DCR (Derwent Chemistry Resource®)

Subject Coverage	• Organic and inorganic chemical compounds • Basic compounds, salts and mixtures as well as oligomers with less than 9 repeating groups, enzymes, proteins, chemically modified polysaccharides and standard polymers
File Type	Structure
Access	The file is only available on STNext
Features	Alerts (SDIs): Monthly, weekly, or with each update (2 updates per week) (every update is the default) In addition, SMARTracker, an automatic crossfile current-awareness search, (SDI XFILE) using a DCR search profile in WPINDEX, WPIX and WPIDS may be run every update, weekly or biweekly (every update is the default). CAS Registry Number® Identifiers: ☐ Keep & Share: ☐ SLART: ☑ Structures: ☑
Record Content	• Chemical compounds from Derwent World Patents Index (DWPI) documents • DCR numbers - unique identifiers for specific chemical compounds and link to corresponding DWPI database records • Systematic chemical names, commonly used chemical names and synonym names • Molecular formulas • Structure diagrams • Specific structure idenitifiers • Substance descriptors • Controlled terms
File Size	• More than 4.3 million specific chemical compounds (04/2022)
Coverage	• 1999-present • Partial coverage 1981-present: Commonly used and significant compounds • Chemical structure diagrams 1992-present
Updates	Updated twice a week with about 3,000 new chemical compounds
Language	English
Database Producer	Clarivate Friars House, 160 Blackfriars Rd. London SE1 8EZ United Kingdom Copyright Holder: Clarivate
Sources	• Claims and examples of patents indexed in the Derwent World Patents Index (DWPI) and classified in Chemical Patents Index (CPI) Sections B (Pharmaceuticals), C (Agrochemicals) and/or E (General Chemicals)

User Aids	• DCR Reference Manual (former implementation) • Building and Searching Structures on STN • Online Helps (HELP DIRECTORY lists all help messages available) • STNGUIDE
Cluster	• STRUCTURE STN Database Cluster Information: http://www.stn-international.com/en/customersupport/customer-support#cluster+%7C+subjects+%7C+features
Related Databases	• WPINDEX, WPIDS, WPIX

Search and Display Fields

Fields that allow left truncation are indicated by an asterisk (*).

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index* (contains single terms from CN; CMT, MF and SCT)	None (or /BI)	S ?PHENYLETHER? S UBIQUINONE/CMT S C19H19FN2O2S S ACETYLCHOLINE-RECEPTOR	CN, CMT, MF, SCT
Accession Number (DCR Number)	/AN	S DCR-5303196/AN	AN
Chemical Name	/CN	S MANDELIC ACID/CN	CN
Chemical Name Segment* (from CN.P, CN.S, SY)	/CNS	S DISULFONYL DIAZIDE/CNS	
Chemical Name, Preferred	/CN.P	S D-GLUCOSE-6-PHOSPHATE/CN.P	CN.P
Chemical Name, Synonym	/SY	S FALUBIN/SY	SY
Chemical Name, Systematic	/CN.S	S DECANE-1,10-DISULFONYL DIAZIDE/CN.S	CN.S
Comment	/CMT	S FIBROBLAST#/CMT	CMT
Component Molecular Formula	/CMF (or /FRAGMF)	S C H3 F6 P/CMF	SMF
Component Molecular Formula, Count	/CMF.CNT	S 6/CMF.CNT	SMF
Controlled Term, Substance	/SCT (or /CT)	S MAO-INHIBITOR/SCT	SCT
Controlled Term, Substance, Drug Activity	/SCT.DA (or /CT.DA)	S MAP-KINASE-INH?/SCT.DA	SCT
Controlled Term, Substance, Mechanism of Action	/SCT.MA (or /CT.MA)	S ADRENALINE/SCT.MA	SCT
Derwent Compound Number, Substance **(2)**	/SDCN	S R20123/SDCN	SDCN
Derwent Drug Registry Name	/DDRN	S 2-184/DDRN	DDRN
Derwent Registry Number, Substance **(2)**	/SDRN	S 1029/SDRN	SDRN
Element Count **(1)**	/ELC	S (S AND O AND C AND H)/ELS AND 4/ELC	Not displayed
Element Count Substance **(1)**	/ELC.SUB	S (S AND C AND H)/ELS AND 4/ELC.SUB	Not displayed
Element Symbol	/ELS	S FE/ELS	Not displayed
Element Symbol, Count **(1)**	/ELS.CNT	S O/ELS(S)7/ELS.CNT	Not displayed
Entry Date, Chemistry Resource **(1)**	/ED (or /EDCR)	S 20210323/ED	ED
Field Availability	/FA	S DDRN/FA	Not displayed
Molecular Formula	/MF	S H CL2 N/MF	MF
Molecular Weight **(1)**	/MW	S 17-21/MW	MW
Number of Components **(1)**	/NC	S 9-11/NC	SMF
Number of Components, total **(1)**	/NC.TOT	S 4/NC.TOT AND L11	SMF
Periodic Group	/PG	S A2/PG	Not displayed
Ring Index Number, Substance **(2)**	/SRIN	S 11895/SRIN	SRIN
Standardized Molecular Formula	/SMF	S "B *1; SI *1; TOTAL *2; TYPE *2"/SMF	SMF
Structured DCR Number	/DCSE	S 70-0-0-0/DCSE	DCSE
Substance Descriptor	/SD (or /CC)	S HALOCARBONS/SD	SD
Substructructure Terms	/SS	S PHOSPHONIC-ACID/SS	SS
Update Date, DCR **(1,3)**	/UP (or /UPCR)	S JAN 2000/UP	UP
Update Date, DWPI Cross Reference **(1,4)**	/UPWX	S 19990719/UPWX	UPWX

(1) Numeric search field that may be searched with numeric operators or ranges.
(2) Cross reference to indexing in bibliographic records. Select data from SDCN or SDRN or SRIN and search in /DCN resp. /DRN, resp. /RIN to retrieve bibliographic records.
(3) UPCR is created when existing records are updated or when new compounds enter the Chemistry Resource Segment.
(4) UPWX is created when DCR compounds are cited in bibliographic records. UPWX may be used in automatic current awareness searches (SDIs) in the Chemistry Resource Segment.

Super Search Fields

Enter a super search code to execute a search in one or more fields that may contain the desired information. Super search fields facilitate crossfile and multifile searching. EXPAND may not be used with super search fields. Use EXPAND with the individual field codes instead.

Search Field Name	Search Code	Fields Searched	Search Examples	Display Codes
Chemical Name	/CN	/CN.P, /CN.S, /SY	S MONDELIC ACID/CN	CN,
Controlled Term, Substance	/SCT	/SCT.MA, /SCT.DA	S ANTIBODY/SCT	SCT

Structure Searching

Terms	Search Examples
L-numbers of structures built using the STRUCTURE editor in STNext	SEARCH L1 FAM
L-numbers of structures built using the STRUCTURE command or uploaded from STN Express or STN on the Web (Boolean logic allowed between L-numbers)	SEA L1 AND L2 SSS
L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L3 OR L4 SSS
L-numbers of structures built using the STRUCTURE command or uploaded from STN Express or STN on the Web combined with L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L1 AND L2 NOT L3

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Substructure (default)	Search for substances which match the query. Substitution is allowed at all open positions. Additional components may be retrieved.	SSS	SEARCH L1 SSS S L2 OR L3 SSS S L7 SSS
Closed Substructure	Search for substances which match the query exactly. Substitution is allowed at positions opened by CONNECT. Additional components may be retrieved.	CSS	SEARCH L1 CSS S L2 NOT L3 CSS S L4 OR L5 CSS
Exact	Search for substances which match the query exactly	EXA	S L5 EXA FUL
Family	Search for substances which match the query exactly. Additional components may be retrieved.	FAM	S L6 FAM

Scopes of Structure Searching

Scope	Definition	Search Code	Search Examples
Sample (default)	Search a fixed 10% of the file (a maximum of 50 records displayed)	SAM	S L6 SSS SAM
Full	Search 100% of the file	FUL	S L5 OR L8 SSS
Subset Sample	Search a fixed sample of an answer set created by a search in DCR	SUB SAM	S L7 SSS SUB=L5 SAM
Subset Full	Search 100% of an answer set created by a search in DCR	SUB FUL	S L7 SSS SUB=L5 FUL

DISPLAY and PRINT Formats

Any combination of formats may be used to display or print answers. Multiple codes must be separated by spaces or commas, e.g., D L1 1-5 TI AU. The fields are displayed or printed in the order requested.

Hit-term highlighting is available for all fields. Highlighting must be ON during SEARCH to use the HIT, KWIC, and OCC formats.

Format	Content	Examples
AN	Accession Number (DCR Number)	D AN.S
CMT	Comment	D CMT
CN **(1)**	Chemical Name	D CN
CN.P **(1)**	Chemical Name, Preferred	D CN.P
CN.S **(1)**	Chemical Name, Systematic	D CN.S 1-5
DCSE	Structured DCR Number	D DCSE
DDRN	Derwent Drug Registry Name	D DDRN L1 1-2
ED (EDCR)	Entry Date, Chemistry Resource	D ED
MF	Molecular Formula	D MF
MW	Molecular Weight	D MF MW
SCT (CT)	Controlled Term, Substance	D SCT
SD (CC)	Substance Descriptor	D SD
SDCN	Derwent Compound Number, Substance	D SCDN
SDRN	Derwent Registry Number, Substance	D SDRN
SMF	Standardized Molecular Formula	D SMF
SRIN	Ring Index Number, Substance	D SRIN 1-10
SS	Substructure Terms	D SS
STR	Chemical Structure Display	D STR
SY **(1)**	Chemical Name, Synonym	D SY
UP (UPCR)	Update Date, DCR	D UP
UPWX	Update Date, DWPI Cross Reference	D UPWX
ALL (FULL)	AN, DCSE, CN.P, CN.S, SY, STR, CMT, MF, SMF, MW, SRIN, SDCN, SDRN, SD, ED, UP, UPWX	D ALL
IALL	ALL, indented with text labels	D IALL
MAX	AN, DCSE, CN.P, CN.S, SY, STR, CMT, MF, SMF, MW, SRIN, SDCN, SDRN, DDRN, SD, SCT.DA, SCT.MA, SS, ED, UP, UPWX	D MAX
IMAX	MAX, indented with text labels	D IMAX
STD (IDE)	AN, DCSE, CN.P, CN.S, SY, STR, CMT, MF, ED, UP, UPWX (STD is the default)	D STD 1-4
ISTD	STD, indented with text labels	D ISTD
SCAN **(2)**	CN.S, MF, STR (random display without answer number)	D SCAN
SAMPLE (SAM)	CN.S, MF, STR	D SAM
HIT	Hit term(s) and field(s)	D HIT
KWIC	Up to 50 words before and after hit term(s) (KeyWord-In-Context)	D KWIC
OCC	Number of occurrences of hit term(s) and field(s) in which they occur	D OCC

(1) All Chemical Names, .Preferred, Systematic and Synonym, are displayed with the CN display code.
(2) SCAN must be specified on the command line, i.e., D SCAN or DISPLAY SCAN.

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Accession Number (DCR number)	AN	Y	Y
Chemical Name	CN	Y **(2)**	N
Chemical Name, Preferred	CN.P	Y	N
Chemical Name, Synonym	SY	Y	N
Chemical Name, Systematic	CN.S	Y	N
Comment	CMT	Y	N
Controlled Term, Substance	SCT	Y	N
Derwent Compound Number, Substance	SDCN	Y	Y
Chemistry Resource Number, Chemistry Resource Segment	DCSE	Y	Y
Derwent Drug Registry Name	DDRN	Y	N
Derwent Registry Number, Substance	SDRN	Y	Y
Entry Date, Chemistry Resource	ED	Y	Y
Molecular Weight	MW	Y	Y
Number of Components	NC	N	Y
Ring Index Number, Substance	SRIN	Y	N
Standardized Molecular Formula	SMF	Y	N
Structure DCR Number	DCSE	Y	Y
Substance Descriptor	SD	Y	N
Update Date, DCR	UP	Y	Y
Update Date, DWPI Cross Reference	UPWX	Y	Y

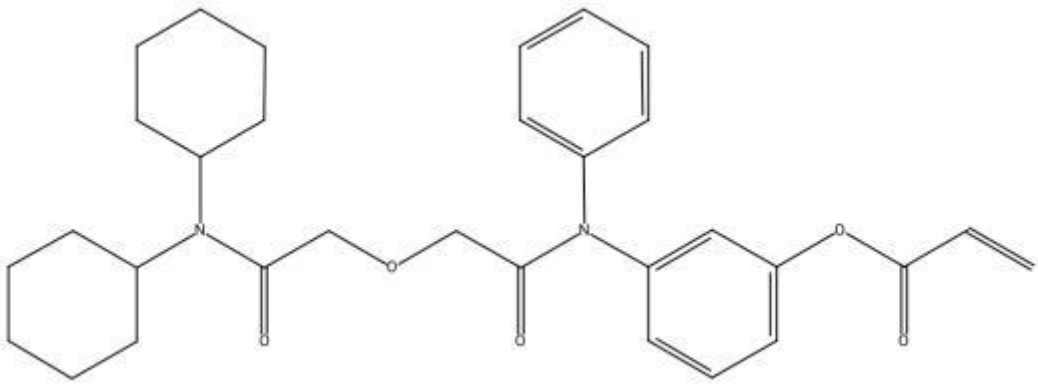
(1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set, e.g. SEL HIT CN.

(2) Selects or analyzes CN.S, CN.P and SY with /CN appended to the terms created by SELECT.

Sample Records

DISPLAY ALL

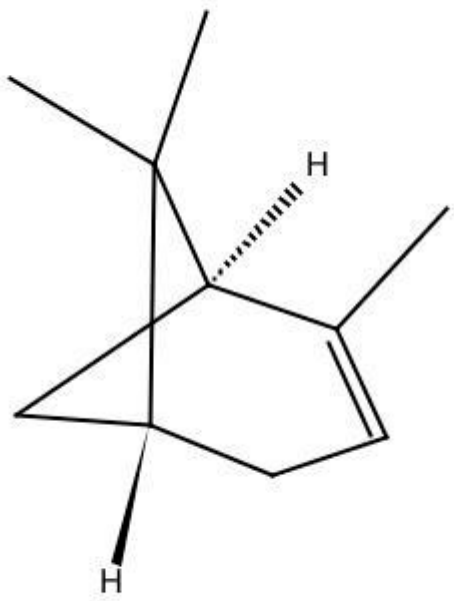
```
L8      ANSWER 1 OF 1 DCR  COPYRIGHT 2021 CLARIVATE on STN.
AN      DCR-1000003   DCR
DCSE    1000003-0-0-0
CN.S    Acrylic acid 3-({[(dicyclohexylcarbamoyl)-methoxy]-acetyl}-phenyl-amino)-
        phenyl ester
STR
```



```
MF      C31 H38 N2 O5
SMF     C31 H38 N2 O5 *1; TOTAL *1; TYPE *1
MW      518.6589
SDCN    RAG9YE
SD      UNSATURATED FATTY ACIDS
ED      Entered STN: 12 Feb 2021
        Last updated on STN: 12 Feb 2021
```

DISPLAY IMAX

```
L11     ANSWER 1 OF 1 DCR  COPYRIGHT 2021 CLARIVATE on STN.
ACCESSION NUMBER:         DCR-4436   DCR
STRUCTURED DCR NO.:       4436-0-0-0
PREF. CHEMICAL NAME:      ALPHA-PINENE
SYSTEMATIC NAME:          2,6,6-Trimethyl-bicyclo[3.1.1]hept-2-ene
SYNONYMS:                 ALPHA PINEN; ALPHA-PINEN; ALPHA-PINENE; PINENE,
                          ALPHA-; PINENE,ALPHA-; PINENE-ALPHA
STR
```

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COMMENT:                  Unspecified stereochemistry
MOLECULAR FORMULA:        C10 H16
STANDARD MOL. FORMULA:    TYPE *1; C10 H16 *1; TOTAL *1
MOLECULAR WEIGHT:         136.2364
RING INDEX NUMBER:        00832
DERWENT COMPOUND NO.:     R00477
DERWENT REGISTRY NO.:     0477
DERWENT DRUG REG. NAME:   PINENEALP
SUBSTANCE DESCRIPTOR:     TERPENES
SCT, MECHANISM OF ACTION:ACETYLCHOLINESTERASE-INHIBITORS; FUNGICIDES;
                          CHOLINESTERASE-INHIBITORS; ANTICHOLINESTERASES;
                          ANALGESICS
SCT, DRUG ACTIVITY:       ANTICHOLINESTERASE; ACETYLCHOLINESTERASE-INHIBITOR;
                          CHOLINESTERASE-INHIBITOR
SUBSTRUCTURE TERM:        OLEFIN; CYCLOBUTANE; CYCLOHEXANE; BRIDGE-STRUCT.;
                          TERPENE
ENTRY DATE:               Entered STN: 12 Feb 2021
                          Last updated on STN: 12 Feb 2021
```