TUTORIAL OChemDb

To access to OChemDb you should go to the url http://www.ba.ic.cnr.it/softwareic/:
- o Insert your credentials (if not inserted before) in the sidebar on the right
- o Go to our portal http://www.ba.ic.cnr.it/ochemdb/

Example 1

- o Select *Molecular editing* in the distance page

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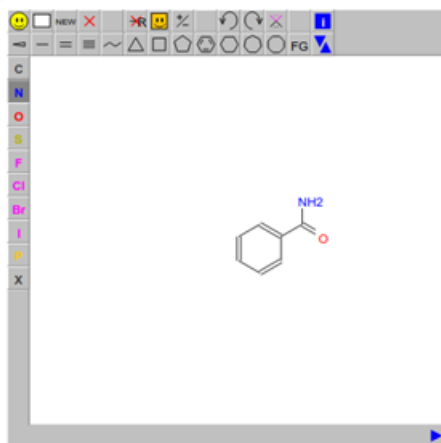
l) Draw molecule

o   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

C(NHH)(c[6]CC)(O)

Atom type 2

O(CCN)

Exact Search ☑

Search

o   Select C1-O1 as pair of bonded atoms
o   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
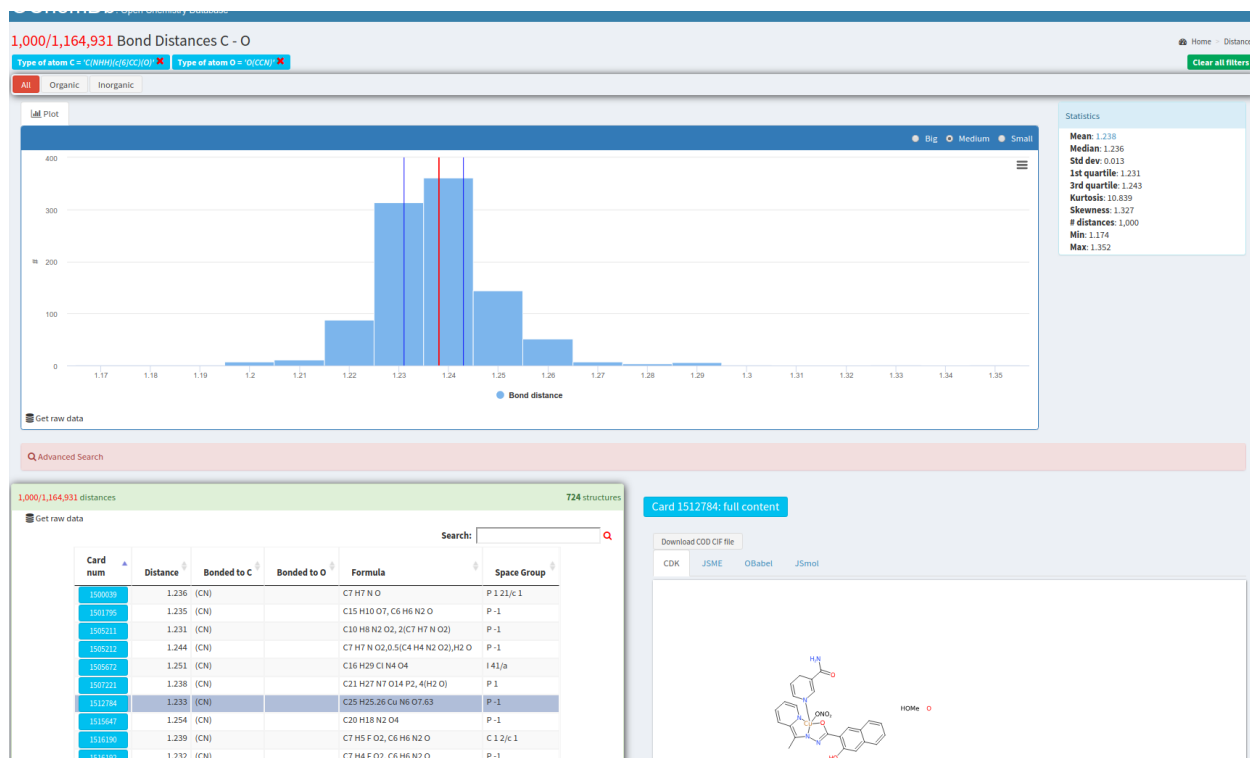
The result page contains several statistical information to be visualized and checked.
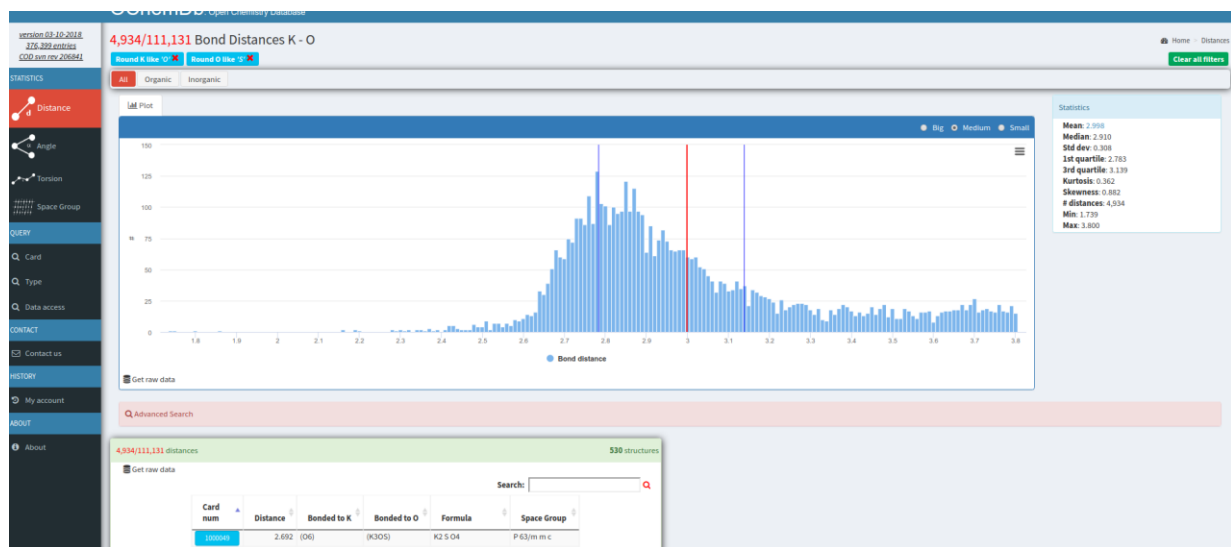
Example 2

o Select *Basic* in the distance page

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

o Click on the *Search* button below

o OChemDb will provide the search results

Example 3

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

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

- Alternatively a radar plot can bee visualized
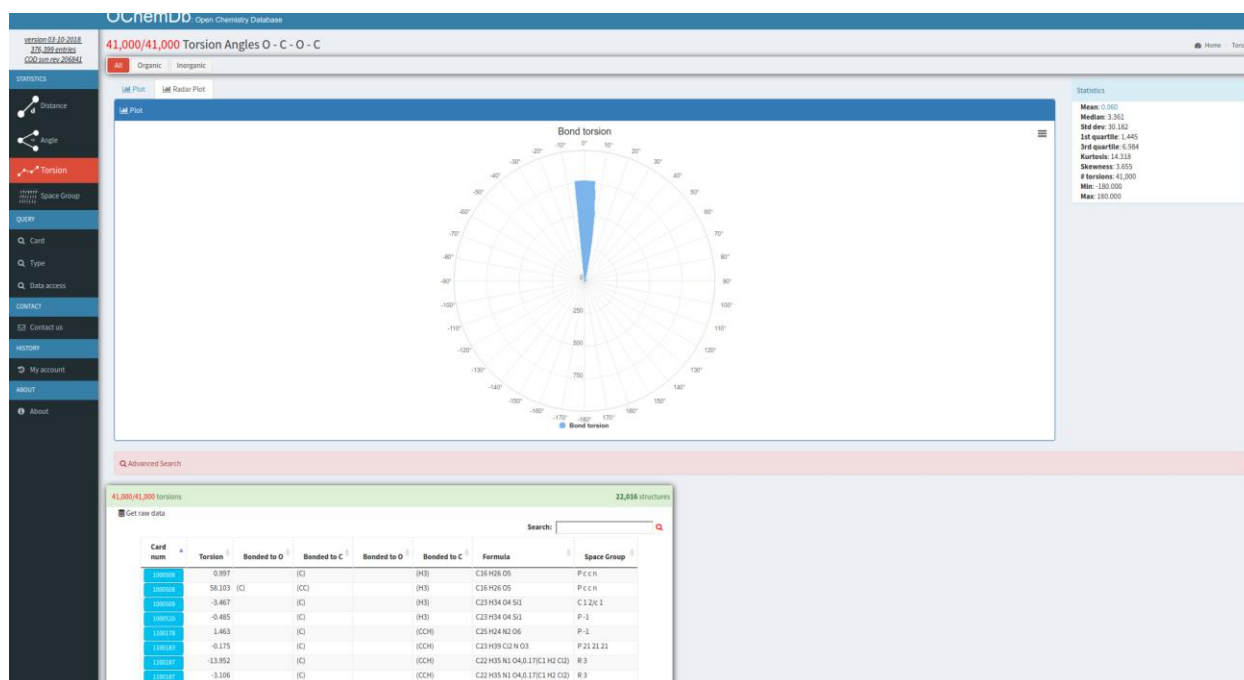
- Details about one database card of the search results can be also inspected