

CAS STN[®]next[®] COFFEE LECTURE



MOLECULAR FORMULA SEARCHING IN THE DERWENT CHEMISTRY RESOURCE (DCR) DATABASE ON CAS STN[®]next[®]

Jim Brown, FIZ Karlsruhe Inc.

Agenda

Searching the Derwent Chemistry Resource (DCR) Database

- Molecular Formula
- Standardized Molecular Formula
- Element Symbol
- Element Symbol Count
- Number of Components
- Number of Fragments

Derwent Chemistry Resource (DCR) database

Substance database containing specific chemical structure records

Not all records have structures

Peptides, polymers, substances with unknown structure, etc.

Searchable by chemical structure and by various text fields

Chemical names, comment field, etc.

Released in 1999, some substance records pre-date 1999

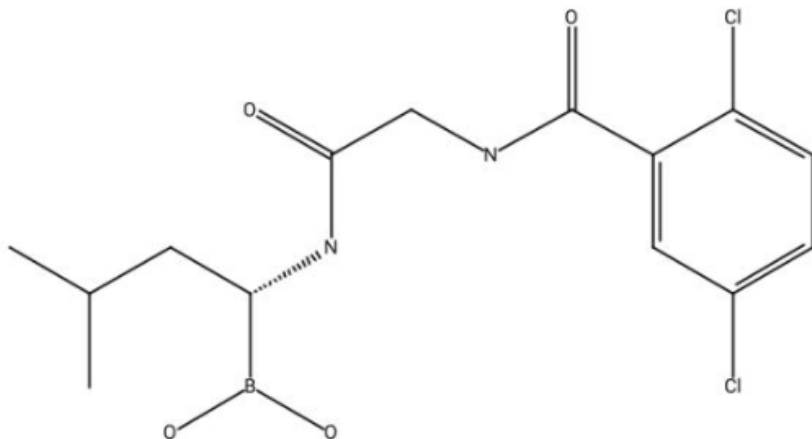
Molecular Formula

Molecular formula is in Hill order

- Carbon first, hydrogen second, all other atoms in alphabetical order
- Fragments are separated by period/hard stop
- May contain words like 'complex' instead of a molecular formula

Molecular formula examples

L7 ANSWER 1 OF 1 DCR COPYRIGHT 2023 CLARIVATE on STN.
AN DCR-1919660 DCR
DCSE 1919660-1-0-0
CN.P IXAZOMIB
CN.S [(1 R)-1-({ [(2,5-dichlorobenzoyl)amino] acetyl)amino)-3-methylbutyl]boronic acid
SY IXAZOMIB; MLN-2238; NINLARO
STR



MF C14 H19 B Cl2 N2 O4

SMF TYPE *1; TOTAL *1; C14 H19 B Cl2 N2 O4 *1
MW 361.0355
SDCN RAZS9G
ED Entered STN: 11 Mar 2009
Last updated on STN: 7 Jun 2017
Update DWPI Cross Ref.: 16 Jun 2023

L8 ANSWER 1 OF 104 DCR COPYRIGHT 2023 CLARIVATE on STN.
AN DCR-2627401 DCR
DCSE 2627401-0-0-0
CN.P ALUMINUM ZIRCONIUM PENTACHLOROHYDREX-GLY
SY ALUMINUM ZIRCONIUM PENTACHLOROHYDREX-GLY
STR

Substance image not available

CMT A coordination complex of aluminum zirconium pentachlorohydrate and glycine of formula $\text{Al}_y\text{Zr}(\text{OH})_{3y+4-x}\text{Cl}_x\text{mGly}_n\text{H}_2\text{O}$ in which some of the water molecules normally coordinated to the metals have been displaced by the glycine.

MF Complex

SDCN RBEXKB

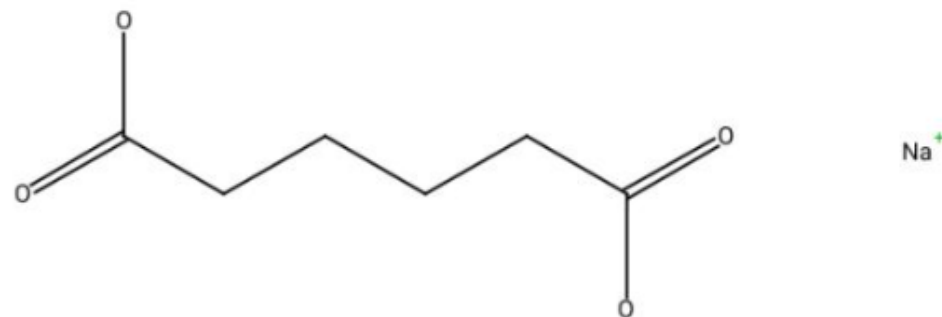
ED Entered STN: 17 Feb 2012

Last updated on STN: 16 Mar 2017

Update DWPI Cross Ref.: 5 Oct 2020

DCR sample record

L1 ANSWER 1 OF 1 DCR COPYRIGHT 2023 CLARIVATE on STN.
AN DCR-20870 DCR
DCSE 20870-0-0-0
CN.P SODIUM ADIPATE
SY ADIPIC ACID - SODIUM SALT; SODIUM ADIPATE
STR



CMT 1:2 Ratio
MF C6 H10 O4 . 2 Na
SMF C6 H10 O4 *1; Na *2; TOTAL *3; TYPE *2
MW 169.131
SDCN R10958
SDRN 1060
ED Entered STN: 4 Oct 1999
Last updated on STN: 4 Oct 1999
Update DWPI Cross Ref.: 8 Feb 2023

Molecular formula search example

```
=> S L1 AND C6H10O4.2NA/MF
```

```
1 C6H10O4.2NA/MF
```

```
L2 1 L1 AND C6H10O4.2NA/MF
```

```
=> S L1 AND C6 H10 O4 . 2 NA/MF
```

```
1 C6 H10 O4 . 2 NA/MF
```

```
L3 1 L1 AND C6 H10 O4 . 2 NA/MF
```

Note: Search input works with and without spaces

```
CMT 1:2 Ratio
```

```
MF C6 H10 O4 . 2 Na
```

```
SMF C6 H10 O4 *1; Na *2; TOTAL *3; TYPE *2
```

Standardized Molecular Formula

Mainly designed for retrieval of coordination compounds and salts

Available for all chemical compounds for consistency

Also in Hill order

Searchable text field containing terms corresponding to chemical fragments

Each formula fragment represents the molecular formula of the ion or ligand

Individual fragments are separated by semicolons

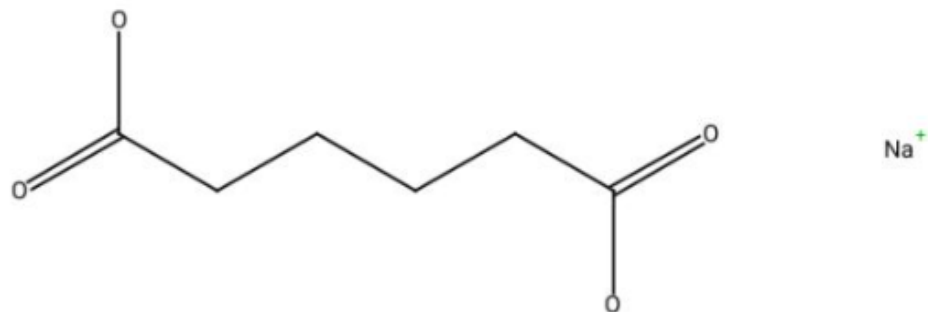
Stoichiometry factors are linked to each formula fragment by an asterisk

Total number of fragments – TOTAL * #

Total number of different types of fragments – TYPE * #

Standardized Molecular Formula

L10 ANSWER 3 OF 3 DCR COPYRIGHT 2023 CLARIVATE on STN.
AN DCR-20870 DCR
DCSE 20870-0-0-0
CN.P SODIUM ADIPATE
SY ADIPIC ACID - SODIUM SALT; SODIUM ADIPATE
STR



CMT 1:2 Ratio
MF C6 H10 O4 . 2 Na
SMF C6 H10 O4 *1; Na *2; TOTAL *3; TYPE *2
MW 169.131
SDCN R10958
SDRN 1060
ED Entered STN: 4 Oct 1999
Last updated on STN: 4 Oct 1999
Update DWPI Cross Ref.: 8 Feb 2023

TOTAL *3 – Total number of components
TYPE *2 – Number of components

Standardized Molecular Formula search examples

```
=> S L1 AND "C6 H10 O4 *1; NA *2; TOTAL *3; TYPE *2"/SMF
```

```
1 "C6 H10 O4 *1; NA *2; TOTAL *3; TYPE *2"/SMF
```

```
L4 1 L1 AND "C6 H10 O4 *1; NA *2; TOTAL *3; TYPE *2"/SMF
```

```
=> S L1 AND "C6 H10 O4 *1"*/SMF
```

```
153 "C6 H10 O4 *1"*/SMF
```

```
L5 1 L1 AND "C6 H10 O4 *1"*/SMF
```

```
=> S L1 AND "C6 H10 O4 *1; NA *2"*/SMF
```

```
2 "C6 H10 O4 *1; NA *2"*/SMF
```

```
L6 1 L1 AND "C6 H10 O4 *1; NA *2"*/SMF
```

- Note use of “ “
- Spaces must be used

Element Symbol

A way to search for substances containing a specific element

Qualitative search, no count

/ELS search qualifier

```
=> S L1 AND (C AND O AND NA)/ELS
```

```
4540893 C/ELS
```

```
3816422 O/ELS
```

```
30198 NA/ELS
```

```
L7          1 L1 AND (C AND O AND NA)/ELS
```

Element Symbol Count

A way to search for substances containing a specific element

Quantitative search

/ELS.CNT search qualifier

```
=> S L1 AND O 3-5/ELS.CNT

      3816422 O/ELS
      3026122 3-5/ELS
      1581125 O 3-5/ELS.CNT
              (O/ELS (T) 3-5/ELS)
L8      1 L1 AND O 3-5/ELS.CNT

=> S L1 AND O/ELS(S)3-5/ELS.CNT

      3816422 O/ELS
      3026122 3-5/ELS.CNT
      1581125 O/ELS(S)3-5/ELS.CNT
L9      1 L1 AND O/ELS(S)3-5/ELS.CNT
```

Number of Components

Number of components in structured molecule

/NC search qualifier

Shown in Standard Molecular Formula field as TYPE *#

```
=> S L1 AND 2/NC
```

```
273467 2/NC
```

```
L10          1 L1 AND 2/NC
```

```
CMT      1:2 Ratio
```

```
MF       C6 H10 O4 . 2 Na
```

```
SMF      C6 H10 O4 *1; Na *2; TOTAL *3; TYPE *2
```

Total Number of Components

Total number of components in structured molecule

/NC.TOT search qualifier

Shown in Standard Molecular Formula field as TOTAL *#

```
=> S L1 AND 3/NC.TOT
```

```
58823 3/NC.TOT
```

```
L11
```

```
1 L1 AND 3/NC.TOT
```

```
CMT 1:2 Ratio
```

```
MF C6 H10 O4 . 2 Na
```

```
SMF C6 H10 O4 *1; Na *2; TOTAL *3; TYPE *2
```

Summary

Derwent Chemistry Resource has many different fields of search

Not every record has every field populated

Consider search options for specific substance search

- Structure search

- Molecular formula options

- Keyword searches (/CMT, CN, CNS, etc.)

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