

# 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/>

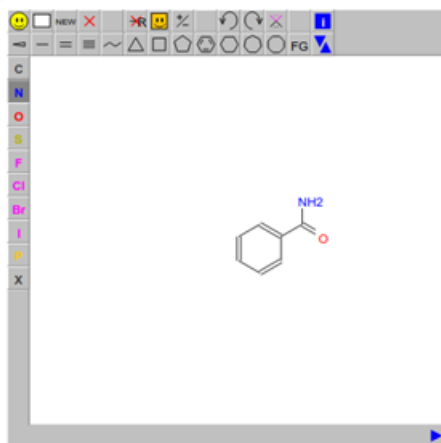
## Example 1

- Select *Molecular editing* in the distance page

The screenshot displays the OChemDb web interface. The top header reads 'OChemDb - Open Chemistry Database'. On the left sidebar, under the 'STATISTICS' section, the 'Distance' option is highlighted. Below this, other options like 'Angle', 'Torsion', and 'Space Group' are visible. The main content area is titled 'Bond Distances' and includes tabs for 'All', 'Organic', and 'Inorganic'. A search bar is present, and below it, three tabs are shown: 'Basic', 'Molecule editing' (which is circled in red), and 'Atom types'. The 'Molecule editing' tab is active, showing a workspace for drawing a molecule. The workspace includes a toolbar with various drawing tools and a list of elements (C, N, O, S, F, Cl, Br, I, P, X) on the left. The text 'The following steps can be carried out' is displayed, followed by two steps: '1) Draw molecule' and '2) Generate atom types'. A 'Generate' button is located next to the second step.

- 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

[Generate](#)

Select bond

- Ⓒ C2 - C3 : c[6](CNO)c[6](CH)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]CH)2(H)
- Ⓒ C2 - C7 : c[6](CNO)c[6](CH)2 - c[6](c[6]CC)c[6](CH)(H)
- Ⓒ C6 - C7 : c[6](c[6]CH)2(H) - c[6](c[6]CC)c[6](CH)(H)
- Ⓒ C5 - C6 : c[6](c[6]CH)2(H) - c[6](c[6]CH)2(H)
- Ⓒ C4 - C5 : c[6](c[6]CH)2(H) - c[6](c[6]CH)2(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](CH)2
- Ⓐ 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]CH)2(H) - H(c[6]CC)
- Ⓒ C5 - H5 : c[6](c[6]CH)2(H) - H(c[6]CC)
- Ⓒ C6 - H6 : c[6](c[6]CH)2(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

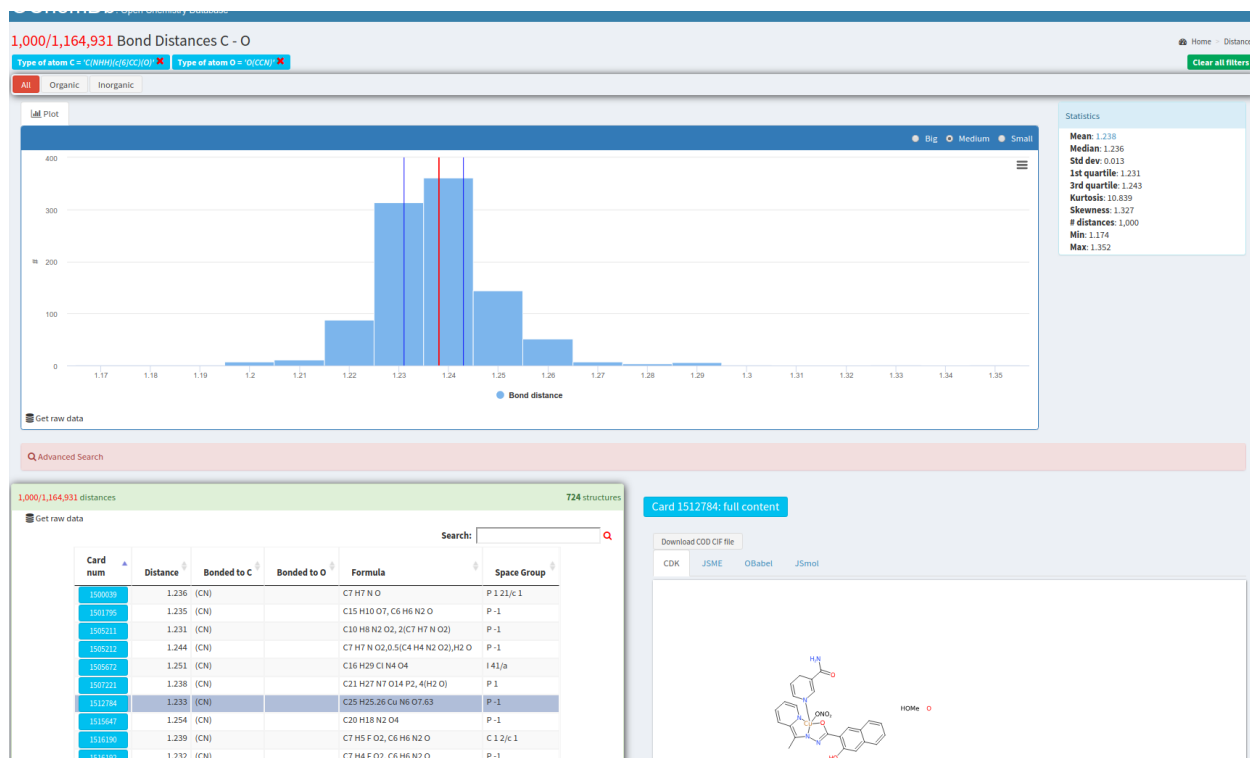
Atom type 2

Exact Search

[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

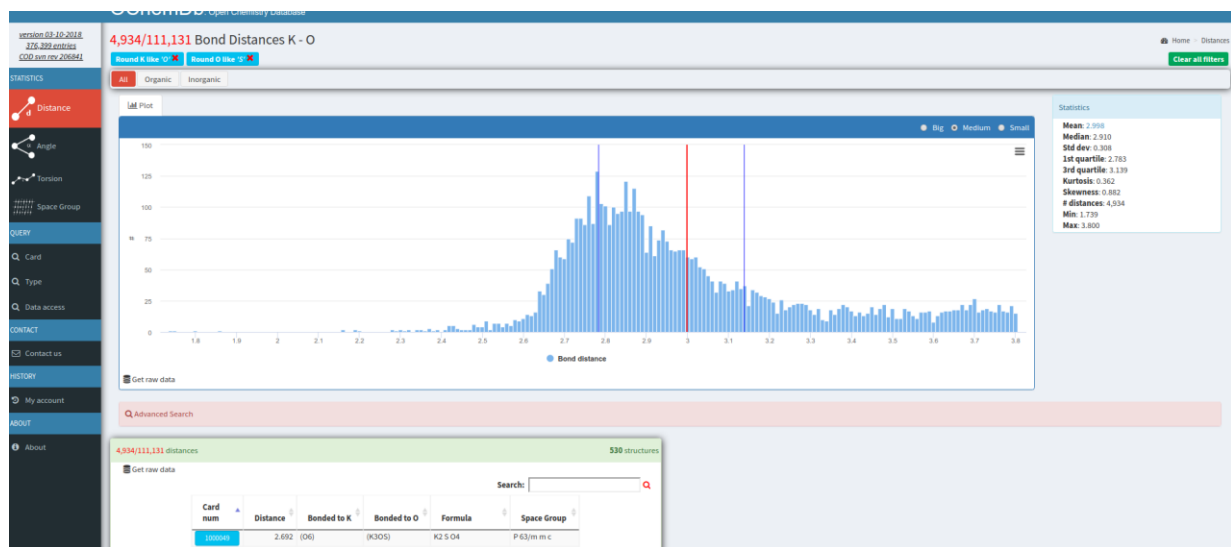
The screenshot shows the 'Bond Distances' web application. The top header includes the version '03-10-2018', the number of entries '476,399 entries', and the DOI '10.26434/chemrxiv-2018-03-10-2018'. The left sidebar contains navigation links: 'Distance', 'Angle', 'Torsion', 'Space Group', 'Query', 'Card', 'Type', 'Data access', 'Contact', 'Contact us', 'History', and 'My account'. The main content area is titled 'Bond Distances' and has tabs for 'Basic', 'Molecule editing', and 'Atom types'. The 'Basic' tab is active. It contains two columns of search criteria. The left column is for 'Atom 1\*' and the right column is for 'Atom 2\*'. Each column has a text input field for the atom symbol, a dropdown for 'First neighbours of Atom 1' and 'First neighbours of Atom 2' (with options 'Any', 'None', 'Select'), a dropdown for 'Oxidation nr. Atom 1' and 'Oxidation nr. Atom 2' (with an option 'Any'), and a text input for 'Minimum distance' and 'Maximum distance'. A 'Search' button is at the bottom left. Below the search area, there is a section titled 'Table of chemical bonds' with the subtitle '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

This screenshot shows the same 'Bond Distances' web application interface, but with the search criteria filled in. In the 'Atom 1\*' column, the text input contains 'K', the 'First neighbours of Atom 1' dropdown is set to 'Select' and the text input below it contains 'O', the 'Oxidation nr. Atom 1' dropdown is set to 'Any', and the 'Minimum distance' text input is empty. In the 'Atom 2\*' column, the text input contains 'O', the 'First neighbours of Atom 2' dropdown is set to 'Select' and the text input below it contains 'S', the 'Oxidation nr. Atom 2' dropdown is set to 'Any', and the 'Maximum distance' text input is empty. The 'Search' button is still at the bottom left. The 'Table of chemical bonds' section is still at the bottom.

- Click on the *Search* button below

- OCChemDb will provide the search results



## Example 3

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

OChemDb Open Chemistry Database

103.10.2018  
208 entries  
1.000 km km 200561

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	1,251,513	126,709	-180	180	0.178	110.18
C-C-P	603,513	31,758	-180	180	-0.011	106.063
C-C-O	588,355	90,180	-180	180	0.357	111.694
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-O-C	236,364	50,702	-180	180	0.261	135.516
C-C-F	177,346	8,021	-180	180	0.125	104.277
F-S-O	94,016	5,744	-180	180	-0.456	112.543
C-N-O	83,117	13,172	-180	180	-0.102	117.795
C-S-O	79,833	11,449	-180	180	0.361	108.107
O-N-C	72,423	23,534	-180	180	-0.694	99.687
O-C-F	59,246	4,150	-180	180	0.092	107.295
N-C-N	53,713	15,086	-180	180	-0.367	127.002
N-C-O	52,737	19,819	-180	180	2.747	113.414
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	124.027
O-C-O-C	41,800	22,016	-180	180	-0.078	32.978
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	33,379	8,347	-180	180	-0.517	111.598

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

version 03-10-2018  
135,209 entries  
1.000 km km 200561

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

Organic Inorganic

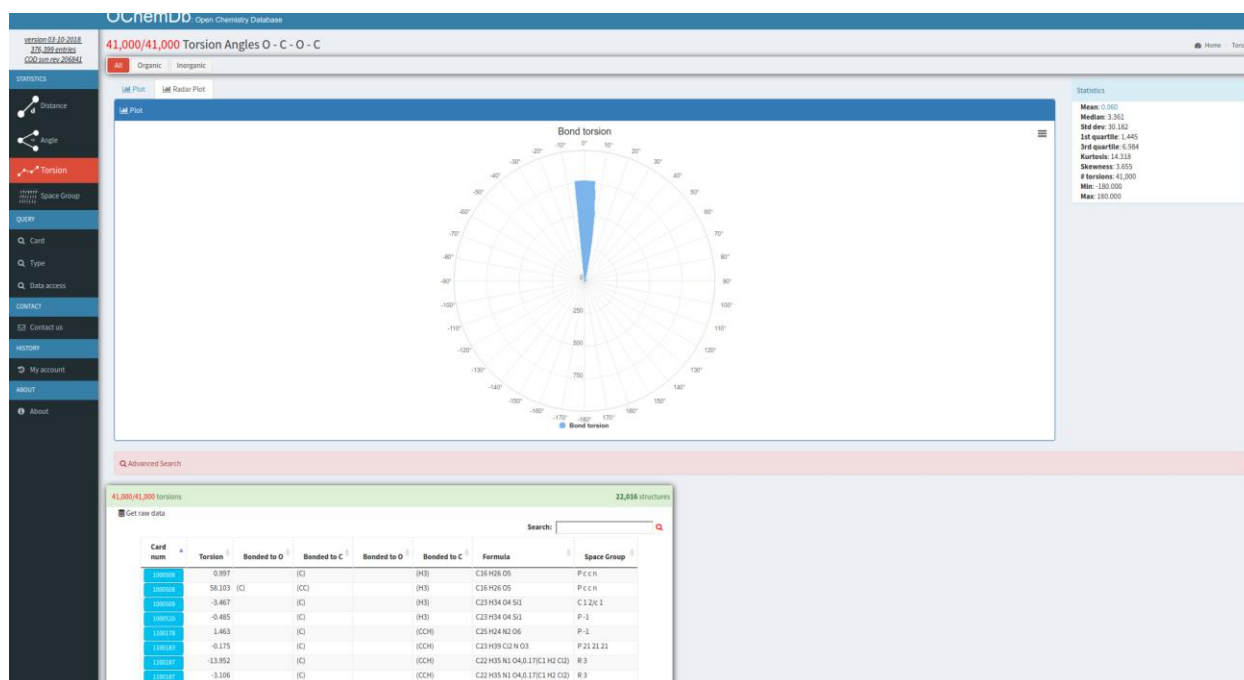
Statistics

Mean: 0.003  
Median: 1.361  
Std dev: 50.302  
1st quartile: 1.445  
2nd quartile: 1.594  
Kurtosis: 14.518  
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
139890	0.997	(C)		(H3)		C16 H26 O5	Pc c n
139891	58.103 (C)	(CC)		(H3)		C16 H26 O5	Pc c n
139892	-3.467	(C)		(H3)		C23 H34 O4 S1	C 1 2/c 1
139893	-0.485	(C)		(H3)		C23 H34 O4 S1	P -1
139894	1.483	(C)		(CC)		C25 H24 N2 O6	P -1
139895	-0.175	(C)		(CC)		C23 H39 Cl2 N O3	P 21 21 21
139896	-13.952	(C)		(CC)		C22 H35 N1 O4 O.17(C1 H2 Cl2)	R 3
139897	-3.106	(C)		(CC)		C22 H35 N1 O4 O.17(C1 H2 Cl2)	R 3
139898	41.243 (C)	(CC)		(CH)		C16 H27 N1 O3	P -1
139899	5.117	(C)		(CC)		C19 H23 N1 O4	P 1 21/a 1
139900	-4.869	(C)		(H3)		C16 H23 N1 O4	C 1 2/c 1
139901	-0.625	(N)		(C3)		C16 H23 N1 O4	C 1 2/c 1
139902	2.625	(N)		(C3)		C16 H23 N1 O3	P 1 21/c 1
139903	-52.414 (C)	(CC)	(C)	(CH)		C21 H29 N1 O3	P 1 21/c 1
139904	-93.206 (C)	(CC)	(C)	(CH)		C21 H29 N1 O3	P 1 21/c 1
139905	11.597	(N)		(CC)		C21 H29 N1 O3	P 21 21 21

- Alternatively a radar plot can be visualized



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

Get raw data

Card num	Torsion	Bonded to O	Bonded to C	Bonded to O	Bonded to C	Formula	Space Group
1296000	0.997	(C)			(H)	C16 H26 O5	P c c n
1296001	58.103	(C)	(CC)		(H)	C16 H26 O5	P c c n
1296002	-3.467	(C)	(H)		(H)	C23 H34 O4 S1	C 1 2/c 1
1296003	-0.485	(C)			(H)	C23 H34 O4 S1	P -1
1296004	1.463	(C)			(CH)	C25 H24 N2 O6	P -1
1296005	-0.175	(C)			(CH)	C23 H29 N2 O3	P 21 21 21
1296006	-13.953	(C)			(CH)	C23 H35 N1 O4 0.17C1 H2 C2	R 3
1296007	-3.106	(C)			(CH)	C23 H35 N1 O4 0.17C1 H2 C2	R 3
1296008	61.243	(C)	(CC)		(CH)	C16 H27 N1 O3	P -1
1296009	5.117	(C)			(C)	C19 H23 N1 O4	P 1 21/n 1
1296010	-4.869	(C)			(H)	C16 H23 N1 O4	C 1 2/c 1
1296011	-0.625	(N)			(C)	C16 H23 N1 O4	C 1 2/c 1
1296012	2.625	(N)			(C)	C16 H23 N1 O3	P 1 21/c 1
1296013	-52.414	(C)	(CC)	(C)	(CH)	C21 H29 N1 O3	P 1 21/c 1
1296014	-93.206	(C)	(CC)	(C)	(CH)	C21 H29 N1 O3	P 1 21/c 1
1296015	11.597	(N)			(CH)	C21 H29 N1 O3	P 21 21 21
1296016	-61.571	(C)	(CC)		(H)	C10 H14 O4	P 1 21/n 1
1296017	-0.431	(C)			(H)	C19 H24 O8	P 21 21 21
1296018	-2.426	(C)			(CH)	C19 H24 O8	P 21 21 21
1296019	1.166	(C)			(H)	C13 H9 N O5	P -1
1296020	-1.086	(C)			(H)	C30 H32 N4 O4	P -1
1296021	0.552	(C)			(CH)	C30 H32 N4 O4	P -1
1296022	61.337	(C)	(CH)		(H)	C31 H32 O7	P 21 21 21
1296023	-3.978	(C)			(H)	C31 H32 O7	P 21 21 21
1296024	-89.804	(C)	(CH)		(C)	C14 H18 O7	P -1
1296025	-0.059	(C)			(C)	C14 H18 O7	P -1
1296026	-0.159	(C)			(H)	C14 H18 O7	P -1
1296027	2.529	(C)			(CH)	C14 H18 O7	P -1
1296028	-0.086	(C)			(H)	C11 H14 O5	P 21 21 21
1296029	-4.130	(C)	(N)		(C)	C17 H17 C N O6	C 1 2/c 1
1296030	-5.188	(N)			(CH)	C30 H38 N2 O5	P -1
1296031	3.745	(N)			(CH)	C20 H28 N2 O4	P 21 21 21
1296032	-8.329	(N)			(C)	C20 H28 N2 O4	P 21 21 21
1296033	-30.741	(C)	(C)		(CH)	C19 H21 C O6 P	P 1 21/c 1
1296034	-1.101	(C)			(H)	C53 H71 Co N6 O14	P 21 21 21
1296035	0.819	(C)			(H)	C53 H71 Co N6 O14	P 21 21 21
1296036	-11.047	(C)			(H)	C53 H71 Co N6 O14	P 21 21 21
1296037	-3.298	(C)			(H)	C53 H71 Co N6 O14	P 21 21 21
1296038	9.088	(C)			(H)	C53 H71 Co N6 O14	P 21 21 21
1296039	-2.559	(C)			(C)	C23 H25 C N O7	P 1 21/n 1
1296040	6.405	(C)	(N)		(C)	C17 H17 C N O6	C 1 2/c 1

Card 1100187: full content

Download CSD CIF file

CDK JSME OLabel JSmol

Chemical structure visualization of a complex molecule.

Information

Name: p-Nitro-3-yl-1,3,5-trimethylcyclohexene-2,3-dicarboximide-5-carboxylate dichloromethane solvate

Space group: P 1

Chemical formula: C22 H35 N1 O4 0.17C1 H2 C2

Crystal system: Trigonal (hexagonal axes)

Cell Parameters

a: 28.224 Å, b: 28.224 Å, c: 15.262 Å

α: 90°, β: 90°, γ: 120°

Info

Z: 18

p(CaK): 16.502

Volume: 10528.808

Color: colorless

Calc. density: 1.178

Reference

Authors: Bach, Thorsten Bergmann, Hermann Gress, Benjamin Harms, Klaus Herdewick, Eberhardt

Journal: Synthesis, 2002, 9, 1395-1405