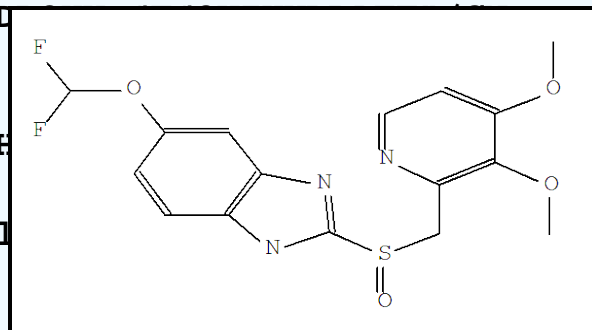
=> D TRIAL

L1 ANSWER 1 OF 13 WPINDEX COPYRIGHT 2009

CN.P PANTOPRAZOLE

CN.S 5-Difluoromethoxy-2-(3,4-dimethoxy-pyridin-2-yl)benzoimidazol e

MF C16 H15 F2 N3 O4 S



# Chemical Name Searching /CN

=> S L1/DCR

L2 454 L1/DCR

*pantoprazole* has been indexed in **454**  
DWPI patent records

=> D FULL HITSTR 1-

L2 ANSWER 1 OF 454 WPINDEX COPYRIGHT 2009

THOMSON REUTERS on STN

AN 2009-A81546 [04] WPIX

DNC C2009-035056 [04]

TI Freeze-dried powder injection for preparing medicine for treating gastric ulcer, duodenal ulcer, gastroesophageal reflux, *Helicobacter pylori* infection and Zollinger-Ellison syndrome, comprises proton pump inhib...

IN CHEN W; DAI J; YE D; ZHAO J

PA (JIAN-N) JIANGSU AOSAIKANG PHARM CO LTD

PI CN 101313894 A 20081203 (200904)

ADT CN 101313894 A CN 2008-10122760 2008

PRAI CN 2008-10122760 20080626

IPCI A61K0031-4164 [I,A]; A61K0031-4164 [I,A]

AB CN 101313894 A UPAB: 20090116

NOVELTY - A freeze-dried powder injection comprises proton pump inhibitor as active component, and is prepared by freeze drying after crystallizing and filtering steps....

.....

AN.S DCR-111250

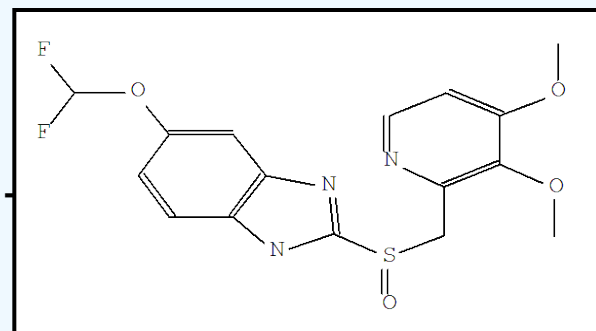
CN.P PANTOPRAZOLE

CN.S 5-Difluoromethoxy-2-  
benzimidazole

SDCN R22667

HITSTR-display

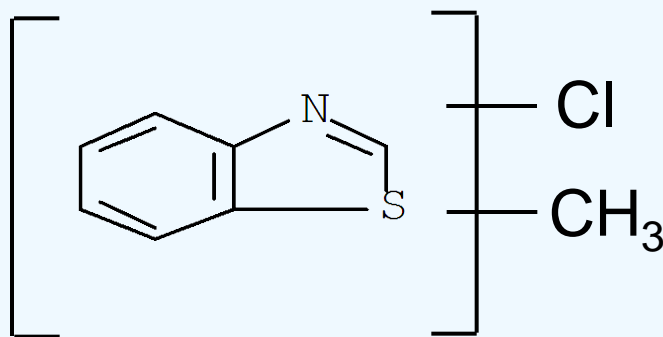
The hit structure display HITSTR is useful for reviewing in-context results following a DCR-search



# Name segment search **/CNS** combined with a molecular formula search **/MF**

## Search Question:

Search for DWPI patent references to  
benzothiazole substituted with chlorine and methyl



# Name segment search /**CNS** combined with a molecular formula search /**MF**

=> S (BENZOTHAZOLE AND METHYL AND CHLORO)/CNS

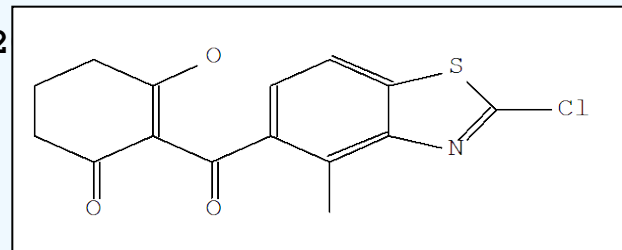
L1 41 (BENZOTHAZOLE AND METHYL AND CHLORO)/CNS

=> D TRIAL

L1 ANSWER 1 OF 41 WPINDEX COPYRIGHT 200

CN.S 2-(2-Chloro-4-methyl-benzothiazole  
-5-carbonyl)-3-hydroxy-cyclohex-2-enone

MF C15 H12 Cl N O3 S



=> S L1 AND C8 H6 CL N S/MF

4 C8 H6 CL N S/MF

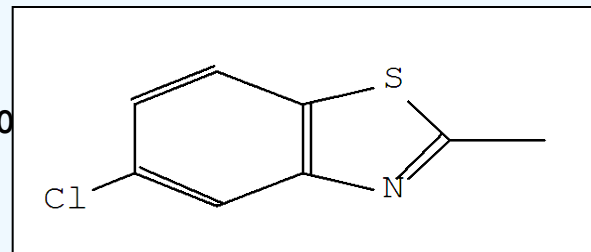
L2 3 L1 AND C8 H6 CL N S/MF

=> D TRIAL

L2 ANSWER 1 OF 3 WPINDEX COPYRIGHT 200

CN.S 5-Chloro-2-methyl-benzothiazole

MF C8 H6 Cl N S



# DWPI Structure Search Options

- **Exact (EXA)**-Search  
retrieves specific compounds and isotopes
- **Family (FAM)**-Search  
retrieves specific compounds, isotopes, salts and mixtures
- **Closed Substructure (CSS)**-Search  
allows for substitution at defined positions
- **Substructure (SSS)**-Search  
allows for substitution at any position
- **SAMPLE (SAM)**-Search: free of charge pre-search
- **SUBSET**-Search: structure search based on subset
- **BATCH**-Search  
for generic structure searches when system limits are reached

# 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 the patent records and the hit structures in context, e.g.: => D L3 1- FULLG HITSTR

DM

The screenshot shows the STN Online and Results application window. The main window displays a list of search results for 'stn\_1503'. A 'Structure File' dialog box is open, showing a list of files in the 'Queries' folder. The file 'aciclovir.str' is selected, and the 'Öffnen' (Open) button is circled in red. A callout box points to the 'Q' button in the main window's toolbar, indicating that it is used to upload the structure query to STN. Another callout box points to the 'Öffnen' button, indicating that it is used to choose the structure query. The chemical structure of aciclovir is displayed at the bottom of the dialog box.

STN Online and Results

File Edit Online Query Results Preferences! Web Window Help

stn\_1503

MOST RECENT THOMSON SCIENTIFIC UPDATE: 200721 <200721/DM>  
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> New re...  
>>> YOU AP...  
>>> New di...  
SEE ON...  
<http://www...>  
>>> IPC Re...  
2006.  
docume...  
200612...  
FOR A COPY...  
PLEASE VIS...  
<http://www...>  
FOR DETAIL...  
<http://sci...>  
PLEASE BE...  
<http://www...>  
<http://sci...>  
>>> FOR DE...  
PLEASE...  
<http://www...>  
\*\*\* YOU HAVE NEW MAIL \*\*\*

Structure File:

Suchen in: Queries

<input type="checkbox"/> aciclovir.str	<input type="checkbox"/> pantochem.str	<input type="checkbox"/> testt.str
<input type="checkbox"/> aspirine.str	<input type="checkbox"/> pantoprazole.str	
<input type="checkbox"/> benz2.str	<input type="checkbox"/> pantow.str	
<input type="checkbox"/> benzoes.str	<input type="checkbox"/> sulfo.str	
<input type="checkbox"/> cetirizine.str	<input type="checkbox"/> sulfonlurea.str	
<input type="checkbox"/> indole.str	<input type="checkbox"/> test.str	

Dateiname: aciclovir.str

Dateityp: Query Files (\*.str)

Öffnen

Abbrechen

Hilfe

Please make sure you have switched to a file suitable for structure searching.

Modifiable Queries  Use Filters

Standard

C1=NC2=C(N1)N=CN=C2C3=NC(=O)NC(=O)N3CCOCCO

Upload the structure query to STN with the 'Q' button

Choose structure query

STN

ne

# DWPI Structure Search: Aciclovir

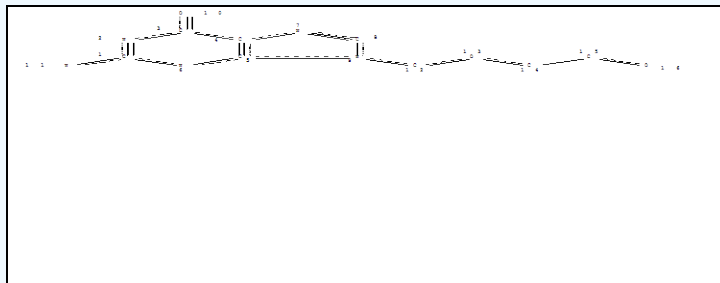
=> **FIL WPINDEX**

=>

Uploading C:\Programme\STNEXP\Queries\aciclovir.str

L1           STRUCTURE UPLOADED

=> **D**



Display the structure query L1 to verify that the upload was successful

=> **S L1 FAM SAM**

FULL FILE PROJECTIONS:   ONLINE   \*\*COMPLETE\*\*  
                          BATCH     \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:       1 TO       40  
PROJECTED ANSWERS:           1 TO       40

Run a free-of-charge sample search

L2                   1 SEA FAM SAM L1

=> **D TRIAL**

.....

Display answers from the sample search with the TRIAL format

# DWPI Structure Search: Aciclovir

=> S L1 FAM FULL

L3 8 SEA FAM FUL L1

Full file structure search  
retrieves **8** compounds

=> D TRIAL

.....

=> S L3/DCR

L4 791 L3/DCR

**791** patent family records  
are retrieved

=> D TRIAL HITSTR 1-

L4 ANSWER 1 OF 791 WPINDEX COPYR

AN 2007-283274 [27] WPINDEX

DNC C2007-103756 [27]

TT TT: PREPARATION USEFUL TREAT HERPES ZOSTER CONDENSATION POWDER N

BENZYLOXY CARBONYL VALINE PRESENCE AGENT SOLVENT

DC B02

IPCI C07D0473-00 [I,C]; C07D0473-18 [I,A]

MC CPI: B06-D09; B14-A02A3

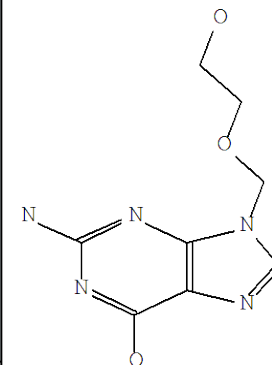
AN.S DCR-86437

CN.P ACICLOVIR

CN.S 2-Amino-9-(2-hydroxy-ethoxymethyl)-1,9-dihydro-purin-6-one

SDCN R04178; RA04GU

TRIAL HITSTR: free-of-charge display  
for a fast relevance check



# DWPI Structure Search: Aciclovir

=> D FULLG HITSTR 3-4 7 9 12 13-20 23

Selected patent records could be displayed in the format FULLG HITSTR

L6 ANSWER 3 OF 791 WPINDEX COPYRIGHT 2005 TH  
AN 2005-725393 [74] WPINDEX  
DNC C2005-220711

TI Liposomal formulation containing hydrophilic active agent, useful e.g. for topical treatment of cancer of skin and musosa, comprises bilayer comprising neutral and charged lipids.

.....

TECHNOLOGY FOCUS - PHARMACEUTICALS - Preferred Materials: (I) is a low molecular weight compound, specifically FU; acyclovir (ACV); iododeoxyuridine; methotrexate and cyprofloxacin. Especially FU is encapsulated in liposomes made of distearoyl-PC (DSPC) and distearoyl-PG (DSPG), or of DSPC and phosphatidylserine; and ACV is encapsulated in liposomes made of dipalmitoylPC, cholesterol and dipalmitoylPG, or of DSPC and DSPG.

FS CPI

FA AB; DCN

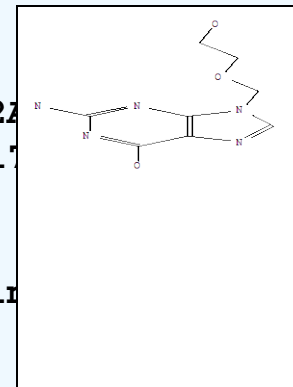
MC CPI: B01-D02; B04-B01B; B04-B03A; B05-B01P; B05-B02A  
B07-D12; B10-B04B; B14-A02A3; B14-H01B; B14-N17

AN.S DCR-86437

CN.P ACICLOVIR

CN.S 2-Amino-9-(2-hydroxyethoxymethyl)-1,9-dihydro-purin

SDCN R04178; RA04GU



B07-A02B;

# DCR is a useful source for synonyms

AN.S DCR-90453

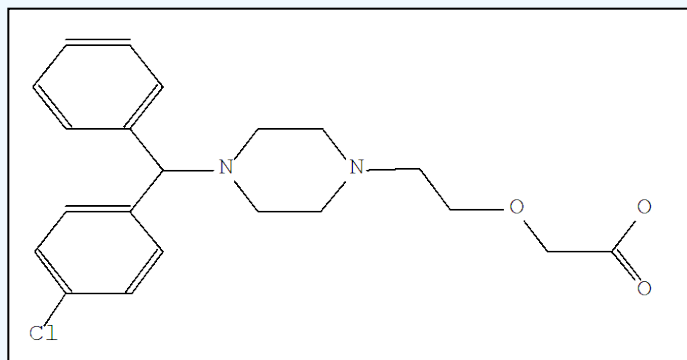
DCSE 90453-0-0-0

CN.P CETIRIZINE

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

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

ALL-display format



MF C21 H25 Cl N2 O3

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

MW 388.8925

SDCN R14937; R16291

# DCR is a useful source for synonyms

=> E CETIRIZINE/CN

E#	FILE	FREQUENCY	TERM
--	----	-----	----
E1	WPINDEX	1	CETIPRIN/CN
E2	WPINDEX	1	CETIPRIN-NOVUM/CN
E3	WPINDEX	1 -->	CETIRIZINE/CN
E4	WPINDEX	1	CETIRIZINE DIHYDROCHLORIDE/CN

1. EXPAND on compound name

=> S E3

L1 1 CETIRIZINE/CN

2. Search for compound name

=> SEL SY

E1 THROUGH E8 ASSIGNED

3. Select synonym names

=> D SEL

E#	FILE	FREQUENCY	TERM
--	----	-----	----
E1	WPINDEX	1	ALERLISIN/SY
E2	WPINDEX	1	CETIRIZINE/SY
E3	WPINDEX	1	CIRRUS/SY
E4	WPINDEX	1	P-071/SY
E5	WPINDEX	1	REACTINE/SY
E6	WPINDEX	1	SM-12800/SY
E7	WPINDEX	1	VIRLEX
E8	WPINDEX	1	ZIRTEC/SY

4. Display selected synonyms

# DCR is a useful source for synonyms

=> S CETIRIZIN? OR ALERLISIN OR CIRRUS OR P(W)071 or P071 OR  
REACTINE OR SM(W)12800 OR SM12800 OR VIRLEX OR ZIRTEC

L1 463 CETIRIZIN? OR ALERLISIN OR CIRRUS OR P(W)071 OR P071 OR  
REACTINE OR SM(W)12800 OR SM12800 OR VIRLEX OR ZIRTEC

5. Compile your own keyword query from the selected synonyms, considering truncations and different spellings

# Which DCR-numbers have been assigned for a patent publication?

```
=> S WO2007009775/PN
```

```
L1          1 WO2007009775/PN
```

1. Search patent number

```
=> SEL DCR
```

```
E1 THROUGH E52 ASSIGNED
```

2. Select DCR-numbers from patent record

```
=> S E1-52/AN.S
```

```
L2          16 (DCR-1149334/AN.S OR DCR-130212/AN.S OR DCR-133845/AN.S .....
```

3. Search selected DCR-numbers in the DCR-field **AN.S**

**16** compounds have been indexed for **WO2007009775**

# Which DCR-numbers have been assigned for a patent publication?

=> D TRIAL

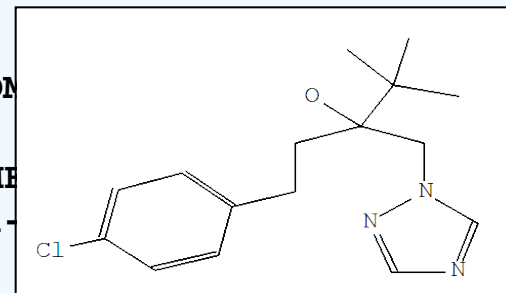
4. The selected compounds could be displayed in the TRIAL format

L2 ANSWER 1 OF 16 WPIX COPYRIGHT 2007 THE THOMSON

CN.P TEBUCONAZOLE

CN.S (ALPHA)-(2-(4-CHLOROPHENYL)ETHYL)-(ALPHA)-(1,1-DIMETHYL-1H-1,2,4-TRIAZOLE-1-ETHANOL)-1-(4-Chloro-phenyl)-4,4-dimethyl-1-pentanol

MF C16 H22 Cl N3 O

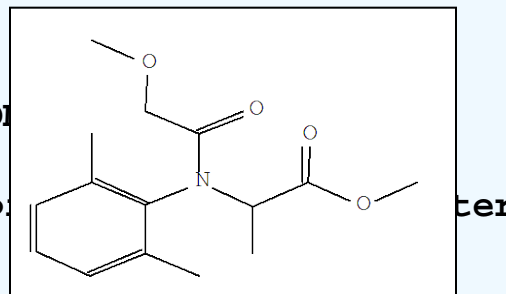


L2 ANSWER 2 OF 16 WPIX COPYRIGHT 2007 THE THOMSON

CN.P METALAXYL

CN.S 2-[(2,6-Dimethyl-phenyl)-methoxyacetyl-amino]-propylamine

MF C15 H21 N O4

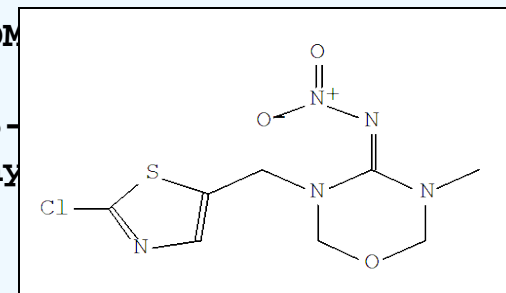


L2 ANSWER 3 OF 16 WPIX COPYRIGHT 2007 THE THOMSON

CN.P THIAMETHOXAM

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

MF C8 H10 Cl N5 O3 S



.....

# Agenda

- What is DWPI Chemistry Resource?
- How to search DCR
- **How to refine DCR searches**
- How to run a multiframe-structure-search including DWPI/DCR and the 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 2007 THE THOMSON CORP 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

the index term field (IT)  
covers the **DCR**-roles

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 M72  
M905 M904 M910  
DCN: R00708-K R00708-P  
DCR: 368-K 368-P 368-U

the chemical code field (CMC)  
covers the **DCN**-roles

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

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

# Example 1 for DCR-role searching: *Preparation of pantoprazole*

=> S L1/DCR (T) (PRD OR P OR NEW OR N)/DCR

L2 66 L1/DCR(T)(PRD OR NEW OR N OR P)

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

=> D BIB IT CMC

L2 ANSWER 1 OF 66 WPINDEX COPYRIGHT 2009

AN 2009-A43434 [02] WPIX

DNC C2009-020385 [02]

TI Preparing optionally substituted chiral pharmaceutical substances involves reacting

L1 – pantoprazole answer  
set from slide 14

IN GAWARI P S; GHARPURE M M; GURJAR M K;

PA (EMCU-N) EMCURE PHARM LTD

PIA WO 2008152462 A1 20081218 (200902)\*

ADT WO 2008152462 A1 WO 2008-IB1423 20080

PRAI IN 2008-MU35 20080107

IN 2007-MU1124 20070615

IT UPIT 20090112

1034-56201-CL 1034-56201-PRD; 105350-CL 105350-PRD; 109574-CL 109574-PRD;

1023326-CL 1023326-PRD; 111250-CL **111250-PRD**; 99135-CL 99135-PRD;

93863-CL 93863-PRD; 269446-CL 269446-PRD

PRD, P – preparation roles  
NEW, N – new compound roles

CMC UPB 20090112

M2 \*05\* C216 D012 D022 D711 F012 F013 F014 F431 H5 H522 H541 H6 H601

H608 H684 H8 K0 K4 K442 L922 M210 M211 M272 M282 M311 M322 M342

M343 M362 M373 M391 M412 M511 M521 M530 M540 M720 N383 ....

DCN: R22667-K R22667-P

DCR: 111250-K **111250-P**

# Example 2 for DCR-role searching: *Mixtures/Use of Pantoprazole*

=> S L1/DCR (T) (USE OR U OR CMP OR M)/DCR

L2 296 L1/DCR(T)(USE OR CMP OR U OR M)/DCR

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

=> D BIB HIT

L3 ANSWER 1 OF 296 WPINDEX COPYRIGHT 2007

THE THOMSON CORP on STN

AN 2007-292142 [28] WPINDEX

DNC C2007-107194 [28]

HIT-display

TI Enteric coating, useful in enteric coated oral dosage form or pancreatin, which is useful to treat e.g. pancreatitis, comprises film-forming agent e.g. pectin and chitin; plasticizer e.g. cetyl alcohol; and optionally...

IN KOELLN C; KOERNER A; ONKEN J; SCZESNY F; SHLIEOUT G

PA (SOLV-C) SOLVAY PHARM GMBH

PI WO 2007020259 A2 20070222 (200728)\* EN 31[0]

PRAI US 2005-708692P 20050815

EP 2005-107472 20050815

IT UPIT 20070430

97485-CL 97485-USE; 97487-CL 97487-USE; 100739-CL 100739-USE; 166937-CL

166937-USE; 105350-CL 105350-USE; 111250-CL 111250-USE; 76120-CL

76120-USE; 99239-CL 99239-USE; 99135-CL 99135-USE; 269446-CL 269446-USE;...

CMC UPB 20061101

M2 \*23\* C216 D012 D022 D711 F012 F013 F014 F431 H5 H522 H541 H6 H601

H608 H684 H8 K0 K4 K442 L922 M210 M211 M272 M282 M311 M322 M342

M343 M362 M373 M391 M412 M431 M511 M521 M530 M540 M782 M905 M904

DCN: R22667-K R22667-M

DCR: 111250-K 111250-M

# DCR searches can be refined using fragmentation codes

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

=> S L1/DCR(P)Q25#/M0,M2,M3,M4  
L5 127 L1/DCR(P)Q25#/M0,M2,M3,M4

Q25# - cosmetic application

=> D AN TI CMC

L1 – taurine: DCR=733384

L5 ANSWER 1 OF 127 WPIX COPYRIGHT 2009 THOMSON REUTERS on STN  
AN 2009-A87761 [04] WPIX  
TI Composition for use as external application for protecting from scalp irritation caused by hair-dye, comprises taurine, amino acid methionine and histidine, which is selected from vitamin E and Leontopodium alpinum..  
CMC UPB 20090116  
DRN: 0187-U 0828-U 1636-U  
DCR: 129481-U 132389-U 132390-U 134498-U 145033-U 21317-U 72864-U 73384-U.  
M2 \*01\* H1 H100 H181 K0 K4 K431 M280 M312 M321 M332 M342 M383 M391 M416  
M431 M620 M782 P420 P930 P943 Q252 M905 M904 M910  
DCN: R00828-K R00828-M  
DCR: 73384-K 73384-M 73384-U

# Agenda

- What is DWPI Chemistry Resource?
- How to search DCR
- How to refine DCR searches
- How to run a multiframe-structure-search including DWPI/DCR and the CAS files

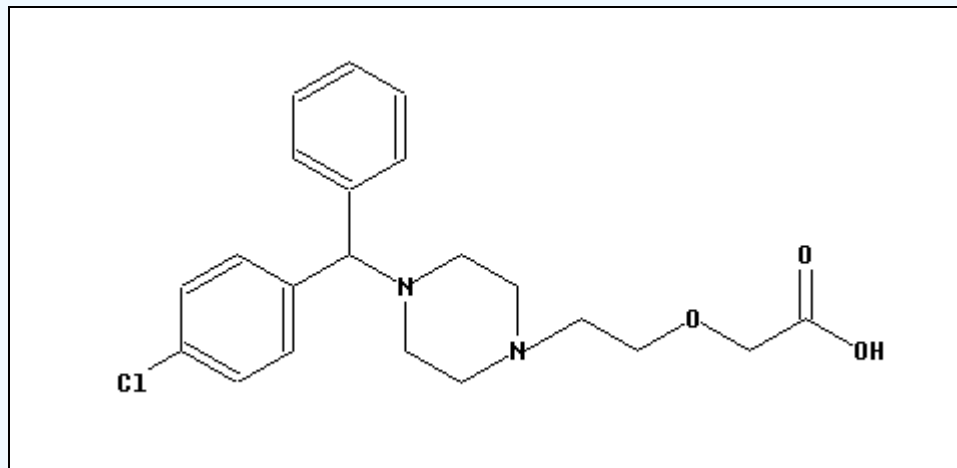
# Multifile structure searching using DWPI/DCR and REGISTRY/CAPLUS

1. Prepare a suitable standard structure query for REGISTRY/MARPAT and WPINDEX
2. Run the search in REGISTRY/CAPLUS 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 DCR/WPINDEX
5. Remove duplicates between CAPLUS/MARPAT and WPINDEX, display additional WPINDEX records

# Multifile-Structure-Search Example: DCR/DWPI and CAS files

## Search Question:

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



# Multifile-search: REGISTRY

=> **FIL REGISTRY**

=>

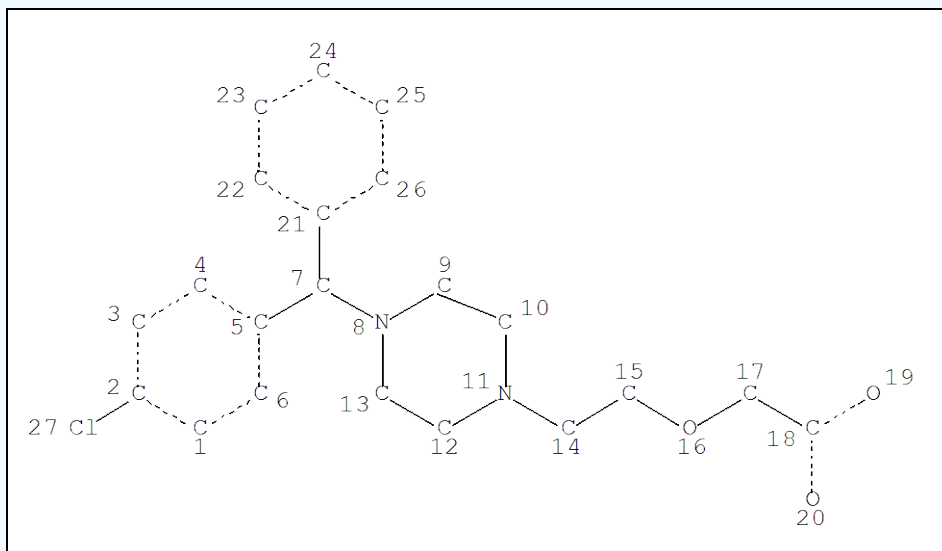
Uploading C:\STNEXP\QUERIES\cetirizine.str  
L1 STRUCTURE UPLOADED

Upload the structure query  
to STN

=> **D**

L1 HAS NO ANSWERS  
L1 STR

Display the query to  
verify that the upload  
was successful



# Multifile-search: REGISTRY

=> S L1 FAM SAM

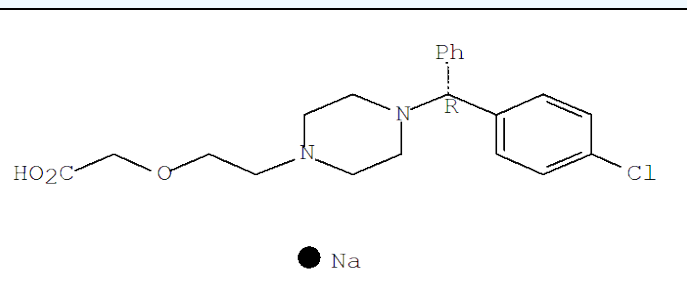
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 7 TO 2  
PROJECTED ANSWERS: 3 TO 163

Run a free sample search and review some of the answers with **D SCAN** to confirm the query is ok

L2 3 SEA FAM SAM L1

=> D SCAN

L2 3 ANSWERS REGISTRY COPYRIGHT 2005 ACS  
IN Acetic acid, [2-[4-[(R)-(4-chlorophenyl)piperazinyl]ethoxy]-, sodium salt (9CI)  
MF C21 H25 Cl N2 O3 . Na



Absolute stereochemistry. Rotation (+).

=> S L1 FAM FULL

L3 28 SEA FAM FUL L1

The FULL-file family search retrieves **28** compounds in REGISTRY

# Multifile-search: CAPLUS

=> FIL CAPLUS

=> S L3 AND P/DT

1097 L3

5720347 P/DT

L4 533 L3 AND P/DT

Crossover to CAPLUS retrieves  
**533** patent records (P/DT)

=> D ALL 1-

L4 ANSWER 1 OF 533 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2009:1498 CAPLUS

ED Entered STN: 01 Jan 2009

TI Multi-day delivery of biologically active substances conjugated to  
carrier, through oral or parenteral administration

IN Kydonieus, Agis

PA Samos Pharmaceuticals, LLC, USA

SO PCT Int. Appl., 54pp.

CODEN: PIXXD2

CC 63-6 (Pharmaceuticals)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	WO 2009002542	A1	20081231	WO 2008-US7983	20080626
PRAI	US 2007-937604P	P	20070627		

Display CAPLUS records  
in ALL-format

.....

# Multifile-search: MARPAT

=> FIL MARPAT

=> S L3 CSS SAM

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 51698 TO 57422  
PROJECTED ANSWERS: 1 TO 97

L5 0 SEA CSS SAM L1

=> S L3 CSS FULL

L6 20 SEA CSS FUL L1

=> S L6 NOT L4

99 L4

L7 8 L6 NOT L4

=> D BIB ABS FHIT 1-

L7 ANSWER 1 OF 8 MARPAT COPYRIGHT 2009 ACS on STN

AN 146:386929 MARPAT

TI Pharmaceuticals for treating viral infections

.....

Use REGISTRY answer set (L3) for MARPAT search

in MARPAT there is no family search option, we use CSS instead

the MARPAT search retrieves 8 additional records

Display MARPAT answers with BIB ABS FHIT

# Multifile-search: DCR/WPINDEX

=> FIL WPINDEX

=> S L1 FAM SAM

PROJECTED ITERATIONS: 3 TO 81  
PROJECTED ANSWERS: 1 TO 40

L8 1 SEA FAM SAM L1

=> D TRIAL

L8 ANSWER 1 OF 1 WPINDEX COPYRIGHT 2005 T

AN.S DCR-1000746

CN.S (2-{4-[(4-Chloro-phenyl)-phenyl-methyl]-  
acid; monohydrochloride

MF C21 H25 Cl N2 O3 . H Cl

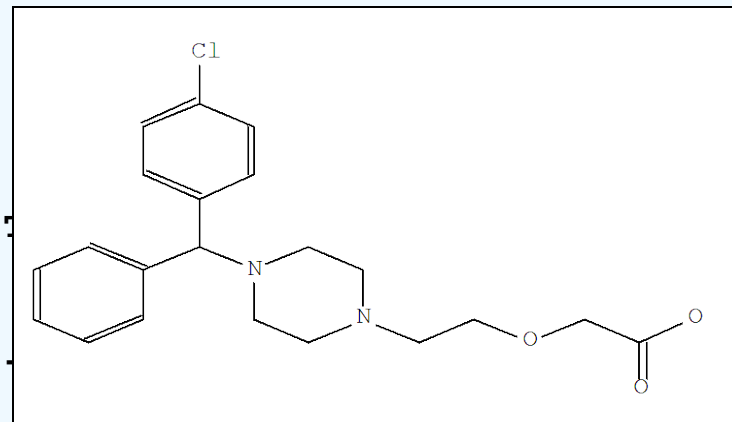
=> S L1 FAM FULL

L9 10 SEA FAM FUL L1

=> D TRIAL

.....

Repeat the family structure  
search in WPINDEX



the full-file structure search  
retrieves **10** DCR-records

# Multifile-search: DCR/WPINDEX

=> S L9/DCR

L10 400 L11/DCR

10 DCR-records retrieve  
400 patent records

=> D TRIAL HITSTR

L10 ANSWER 1 OF 400 WPINDEX COPYRI

AN 2009-A77562 [03] WPINDEX

DNC C2009-033039 [03]

TT TT: COMBINATION USEFUL TREAT ALLERGIC SYMPTOM SKIN MUCOUS MEMBRANE  
CONJUNCTIVA COMPRISE ACTIVE AGENT MADE PANTOTHENIC ACID ANTIALLERGIC  
SUBSTANCE ANTIHISTAMINE CORTICOSTEROID

DC B05

IPCI A61K0031-185 [I,C]; A61K0031-197 [I,A]; A61P0037-00 [I,C]; A61P0037-08...

MC CPI: B01-B01; B01-B02; B01-B03; B01-C02; B01-C05; B03-L; B06-A03;

B06-B02; B06-D04; B06-D05; B06-D06;

B06-F05; B07-B01; B07-D03; B07-D04C

B07-D12; B10-A15; B10-B02H; B10-B02

B14-K01; B14-N03; B14-N04; B14-N17;

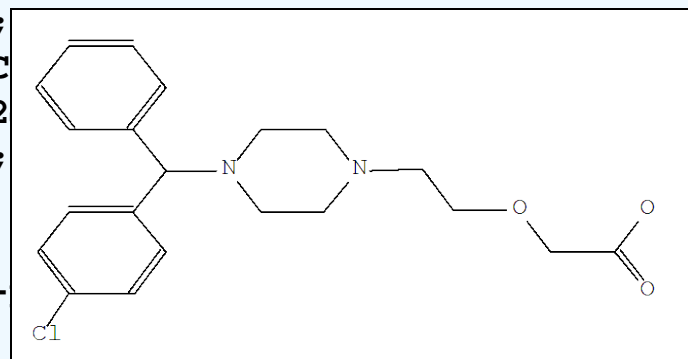
AN.S DCR-90453

CN.P CETIRIZINE

CN.S (2-{4-[(4-Chloro-phenyl)-phenyl-methyl]-  
acid

SDCN R14937; R16291

Use the free format **TRIAL HITSTR**  
for a fast relevance check



# Multifile-search: duplicate removal

```
=> DUP IDE L4 L7  
L11          541 DUP IDE
```

the command **DUPLICATE IDENTIFY** is useful to merge the CAPLUS (L4) and MARPAT (L7) answer set = L11

```
=> FIL WPINDEX
```

Enter the file WPINDEX again

```
=> TRA L11 PN  
L12          TRANSFER L11  
L13          661 L12
```

Use the **TRANSFER**-command to transfer all patent numbers from the CAS files to WPINDEX

```
=> S L10 NOT L13  
L14          73 L10 NOT L13
```

the WPINDEX search retrieves **73** additional inventions

# Multifile-search: WPINDEX-display

=> D FULL HITSTR 1-

Display the additional records from the WPINDEX search

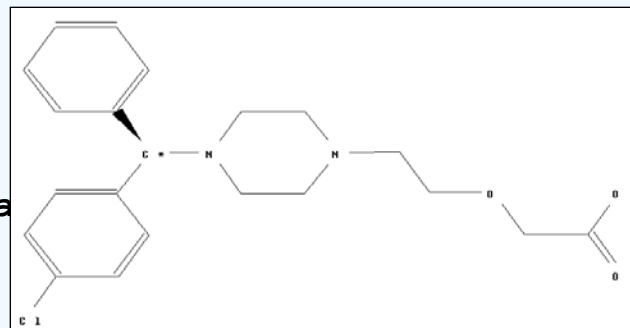
...  
AN 2008-009865 [82] WPINDEX  
DNC C2008-450962 [82]  
DNN N2009-040675 [82]  
TI Method of preparation of levorotatory  
(2-(4-((4-chlorophenyl)uphenylmethyl)ul-piperazimyl) ethoxy acetic acid  
dihydrochloride  
DC E13  
IN BURAD D; CHAUDHARY B; MEHTA H; PARMAR S; TALIA Y  
PA (PRAV-N) PRAVEEN LAB PTE LTD  
PI IN 2005MU01319 I3 20080815 (200882)\* EN [0]  
ADT IN 2005MU01319 I3 IN 2005-MU1319 20051020  
PRAI IN 2005-MU1319 20051020  
AB IN 200501319 I3 UPAB: 20081222  
NOVELTY - The synthesis of L-cetirizine using commercially available and  
economical reagents, is disclosed. Also disclosed is the conversion of  
p-chlorobenzophenone to L-cetirizine hydrochloride with higher chemical  
and optical purity...

AN.S DCR-174423

CN.P LEVOCETIRIZINE

CN.S (2-{4-[(4-Chloro-phenyl)-phenyl-methyl]-piperaz  
acid

SDCN RA0WVA



# What is unique to DCR/DWPI?\*

• preparations	<b>2</b>
• preparation of intermediate	<b>1</b>
• highly relevant formulations	<b>16</b>
• other formulations	<b>38</b>
• methods of disease treatment	<b>9</b>
• delivery devices	<b>7</b>
	<hr/>
	<b>73</b> unique

\* 20<sup>th</sup> of January 2009

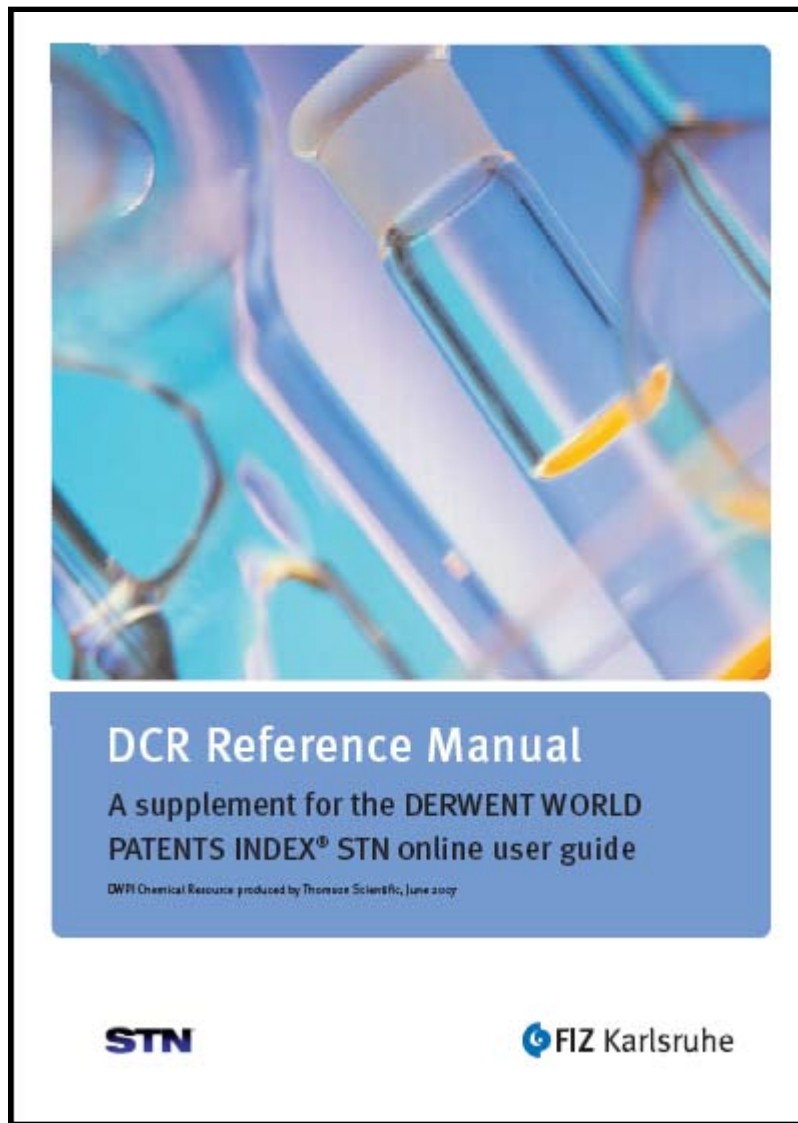
# Why are the CAS files and Derwent World Patents Index required for comprehensiveness?

- 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

Available at (PDF):

[www.stn-international.de/  
training\\_center/patents/dcr\\_  
rm.pdf](http://www.stn-international.de/training_center/patents/dcr_rm.pdf)



# Summary

- DWPI Chemistry Resource (DCR) is an important source for specific compounds from patents
- You can use the same structure queries for DWPI/DCR-structure searches like in REGISTRY and BEILSTEIN
- DCR provides various options to search with substance-specific information
- DCR searches can be refined using **roles** and **fragmentation codes**
- DCR-records are very useful for retrieving **synonyms** of chemical compounds

**STN<sup>®</sup>**

**Searching in DWPI Chemistry  
Resource (DCR)**

**- [www.stn-international.com](http://www.stn-international.com) -**