NCiweb
NCiplot web interface

NCIweb

We will analyze interactions in biosystems using nciweb

https://lct-webtools.sorbonne-universite.fr/nciweb/index.php

Exercise 1. Analysis of different non-covalent interaction types
Files are available at: https://www.lct.jussieu.fr/pagesperso/contrera/label2023/ex1.zip

1.1. We are now going to analyze different systems that you already know. Describe the different interactions you see, identifying them with what you expected:

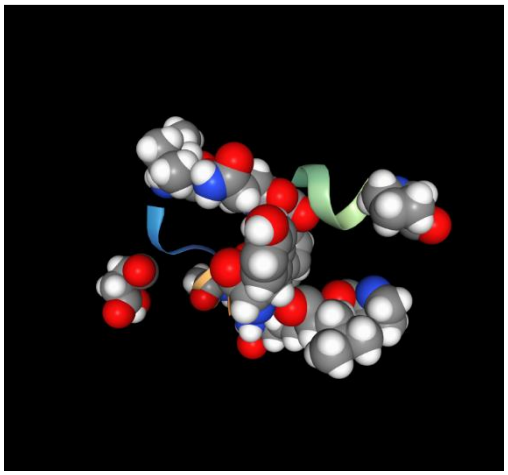
- Water dimer
- Benzene dimer (parallel conformation)
- Bicyclooctene

1.2. With what you have learnt in the previous exercise, describe the interactions you find in more complex situations:

- Adenine-thymine
- Phenol dimer
- Formic acid dimer

Exercise 2. Stretching bonds: the hydrogen molecule

You can download the wfn files at
https://www.lct.jussieu.fr/pagesperso/contrera/label2025/H2.zip
This exercise is a connection with the model system in the python exercise. We will now study H_2 molecule at several distances.
Calculate NCI at d=2.0 and 2.5Å. What changes do you expect in the isosurfaces (size, colour)?



Exercise 3. Biosystems

Upload the file 3NIR (pdbs can be uploaded directly by its name) and analyze the intermolecular interactions with what you have learnt. Do not forget to add the hydrogens!
You can also visualize the ligand-protein interactions in 1STP. Since these files are big, results are directly available here. In order to visualize the ligand, you can increase the size of its atoms (*b&s sizes*).