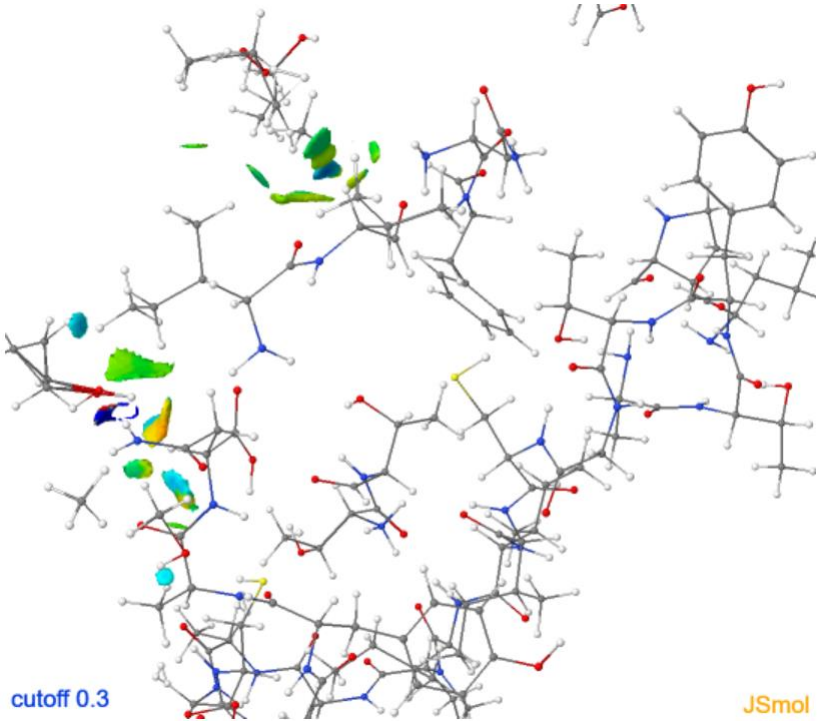
Non covalent interactions

Computational Lab



Julia Contreras García &

Peter Reinhardt

CNRS/Sorbonne Université

Instructions

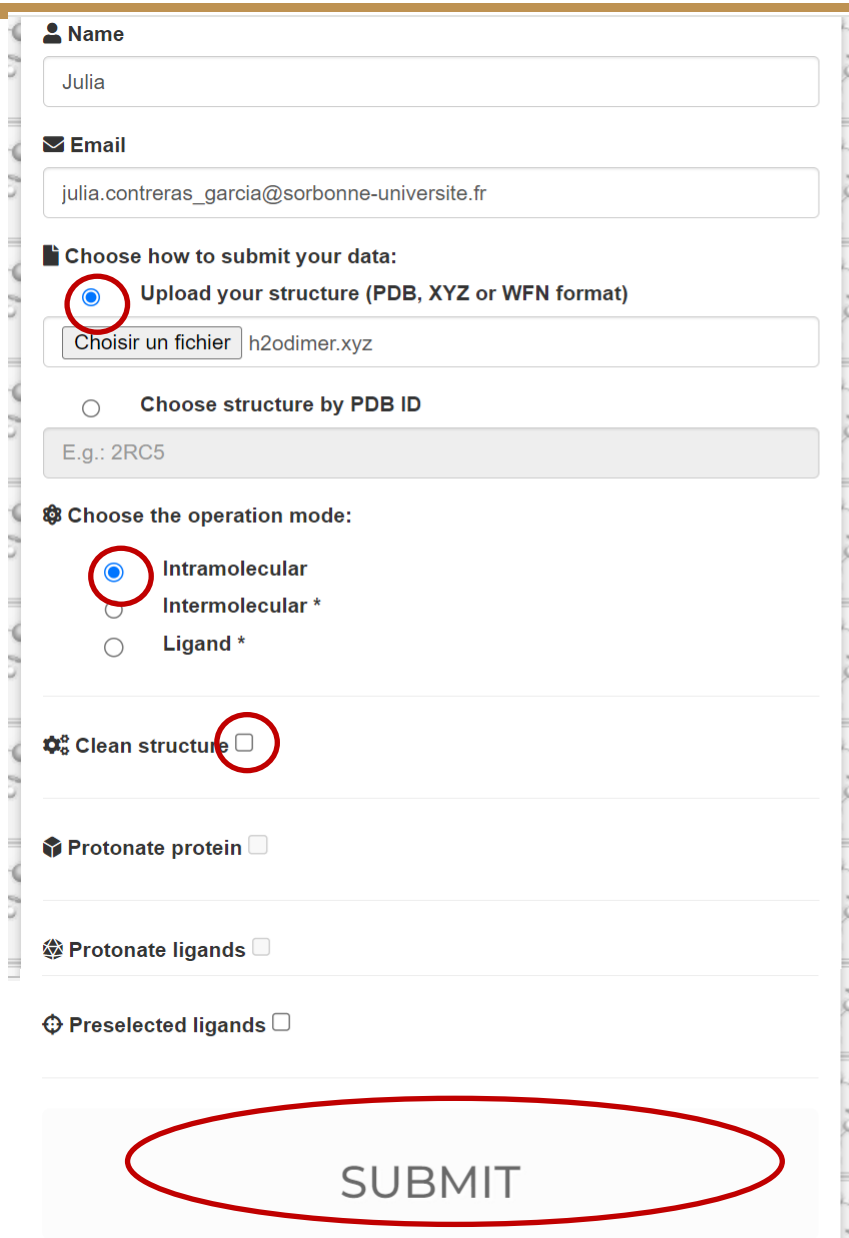
In these exercises we will analyze non-covalent interactions in real molecules, following the models done in Jupiter.

You will be able to do it via our web server NCIweb at:

https://nciweb.dsi.upmc.fr/index.php

- Exercise 1

Loading a file



NCIweb is a web implementation of the popular **NCIplot** code. At the moment, **NCIweb** works with promolecular densities. It provides a representation of the non-covalent interactions of a system based on the reduced density gradient of the electron density. More information on the **NCIplot** code and the theoretical background of the method can be found here.

What do I need to use NCIweb?

To use **NCIweb** you simply need a PDB or XYZ structure to upload, on which the analysis will be performed. You can also fetch a PDB file directly with its PDB ID. Only single structure PDBs are accepted (not NMR ensembles). If everything works fine, you will receive an email with a link to **NCIwebResults** web site. You will find an interface to visualize your results as well as the possibility to download all the result files including a simple VMD script for visualization. Three operation modes are available:

1. Running in **Intramolecular mode** will study all non-covalent interactions in the system.
2. Running in **Intermolecular mode** will require manual definition of two fragments, and will only study interactions between them.
3. Running in **Ligand mode** will require manual definition of a ligand and a receptor, and will only study interactions between the ligand and the receptor in the proximity.

For **PDB files only**, additional options are available:

- The *clean structure* checkbox will selectively remove non-protein fragments from the structure, enabling more processing options.

With our preprocessing pipeline, a PDB structure from a data bank may be directly analyzed. Nevertheless, we recommend manual and careful preparation and protonation whenever possible.

*** Only available if data is updated in PDB format.**
PDB file. This will skip visual selection of ligands.

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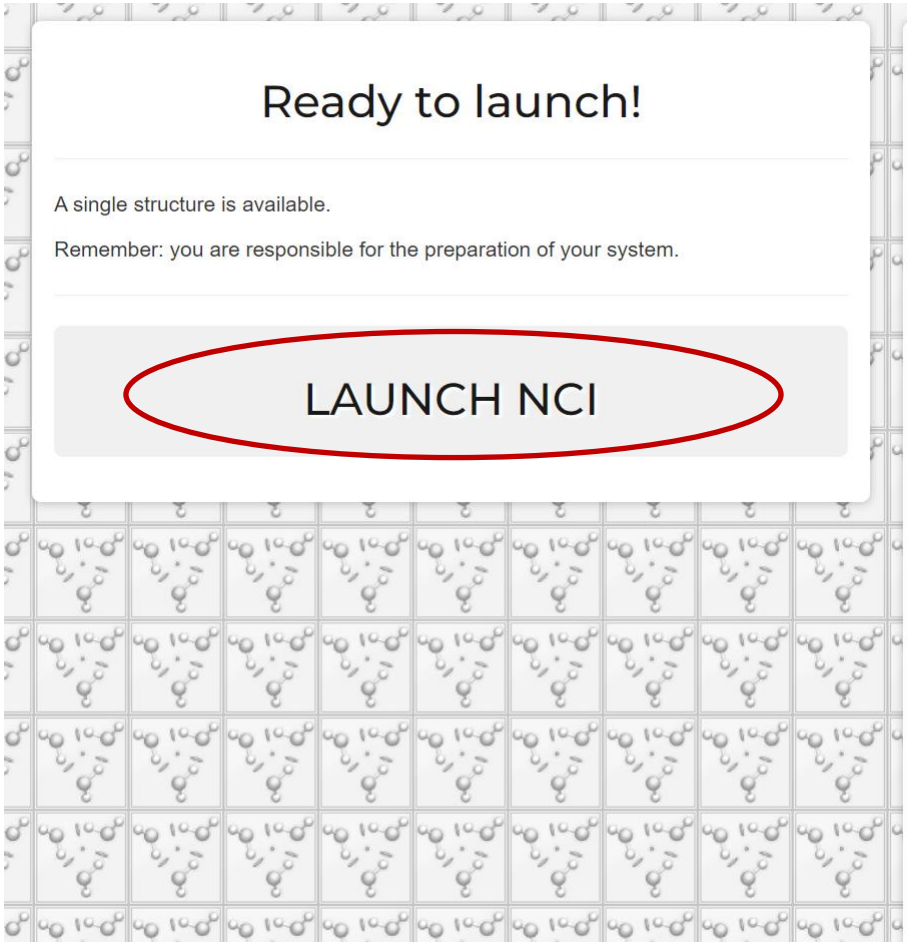
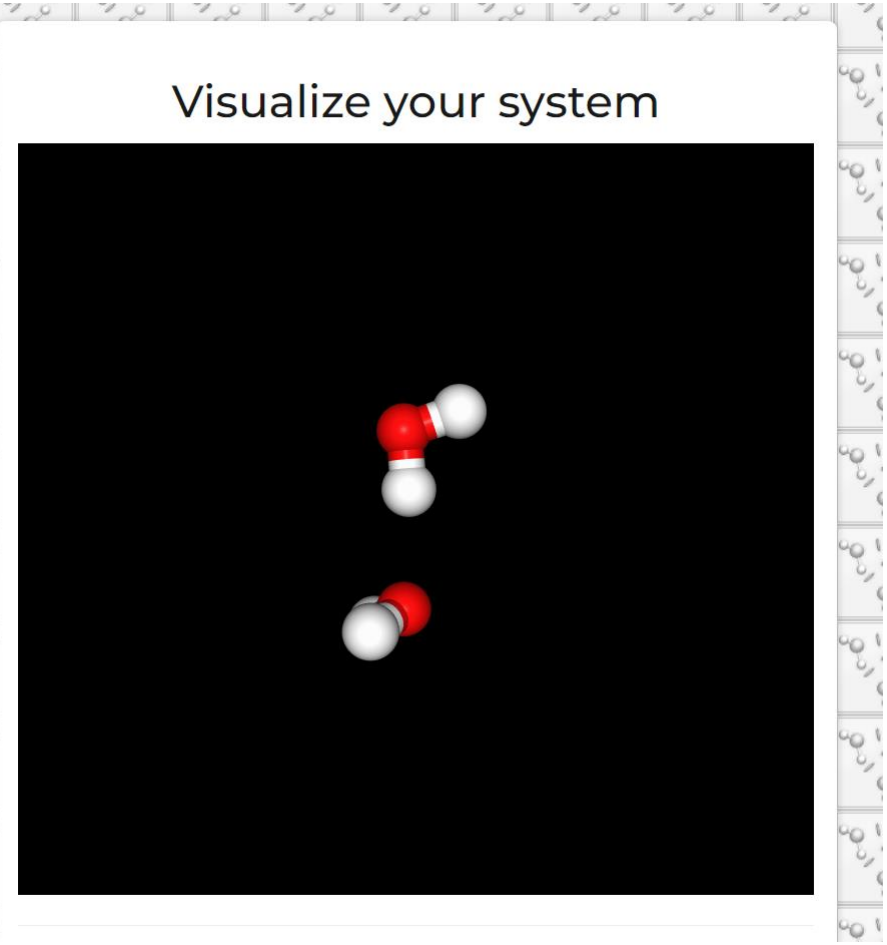
*** Only available if data is updated in PDB format.**

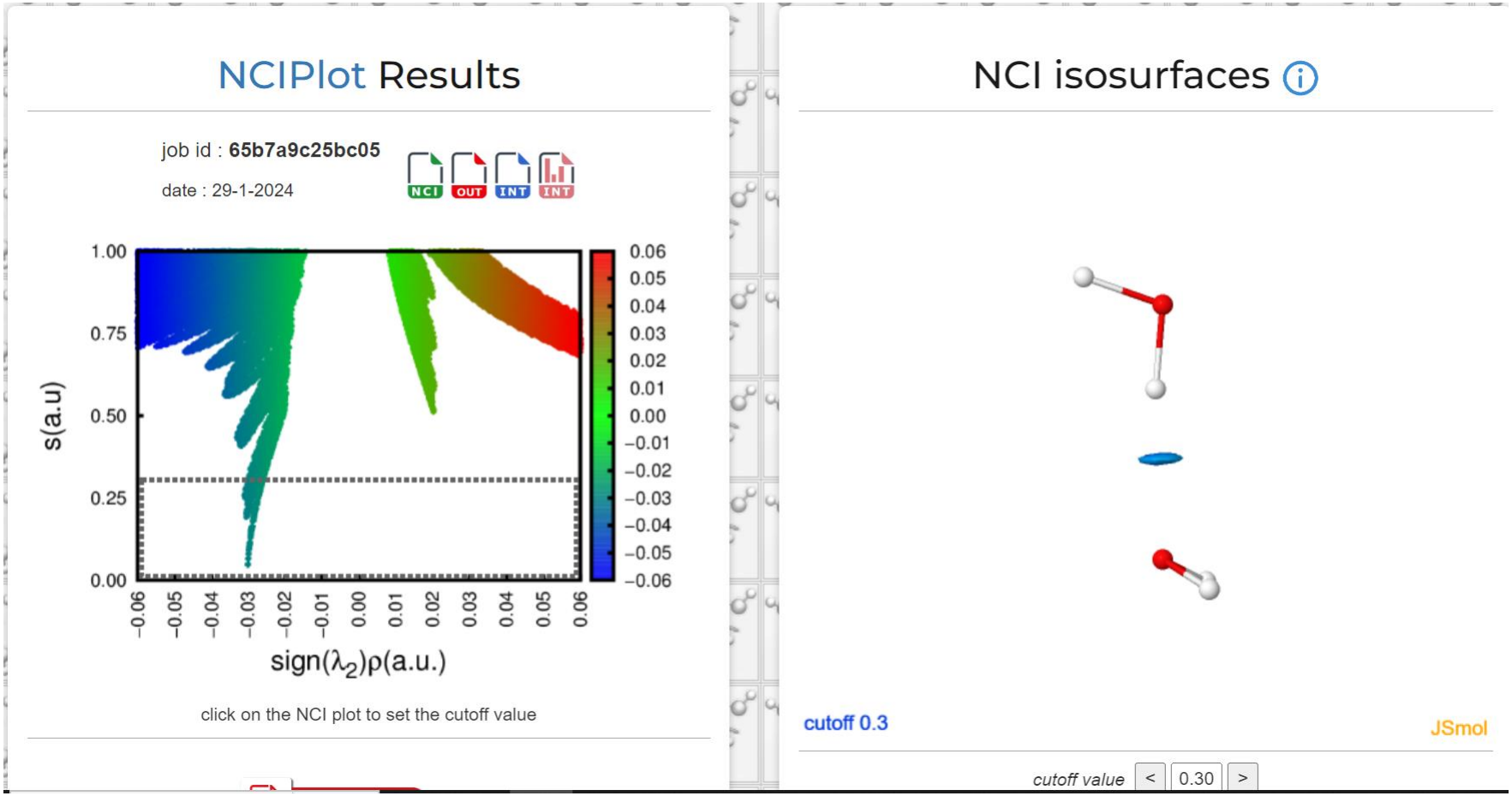
Loading a file





Water dimer

- https://nciweb.dsi.upmc.fr/to_download/65b7a9c25bc05/



Benzene dimer

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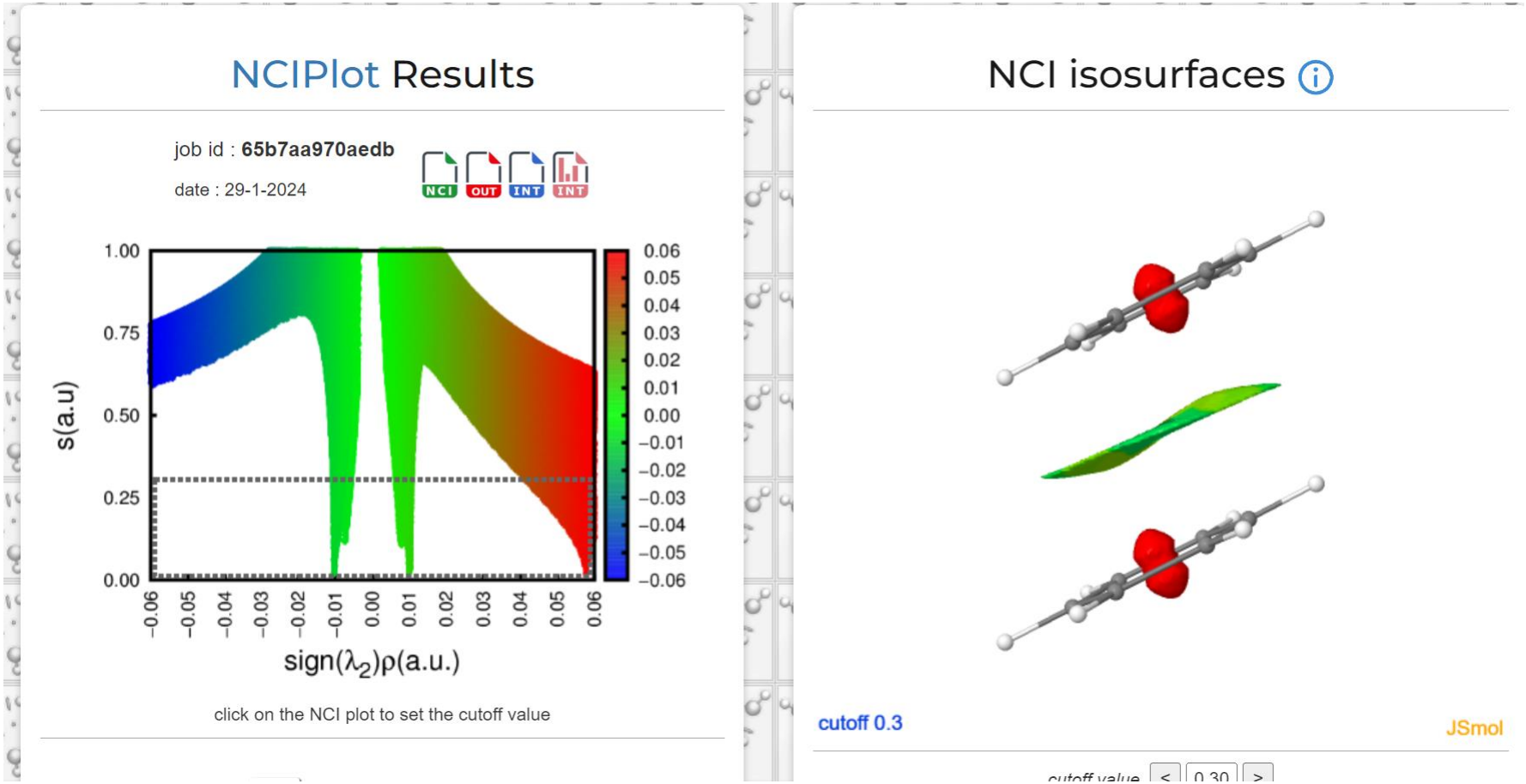

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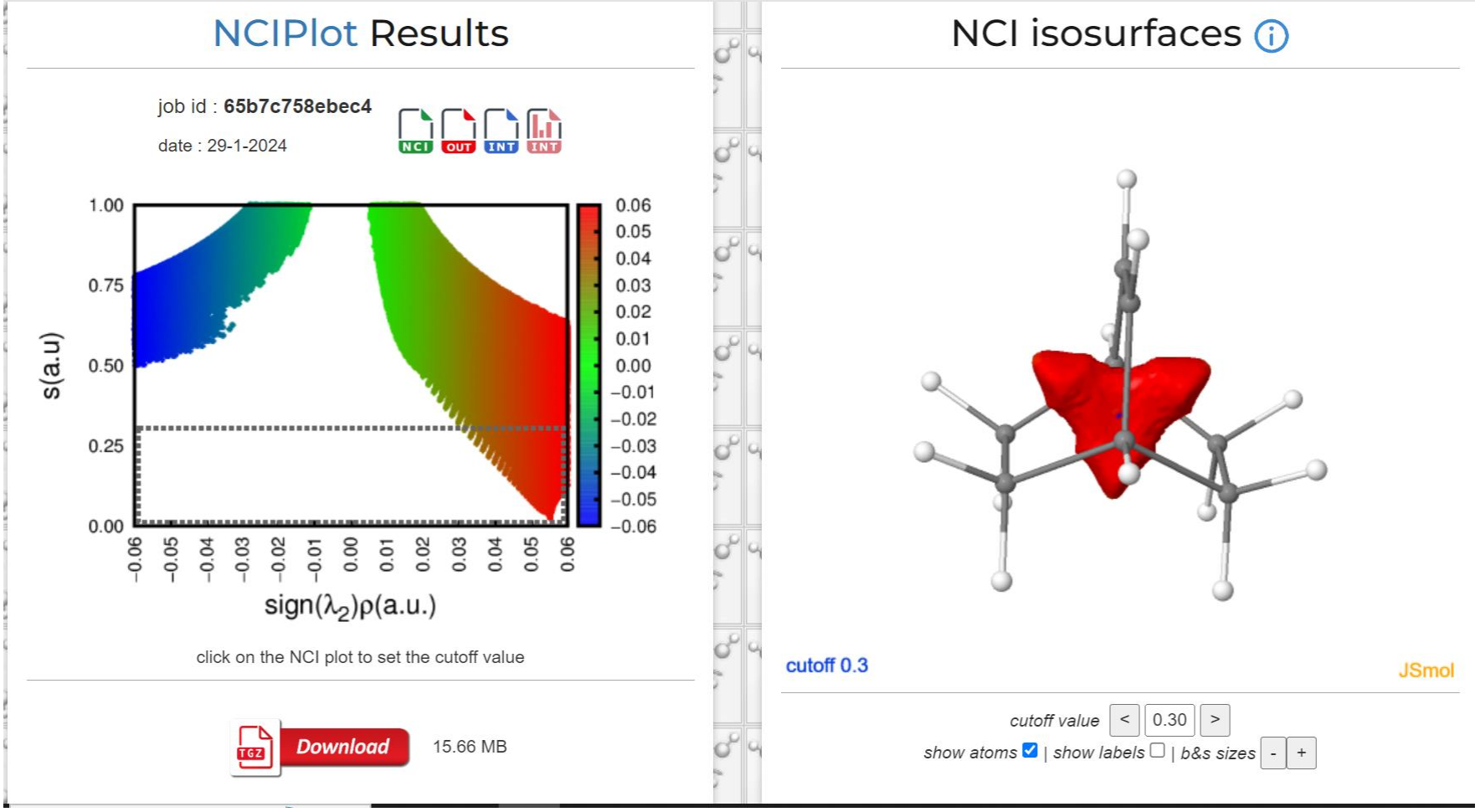

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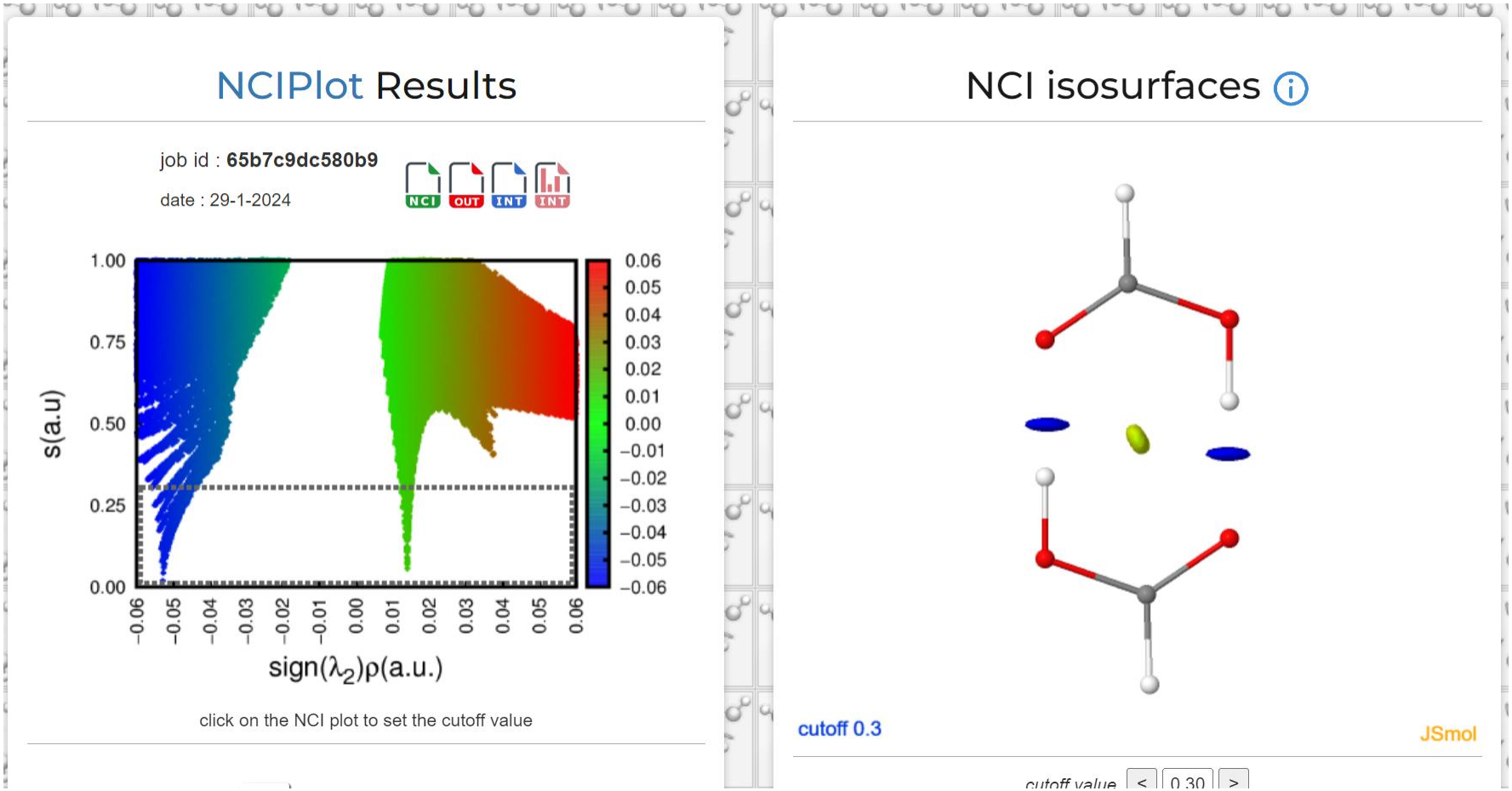

- https://nciweb.dsi.upmc.fr/to_download/65b7ca13a2df6/

NCIPlot Results

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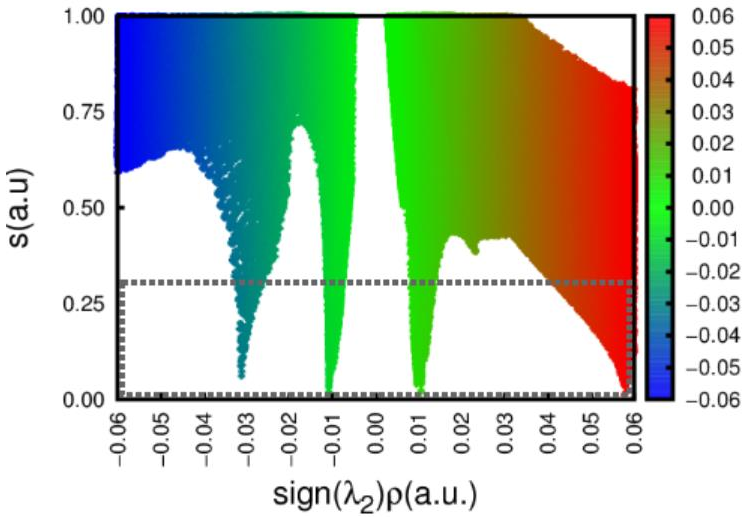
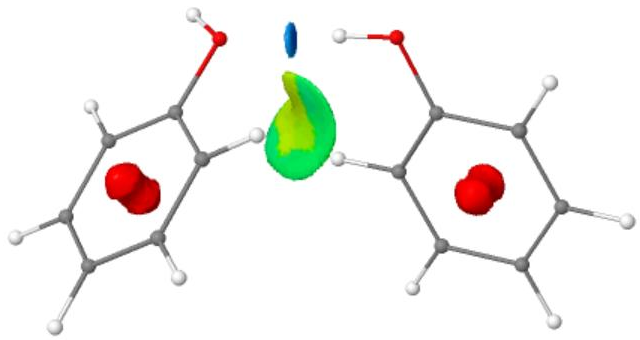
date : 29-1-2024



click on the NCI plot to set the cutoff value

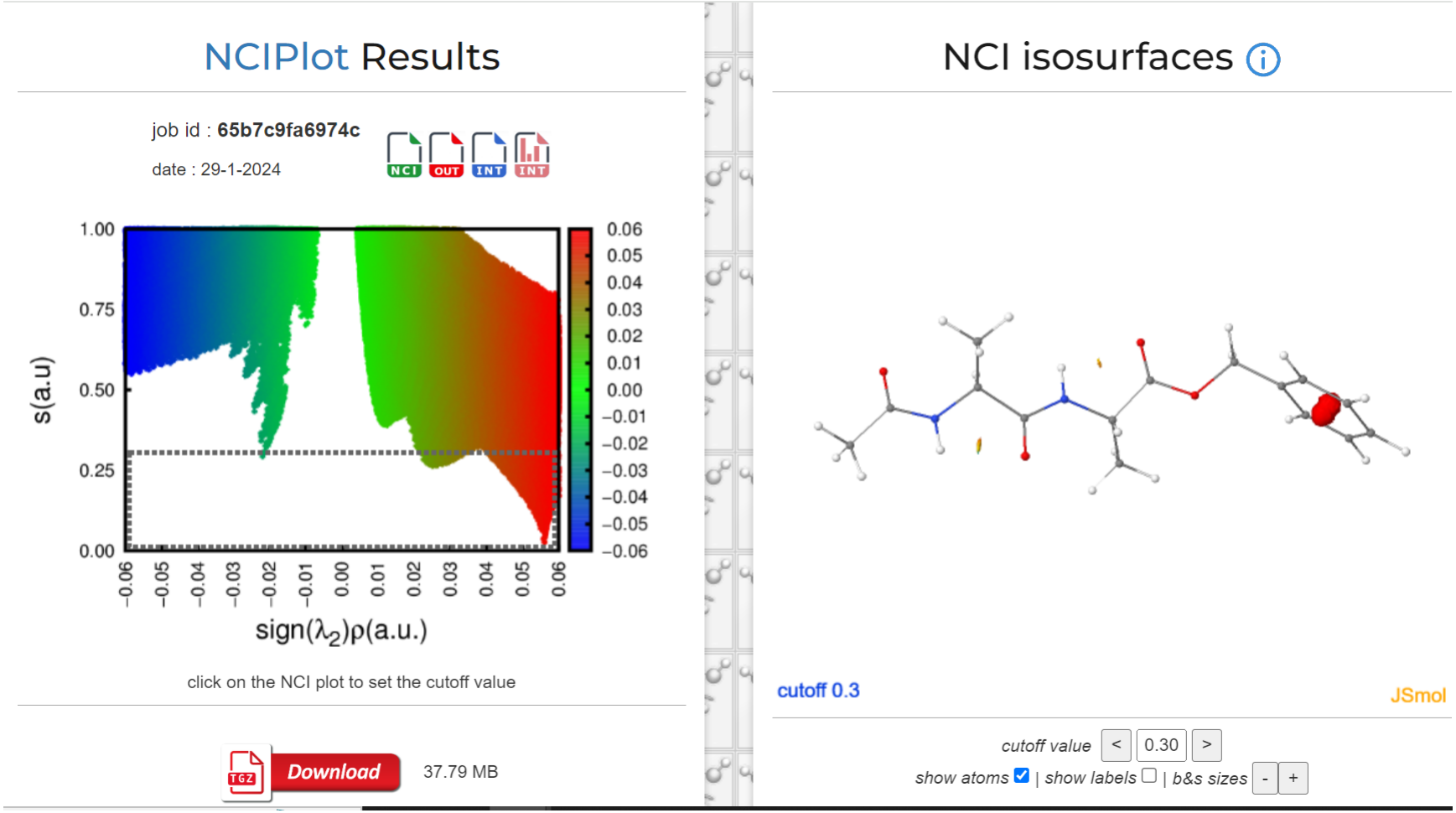
NCI isosurfaces



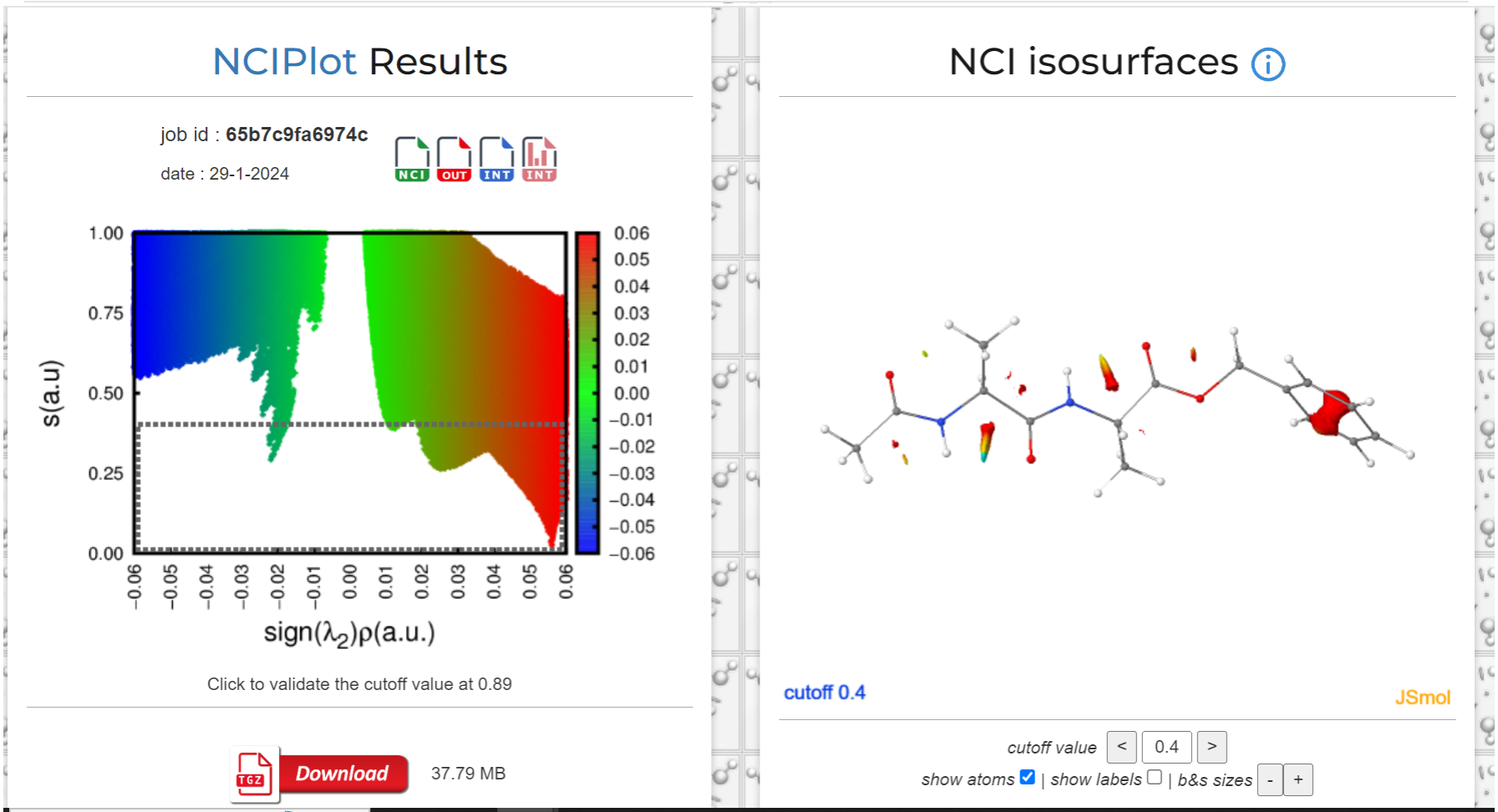
cutoff 0.3

JSmol

- https://nciweb.dsi.upmc.fr/to_download/65b7c9fa6974c/

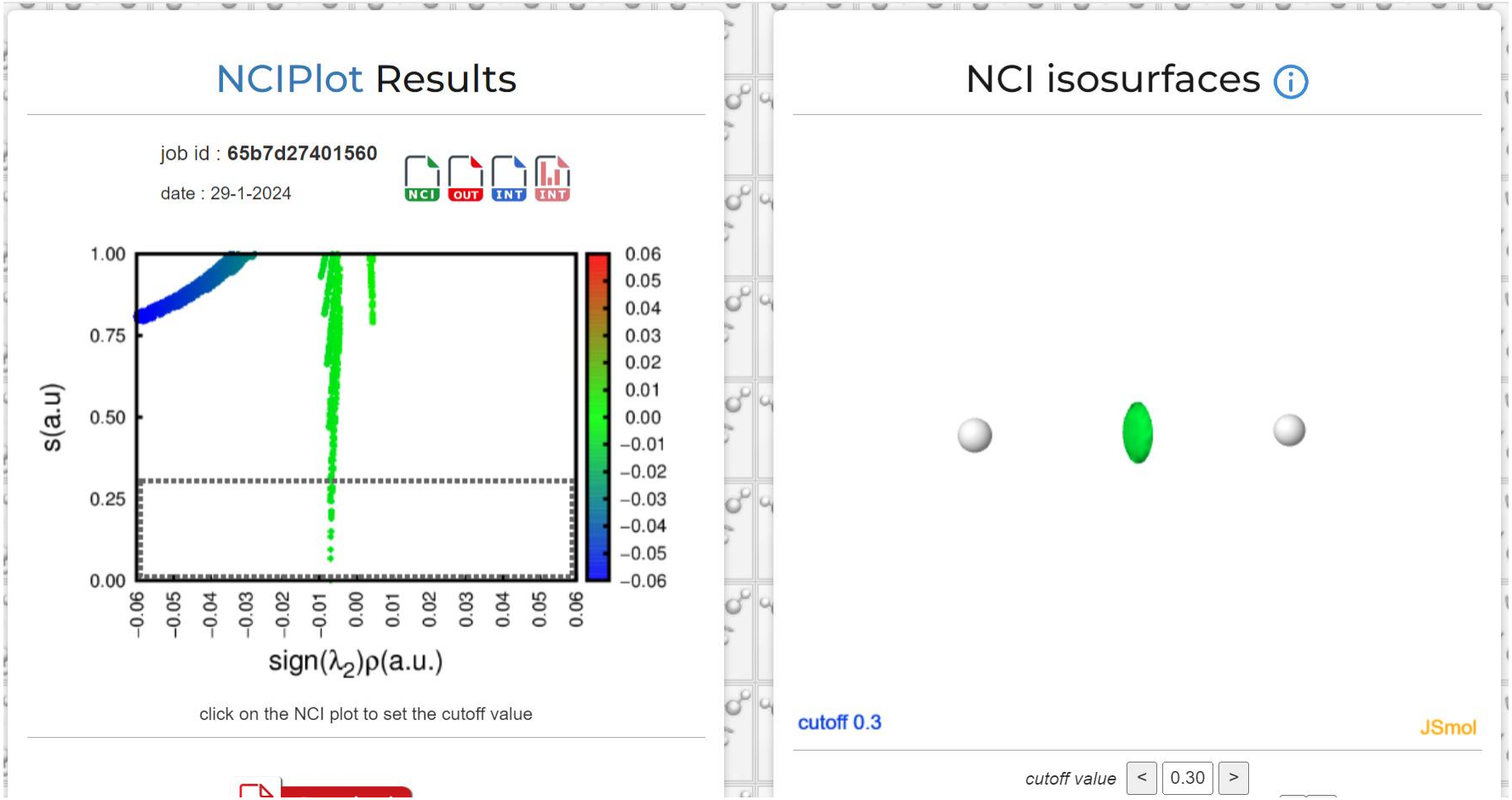


- https://nciweb.dsi.upmc.fr/to_download/65b7c9fa6974c/

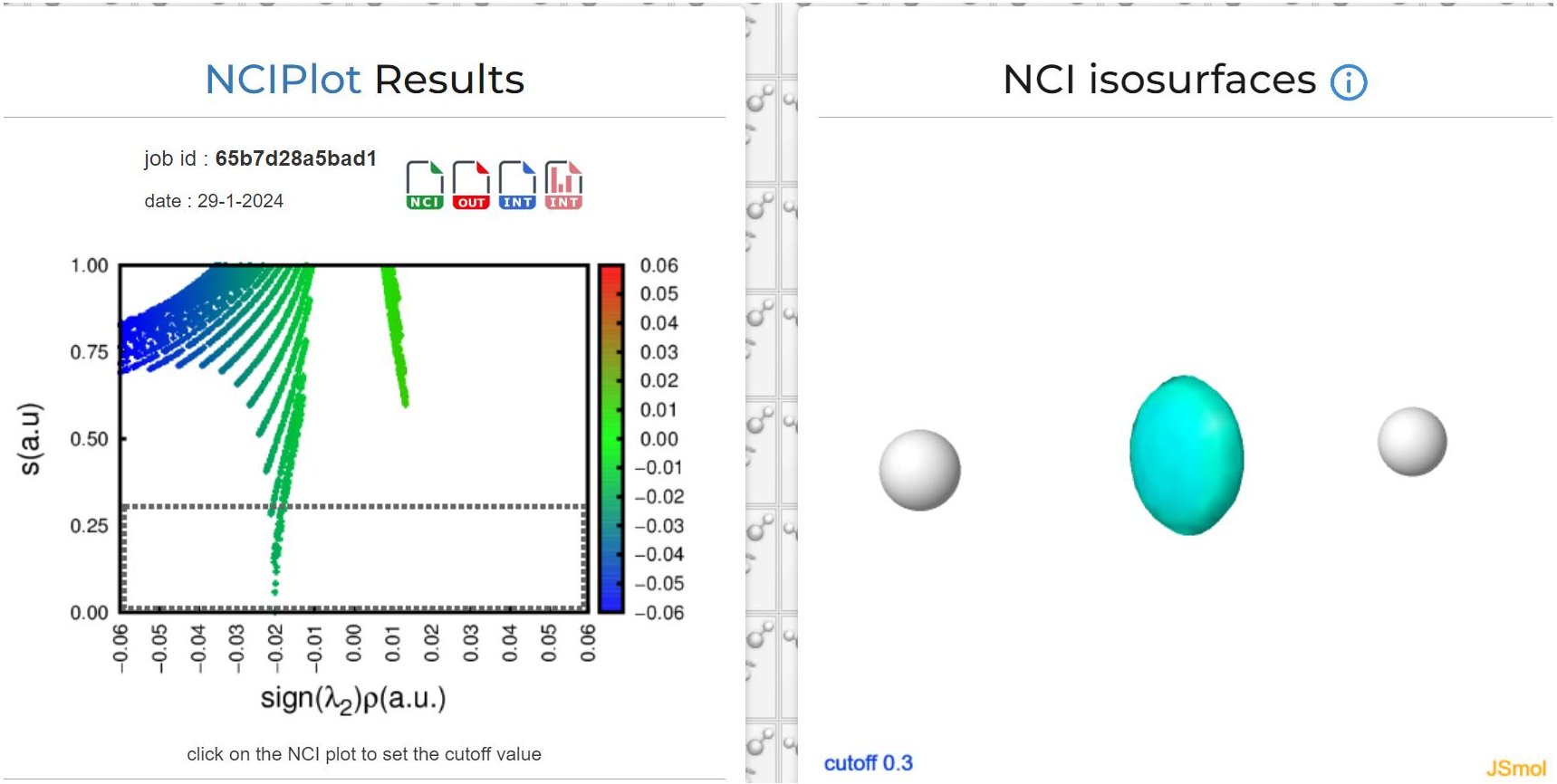


- Exercise 2

- https://nciweb.dsi.upmc.fr/to_download/65b7d27401560/

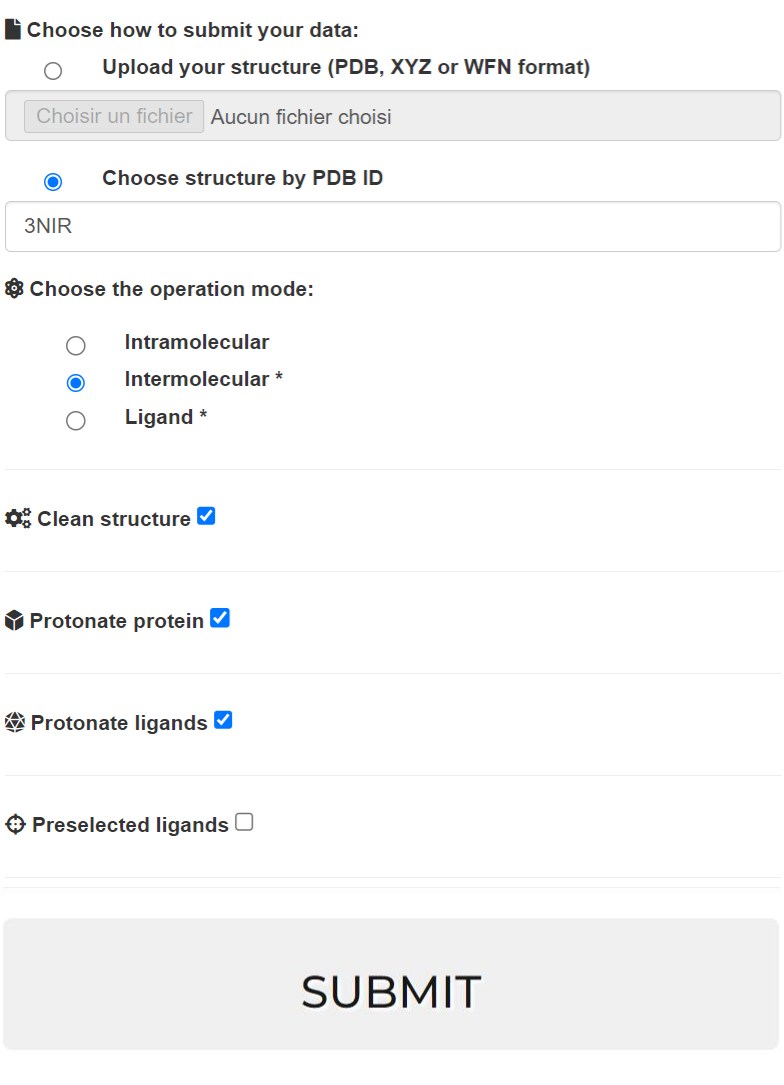


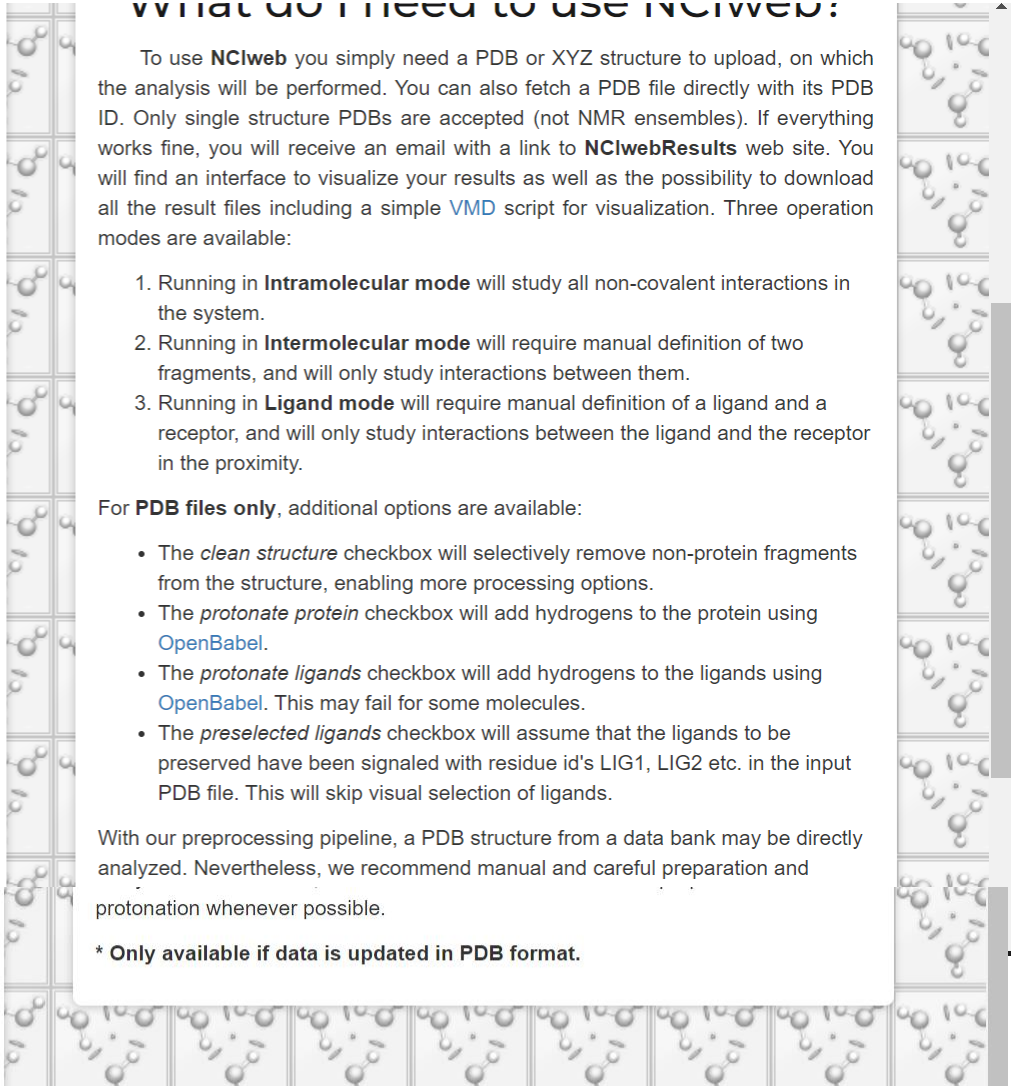
- https://nciweb.dsi.upmc.fr/to_download/65b7d28a5bad1/



- Exercise 3

- 3NIR


Choose how to submit your data:
Upload your structure (PDB, XYZ or WFN format)
Choisir un fichier
Aucun fichier choisi
Choose structure by PDB ID
3NIR
Choose the operation mode:
Intramolecular
Intermolecular *
Ligand *
Clean structure
Protonate protein
Protonate ligands
Preselected ligands
SUBMIT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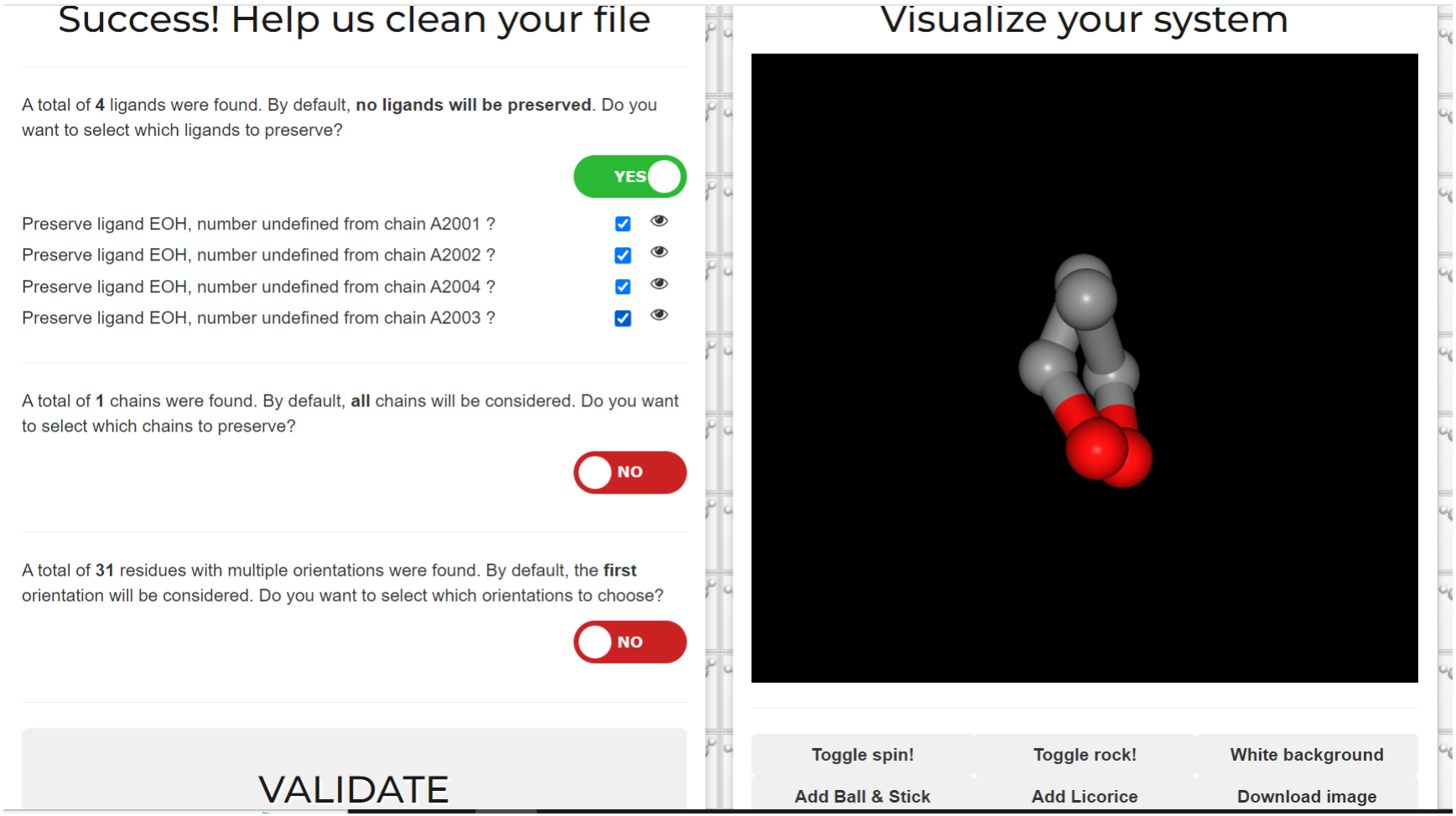
1. Running in Intramolecular mode will study all non-covalent interactions in the system.
2. Running in Intermolecular mode will require manual definition of two fragments, and will only study interactions between them.
3. Running in Ligand mode will require manual definition of a ligand and a receptor, and will only study interactions between the ligand and the receptor in the proximity.
For PDB files only, additional options are available:
The clean structure checkbox will selectively remove non-protein fragments from the structure, enabling more processing options.
The protonate protein checkbox will add hydrogens to the protein using OpenBabel.
The protonate ligands checkbox will add hydrogens to the ligands using OpenBabel. This may fail for some molecules.
The preselected ligands checkbox will assume that the ligands to be preserved have been signaled with residue id's LIG1, LIG2 etc. in the input PDB file. This will skip visual selection of ligands.
With our preprocessing pipeline, a PDB structure from a data bank may be directly analyzed. Nevertheless, we recommend manual and careful preparation and protonation whenever possible.
* Only available if data is updated in PDB format.

- 3NIR


Success! Help us clean your file
A total of 4 ligands were found. By default, no ligands will be preserved. Do you want to select which ligands to preserve?
YES
Preserve ligand EOH, number undefined from chain A2001 ?
Preserve ligand EOH, number undefined from chain A2002 ?
Preserve ligand EOH, number undefined from chain A2004 ?
Preserve ligand EOH, number undefined from chain A2003 ?
A total of 1 chains were found. By default, all chains will be considered. Do you want to select which chains to preserve?
NO
A total of 31 residues with multiple orientations were found. By default, the first orientation will be considered. Do you want to select which orientations to choose?
NO
VALIDATE
Visualize your system
Toggle spin!
Toggle rock!
White background
Add Ball & Stick
Add Licorice
Download image

Fragment Definition

A total of **5** different elements have been selected. **Define your fragments using the checkboxes below.** Interactions within the same fragment will be ignored in order to highlight intermolecular interactions.

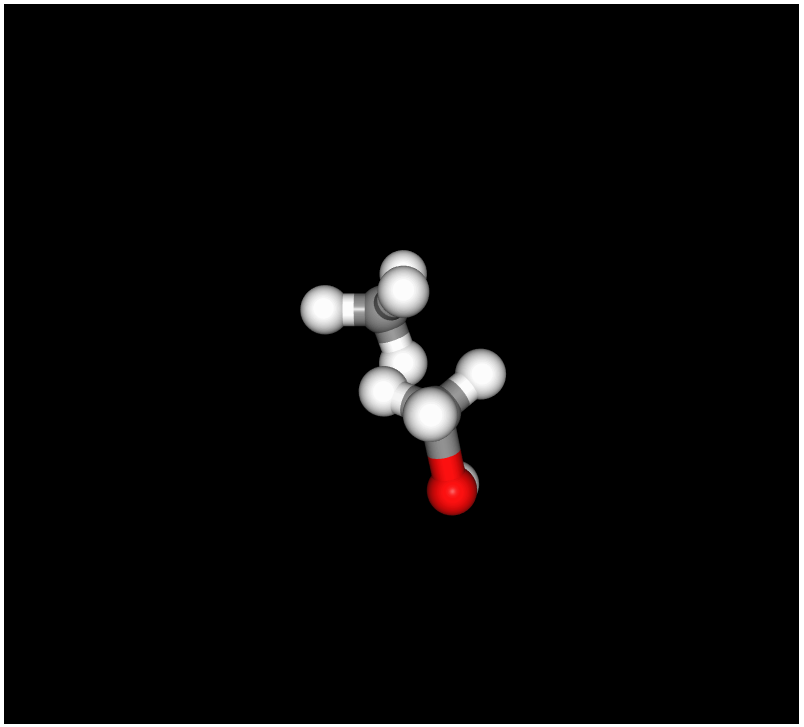
All elements **must** be allocated within a fragment!

0 elements remaining. **Ready!**

		Fragment 1	Fragment 2
Ligand EOH, number undefined from chain A2001.	👁	☑	☐
Ligand EOH, number undefined from chain A2002.	👁	☑	☐
Ligand EOH, number undefined from chain A2004.	👁	☑	☐
Ligand EOH, number undefined from chain A2003.	👁	☑	☐
Chain A.	👁	☐	☑

APPLY

Visualize your system



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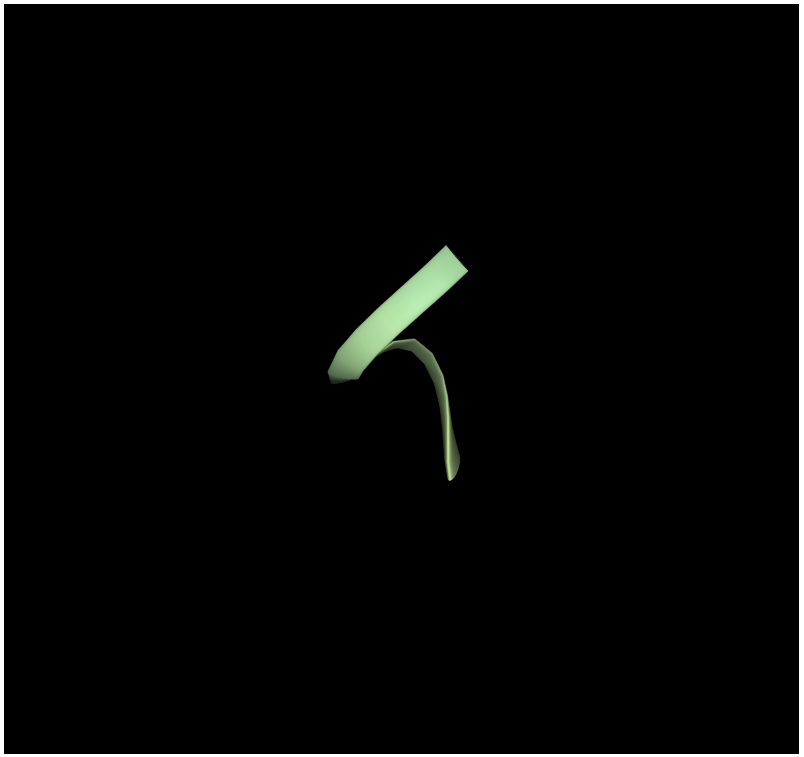
All elements **must** be allocated within a fragment!

0 elements remaining. **Ready!**

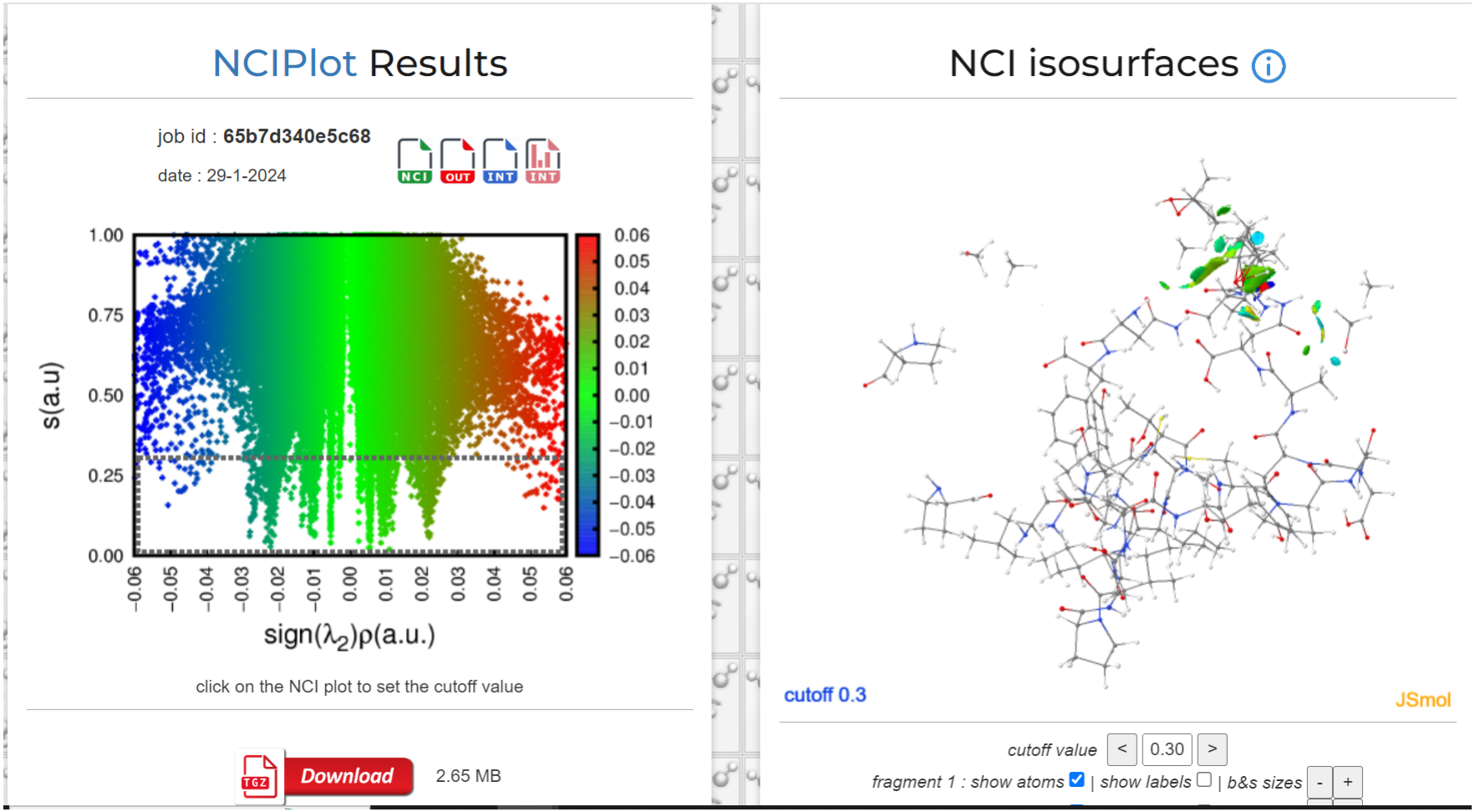
		Fragment 1	Fragment 2
Ligand EOH, number undefined from chain A2001.	👁	☑	☐
Ligand EOH, number undefined from chain A2002.	👁	☑	☐
Ligand EOH, number undefined from chain A2004.	👁	☑	☐
Ligand EOH, number undefined from chain A2003.	👁	☑	☐
Chain A.	👁	☐	☑

APPLY

Visualize your system



- https://nciweb.dsi.upmc.fr/to_download/65b7d340e5c68/



NCIPlot Results

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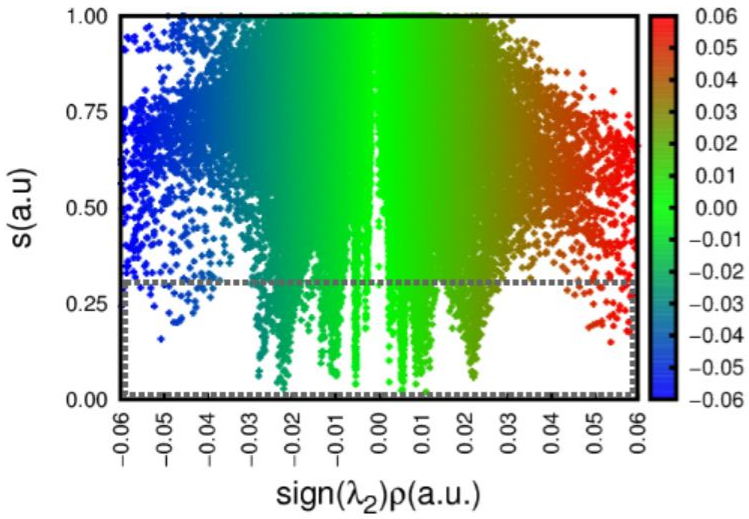
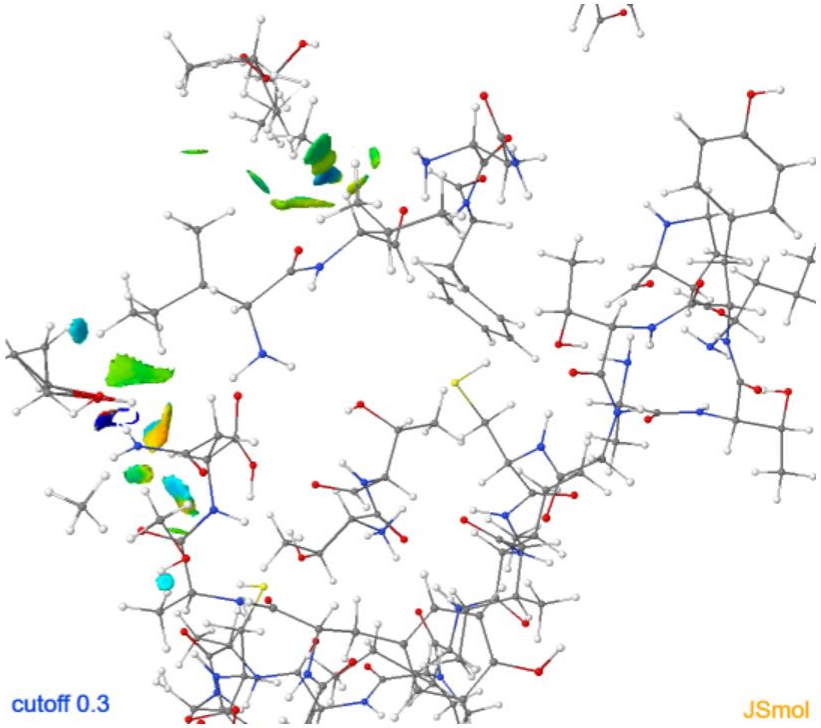
date : 29-1-2024



click on the NCI plot to set the cutoff value

Download 2.65 MB

NCI isosurfaces



cutoff value < 0.30 >

fragment 1 : show atoms ☑ | *show labels* ☐ | *b&s sizes* - +