

TUTORIAL OChemDb

To access to OChemDb you should go to the url <http://www.ba.ic.cnr.it/softwareic/>:

- Insert your credentials (if not inserted before) in the sidebar on the right
- Go to our portal <http://www.ba.ic.cnr.it/ochemdb/>

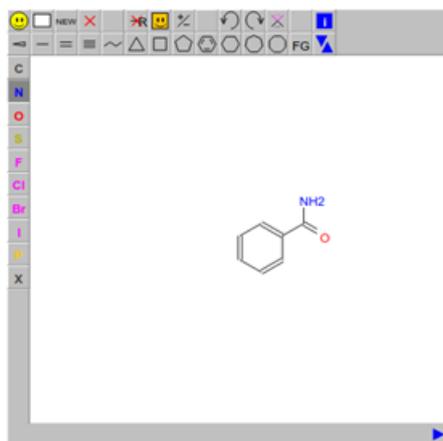
Example 1

- Select *Molecular editing* in the distance page

The screenshot displays the OChemDb interface. At the top, the header reads "OChemDb - Open Chemistry Database". On the left, a sidebar contains navigation options: "STATISTICS", "Distance" (highlighted in red), "Angle", "Torsion", "Space Group", "QUERY" (with sub-options: Card, Type, Data access), "CONTACT" (with sub-option: Contact us), "HISTORY" (with sub-option: My account), and "ABOUT" (with sub-option: About). The main content area is titled "Bond Distances" and includes tabs for "All", "Organic", and "Inorganic". Below these is a search bar and a navigation menu with "Basic", "Molecule editing" (circled in red), and "Atom types". The "Molecule editing" section contains the instruction "The following steps can be carried out" and two numbered tasks: "1) Draw molecule" and "2) Generate atom types". A "Generate" button is located under the second task. The "1) Draw molecule" task includes a toolbar with icons for drawing and editing, and a vertical list of element symbols: C, N, O, S, F, Cl, Br, I, P, X.

- Draw the molecular fragment containing the bond to be sought by using the free molecule editor/viewer in JavaScript JSME

1) Draw molecule



- Click on *Generate* on the right side to generate the atom types corresponding to the molecule sketch

The following steps can be carried out

1) Draw molecule

2) Generate atom types

Select bond

- C2 - C3 : c[6](CNO)c[6](CH2)2 - c[6](c[6]CC)c[6](CH)(H)
- C3 - C4 : c[6](c[6]CC)c[6](CH)(H) - c[6](c[6]CH2)(H)
- C2 - C7 : c[6](CNO)c[6](CH2)2 - c[6](c[6]CC)c[6](CH)(H)
- C6 - C7 : c[6](c[6]CH2)(H) - c[6](c[6]CC)c[6](CH)(H)
- C5 - C6 : c[6](c[6]CH2)(H) - c[6](c[6]CH2)(H)
- C4 - C5 : c[6](c[6]CH2)(H) - c[6](c[6]CH2)(H)
- C1 - N1 : C(NHH)c[6](CC)(O) - N(CCO)(H)2
- C1 - C2 : C(NHH)c[6](CC)(O) - c[6](CNO)c[6](CH2)
- C1 - O1 : C(NHH)c[6](CC)(O) - O(CCN)

- N1 - H1 : N(CCO)(H)2 - H(NCH)
- N1 - H2 : N(CCO)(H)2 - H(NCH)
- C3 - H3 : c[6](c[6]CC)c[6](CH)(H) - H(c[6]CC)
- C4 - H4 : c[6](c[6]CH2)(H) - H(c[6]CC)
- C5 - H5 : c[6](c[6]CH2)(H) - H(c[6]CC)
- C6 - H6 : c[6](c[6]CH2)(H) - H(c[6]CC)
- C7 - H7 : c[6](c[6]CC)c[6](CH)(H) - H(c[6]CC)

3) Search selected atom types

(edit if necessary)

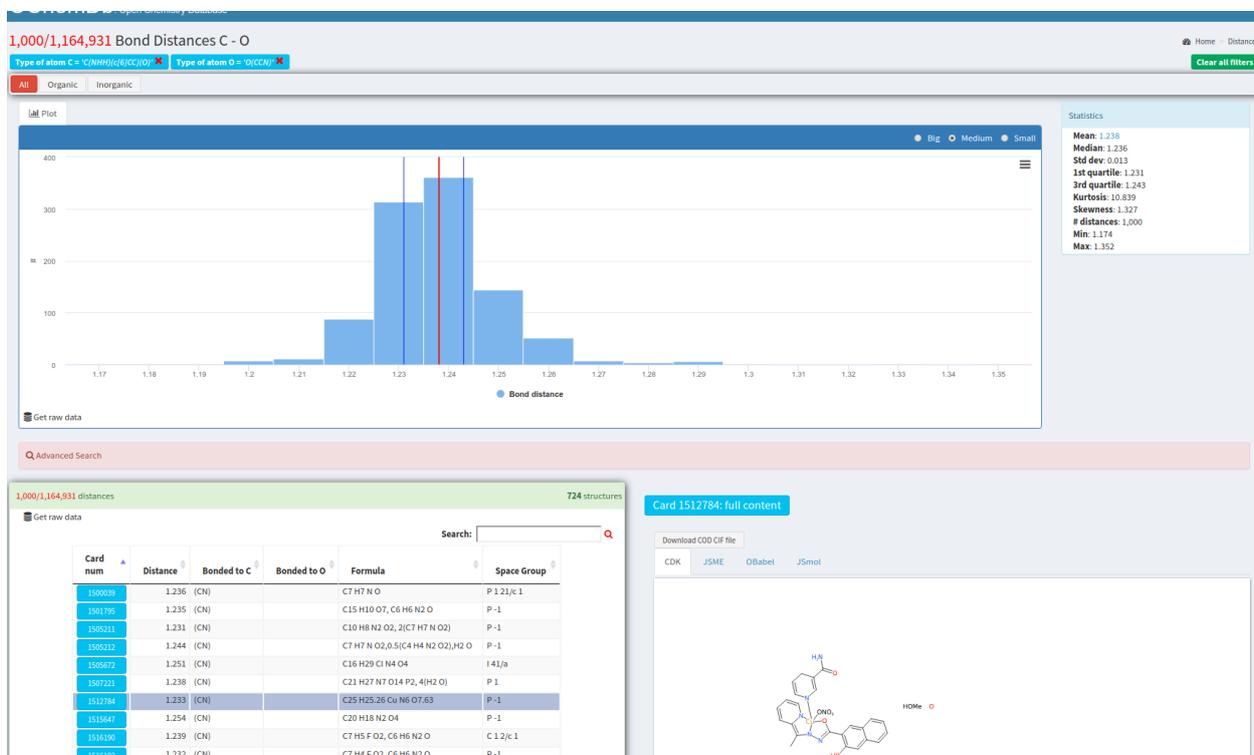
Atom type 1

Atom type 2

Exact Search

- Select C1-O1 as pair of bonded atoms
- Click on the *Search* button on the right side for exactly searching the corresponding atom types in the database.

- OChemDb will provide the result page where you can click on the result table below to show card information to verify results



The result page contains several statistical information to be visualized and checked.

Example 2

- Select *Basic* in the distance page

version: 0.16-2014
276,399 entries
COD:am.rcv.205841

Bond Distances

All Organic Inorganic

Search

Basic Molecule editing Atom types

Atom 1*

Atom 2*

First neighbours of Atom 1
Any None Select

First neighbours of Atom 2
Any None Select

Oxidation nr. Atom 1
Any

Oxidation nr. Atom 2
Any

Minimum distance

Maximum distance

Search

Table of chemical bonds
You can select the desired bond

- Insert K as *Atom 1* and O as *Atom 2*
- Click on *Select* for “*First neighbours of Atom 1*” and put in the textbox O
- Click on *Select* for “*First neighbours of Atom 2*” and put in the textbox S

Search

Basic Molecule editing Atom types

Atom 1*

K

Atom 2*

O

First neighbours of Atom 1
Any None **Select**
O

First neighbours of Atom 2
Any None **Select**
S

Oxidation nr. Atom 1
Any

Oxidation nr. Atom 2
Any

Minimum distance

Maximum distance

Search

Table of chemical bonds
You can select the desired bond

- Click on the *Search* button below

- o OCChemDb will provide the search results



Example 3

- Select the torsion O-C-O-C in the torsion page

OChemDb Open Chemistry Database

103.20.2018
120 entries
12.05.2016

Torsion Angles

Organic Inorganic

Search

Basic Molecule editing Atom types

Atom 1* Atom 2* Atom 3* Atom 4*

First neighbours of Atom 1 First neighbours of Atom 2 First neighbours of Atom 3 First neighbours of Atom 4

Oxidation nr. Atom 1 Oxidation nr. Atom 2 Oxidation nr. Oxidation nr.

Minimum angle Maximum angle

Search

Table of torsion angles
You can select the desired torsion

Show 50 entries

Bond	#	Entries	Min	Max	Mean	Std dev
C-C-C-C	1,251,513	126,709	-180	180	0.178	110.18
C-C-P-C	603,513	31,758	-180	180	-0.011	106.063
C-C-O-C	588,355	90,180	-180	180	0.357	111.604
C-C-N-C	587,335	93,150	-180	180	-0.148	111.288
C-C-N	363,299	89,284	-180	180	-0.547	115.875
C-C-O-C	236,364	50,702	-180	180	0.261	135.516
C-C-C-F	177,346	8,021	-180	180	0.125	104.277
F-C-S-O	94,816	5,744	-180	180	-0.456	112.543
C-C-N-O	83,117	13,172	-180	180	-0.152	117.795
C-C-S-O	79,833	11,449	-180	180	0.361	108.107
O-C-M-C	72,423	23,534	-180	180	-0.694	99.687
O-C-C-F	59,246	4,150	-180	180	0.092	107.295
N-C-M-C	53,713	15,086	-180	180	-0.367	127.002
N-C-C-O	52,737	19,819	-180	180	2.747	113.414
C-C-P-O	44,621	4,952	-180	180	-0.355	107.943
C-C-N-N	44,053	15,522	-180	180	-0.26	121.057
O-C-O-C	41,800	22,016	-180	180	-0.078	32.976
C-C-P-N	34,810	3,660	-180	180	0.33	107.195
N-C-C-N	34,096	15,584	-180	180	2.758	102.02
C-C-S-C	33,179	8,347	-180	180	-0.517	111.598

- The histogram corresponding to the statistical analysis of the search results will be provided.

103.20.2018
120 entries
12.05.2016

41,000/41,000 Torsion Angles O - C - O - C

Organic Inorganic

Histogram Plot Radar Plot

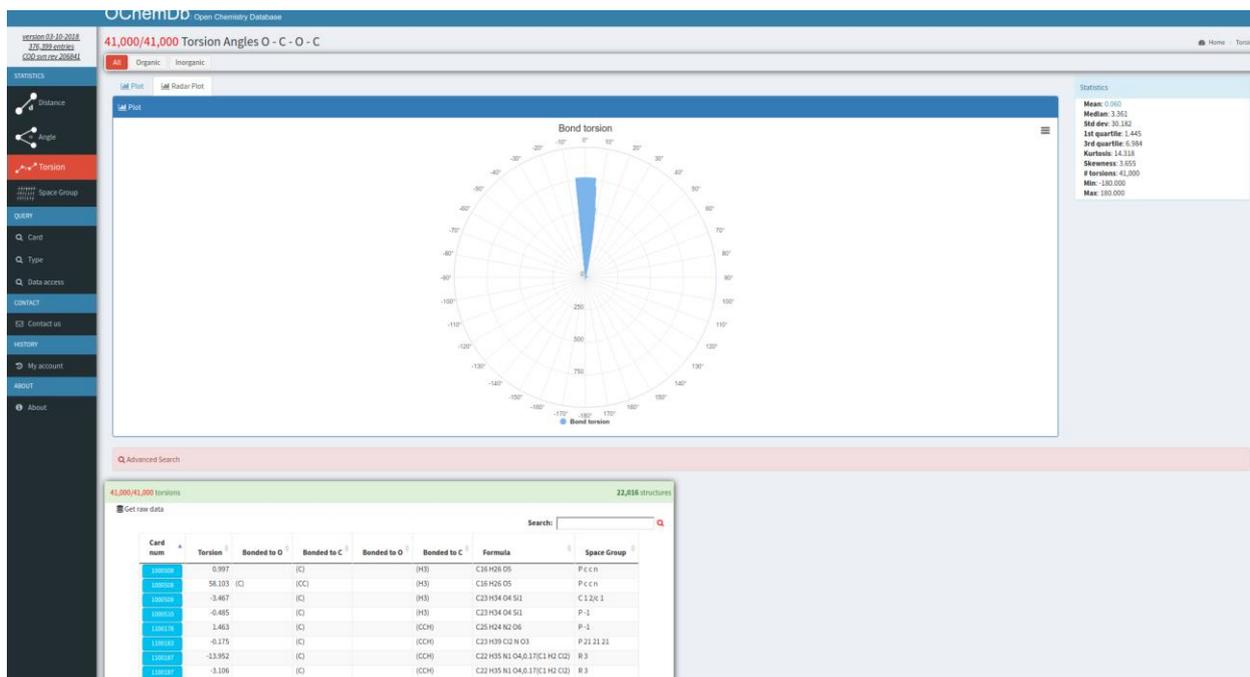
Statistics

- Mean: 0.000
- Median: 1.361
- Std dev: 50.102
- 1st quartile: 1.445
- 2nd quartile: 1.994
- Kurtosis: 14.318
- Skewness: 3.055
- # torsions: 41,000
- Min: -180.000
- Max: 180.000

41,000/41,000 torsions 22,016 structures

Card num	Torsion	Bonded to O	Bonded to C	Bonded to O	Bonded to C	Formula	Space Group
1196000	0.597	(C)				C16H26O5	P c c n
1196001	58.103	(C)	(C)			C16H26O5	P c c n
1196002	-3.467	(C)				C23H34O4S1	C 1 2/c 1
1196003	-0.485	(C)				C23H34O4S1	P -1
1196019	1.463	(C)				C25H24N2O6	P -1
1196020	-0.175	(C)				C23H39Cl2NO3	P 21 21 21
1196021	-13.952	(C)				C22H35N1O4O.17C1H2Cl2	R 3
1196022	-3.106	(C)				C22H35N1O4O.17C1H2Cl2	R 3
1196029	-61.243	(C)	(C)			C16H27N1O3	P -1
1196030	5.117	(C)				C19H23N1O4	P 1 21/a 1
1196031	4.869	(C)				C16H23N1O4	C 1 2/c 1
1196032	-0.625	(N)				C16H23N1O4	C 1 2/c 1
1196033	2.625	(N)				C16H23N1O3	P 1 21/c 1
1196034	-52.414	(C)	(C)	(C)		C21H29N1O3	P 1 21/c 1
1196035	-93.206	(C)	(C)	(C)		C21H29N1O3	P 1 21/c 1
1196036	11.597	(N)				C21H29N1O3	P 21 21 21

- Alternatively a radar plot can be visualized



- Details about one database card of the search results can be also inspected

