

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 | | | | | | |
| Features Alerts (SDIs) Monthly, weekly, or with each update (2 updates per (every update is the default). In addition, SMARTracker, an automatic crossfile or search, (SDI XFILE) using a DCR search profile in WPINDEX, WPIX and WPIDS may be run every up biweekly (every update is the default). | | | | | crossfile current awareness profile in | | |
| | CAS Registry Number® Identifiers | | <u>SLART</u> | Ø | | | |
| | Keep & Share | | Structures | \checkmark | | | |
| 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 identifiers Substance descriptors Controlled terms | | | | | | |
| File Size | More than 5.2 million specific chemical compounds (02/2024) | | | | | | |
| Coverage | 1999-present Partial coverage 1981-present: Commonly used and significant compounds Chemical structure diagrams 1992-present | | | | | | |
| Updates | Updated twice a week with about 3,900 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) | | | | | | |

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| User Aids | Enhanced and restructured DWPI and DCR: What you need to know as DCR user Online Helps (HELP DIRECTORY lists all help messages available) STNGUIDE |
|----------------------|---|
| Cluster | STRUCTURE |
| | STN Database Cluster Information: https://www.cas.org/support/training/stn/database-clusters |
| Related Databases | WPINDEX, WPIDS, WPIX |

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

| | Search | | Display |
|---|--|--|---|
| Search Field Name | Code | Search Examples | 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 | CMT, CN.P, CN.S, MF, SCT.DA, SCT.MA, SY |
| Accession Number (DCR Number) Chemical Name (CN.P, CN.S, SY) Chemical Name Segment * (from CN) | /AN /CN /CNS | S DCR-5303196/AN S MANDELIC ACID/CN S DISULFONYL DIAZIDE/CNS | AN CN.P,CN.S,SY CN.P,CN.S,SY |
| Chemical Name, Preferred Chemical Name, Synonym Chemical Name, Systematic Comment Component Molecular Formula | /CN.P /SY /CN.S /CMT /CMF (or /FRAGMF) | S D-GLUCOSE-6-PHOSPHATE/CN.P S FALUBIN/SY S DECANE-1,10-DISULFONYL DIAZIDE/CN.S S FIBROBLAST#/CMT S C H3 F6 P/CMF | CN.P SY CN.S CMT SMF |
| Component Molecular Formula, Count | /CMF.CNT | S 6/CMF.CNT | SMF |
| Controlled Term, Substance (SCT.DA, SCT.MA) | /SCT (/CT) | S MAO-INHIBITOR/SCT | SCT.DA, SCT.MA |
| Controlled Term, Substance, Drug Activity | /SCT.DA (or /CT.DA) | S MAP-KINASE-INH?/SCT.DA | SCT.DA |
| Controlled Term, Substance, Mechanism of Action | /SCT.MA (or /CT.MA) | S ADRENALINE/SCT.MA | SCT.MA |
| Derwent Compound Number, Substance (2) | /SDCN | S R20123/SDCN | SDCN |
| Derwent Drug Registry Name Derwent Registry Number, Substance (2) | /DDRN /SDRN | S 2-184/DDRN S 1029/SDRN | DDRN SDRN |
| Element Count (1) Element Count Substance (1) Element Symbol Element Symbol, Count (1) Entry Date, Chemistry Resource (1) | /ELC /ELC.SUB /ELS /ELS.CNT /ED (or /EDCR) | S (S AND O AND C AND H)/ELS AND 4/ELC S (S AND C AND H)/ELS AND 4/ELC.SUB S FE/ELS S O/ELS(S)7/ELS.CNT S 20210323/ED | MF MF MF ED |
| Field Availability Molecular Formula Molecular Weight (1) Number of Components (1) Number of Components, Total (1) Periodic Group Ring Index Number, Substance (2) Standardized Molecular Formula Structured DCR Number Substance Descriptor | /FA /MF /MW /NC /NC.TOT /PG /SRIN /SMF /DCSE /SD (or /CC) | S DDRN/FA S H CL2 N/MF S 17-21/MW S 9-11/NC S 4/NC.TOT AND L11 S A2/PG S 11895/SRIN S "B *1; SI *1; TOTAL *2; TYPE *2"/SMF S 70-0-0/DCSE S HALOCARBONS/SD | Not displayed MF MW SMF SMF Not displayed SRIN SMF DCSE SD |
| Substructure Terms Update Date, DCR (1,3) Update Date, DWPI Cross Reference (1,4) | /SS /UP (or /UPCR) /UPWX | S PHOSPHONIC-ACID/SS S JAN 2000/UP S 19990719/UPWX | SS UP 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.

Structure Searching

| Terms | Search Examples |
|---|------------------------------------|
| L-numbers of structures built using the STRUCTURE editor in STNext L-numbers of structures built using the STRUCTURE command (Boolean logic allowed between L-numbers) | SEARCH L1 FAM 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 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

| Туре | 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 by assigning non-hydrogen attachments. Right click on a node or group of nodes and use the Non-Hydrogen Count tab in the STNext structure drawing tool. Additional components may be retrieved. | CSS | SEARCH L1 CSS S L2 NOT L3 CSS S L4 OR L5 CSS |
| Exact Family | Search for substances which match the query exactly Search for substances which match the query exactly. Additional components may be retrieved. | EXA FAM | S L5 EXA FUL 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 CMT CN (1) CN.P (1) CN.S (1) DCSE DDRN ED (EDCR) MF MW SCT (CT) SD (CC) SDCN SDRN SMF SRIN SS STR SY (1) UP (UPCR) UPWX | Accession Number (DCR Number) Comment Chemical Name (includes CN.P,CN.S and SY) Chemical Name, Preferred Chemical Name, Systematic Structured DCR Number Derwent Drug Registry Name Entry Date, Chemistry Resource Molecular Formula Molecular Formula Molecular Weight Controlled Term, Substance (includes SCT.DA and SCT.MA) Substance Descriptor Derwent Compound Number, Substance Derwent Registry Number, Substance Standardized Molecular Formula Ring Index Number, Substance Substructure Terms Chemical Structure Display Chemical Name, Synonym Update Date, DCR Update Date, DWPI Cross Reference | D AN D CMT D CN.P D CN.P D CN.S 1-5 D DCSE D DDRN L1 1-2 D ED D MF D MW D SCT D SD D SDCN D SDCN D SDRN D SMF D SRIN 1-10 D SS D STR D STR D SY D UP D UPWX |
| ALL (FULL) IALL MAX IMAX STD (IDE) ISTD SCAN (2) SAMPLE (SAM) | AN, DCSE, CN.P, CN.S, SY, STR, CMT, MF, SMF, MW, SRIN, SDCN, SDRN, SD, ED, UP, UPWX ALL, indented with text labels 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 MAX, indented with text labels AN, DCSE, CN.P, CN.S, SY, STR, CMT, MF, ED, UP, UPWX (STD is the default) STD, indented with text labels CN.S, MF, STR (random display without answer number) CN.S, MF, STR | D ALL D IALL D MAX D IMAX D STD 1-4 D ISTD D SCAN D SAM |
| HIT KWIC OCC | Hit term(s) and field(s) Up to 50 words before and after hit term(s) (KeyWord-In-Context) Number of occurrences of hit term(s) and field(s) in which they occur | D HIT D KWIC 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.

6 DCR 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 | Ν |
| Chemical Name, Systematic | CN.S | Y | Ν |
| Comment | CMT | Y | Ν |
| Controlled Term, Substance | SCT | Y (3) | Ν |
| Derwent Compound Number, Substance | SDCN | Y | Y |
| Derwent Drug Registry Name | DDRN | Y | Ν |
| Derwent Registry Number, Substance | SDRN | Y | Y |
| Entry Date, Chemistry Resource | EDCR (ED) | Y | Y |
| Molecular Weight | MW | Y | Y |
| Number of Components | NC | Ν | Y |
| Ring Index Number, Substance | SRIN | Y | Ν |
| Standardized Molecular Formula | SMF | Y | Ν |
| Structured DCR Number | DCSE | Y | Y |
| Substance Descriptor | SD | Y | Ν |
| Update Date, DCR | UPCR (UP) | Y | Y |
| Update Date, DWPI Cross Reference | UPWX | Y | Y |

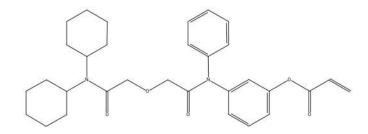
(1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set, e.g. SEL HIT CN.

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

Sample Records

DISPLAY ALL

```
L8 ANSWER 1 OF 1 DCR COPYRIGHT 2024 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: 24 Jan 2005

      Last updated on STN: 24 Jan 2005

      Update DWPI Cross Ref.: 24 Jan 2005
```

DISPLAY IMAX

L11ANSWER 1 OF 1 DCRCOPYRIGHT 2024 CLARIVATE on STN.ACCESSION NUMBER:DCR-4436DCRSTRUCTURED DCR NO.:4436-0-0-0PREF. CHEMICAL NAME:ALPHA-PINENESYSTEMATIC NAME:2,6,6-Trimethyl-bicyclo[3.1.1]hept-2-eneSYNONYMS:ALPHA PINEN; ALPHA-PINEN; ALPHA-PINENE; PINENE,ALPHA-; PINENE, ALPHA-; PINENE-ALPHASTR

.....H

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| COMMENT: MOLECULAR FORMULA: | |
|--------------------------------|--|
| | C10 H16 *1; TOTAL *1; TYPE *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, DRUG ACTIVITY: | ACETYLCHOLINESTERASE-INHIBITORS; ANALGESICS; |
| | ANTICHOLINESTERASES; CHOLINESTERASE-INHIBITORS; |
| | FUNGICIDES |
| SCT, MECHANISM OF ACTION | :ACETYLCHOLINESTERASE-INHIBITOR; ANTICHOLINESTERASE; |
| | CHOLINESTERASE-INHIBITOR |
| SUBSTRUCTURE TERM: | BRIDGE-STRUCT.; CYCLOBUTANE; CYCLOHEXANE; OLEFIN; |
| | TERPENE |
| ENTRY DATE: | Entered STN: 3 May 1999 |
| | Last updated on STN: 12 Aug 2022 |
| | Update DWPI Cross Ref.: 22 Jan 2024 |
| | - |

| In North America | | In Europe | | In Japan | In Japan | | |
|--|--|--|--|-------------------|---|--|--|
| CAS Customer Center: P.O. Box 3012 Columbus, Ohio 43210-0012 U.S.A. | | represent FIZ Karlsi Hermann 76344 Eg | CAS Customer Center EMEA represented by FIZ Karlsruhe - Leibniz-Institute for Information Infrastructure Hermann-von-Helmholtz-Platz 1 76344 Eggenstein-Leopoldshafen Germany | | JAICI (Japan Association for International Chemical Information) Nakai Building 6-25-4 Honkomagome, Bunkyo-ku Tokyo 113-0021 Japan | | |
| Phone: E-mail: | 800-753-4227 (North America) 614-447-3731 (worldwide) help@cas.org | Phone: E-mail: Internet: | +49-721-9588 3155 EMEAhelp@cas.org www.fiz-karlsruhe.de | Phone: E-mail: | +81-3-5978-3601 (Technical Service) +81-3-5978-3621 (Customer Service) support@jaici.or.jp (Technical Service) | | |
| Internet: | www.cas.org | | | Internet: | customer@jaici.or.jp (Customer Service) www.jaici.or.jp | | |