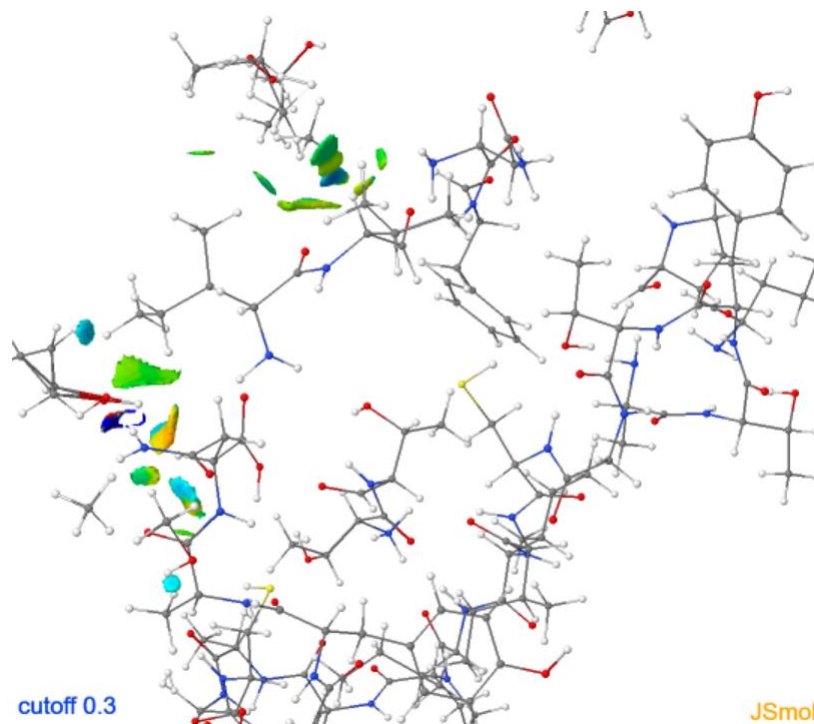


Non covalent interactions

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

You can download the exercises here:

<https://www.lct.jussieu.fr/pagesperso/contrera/nci-exercises.html#label2025>

- Exercise 1

Loading a file

Name
Julia

Email
julia.contreras_garcia@sorbonne-universite.fr

Choose how to submit your data:

☒ **Upload your structure (PDB, XYZ or WFN format)**
Choisir un fichier h2odimer.xyz

☐ **Choose structure by PDB ID**
E.g.: 2RC5

Choose the operation mode:

☒ **Intramolecular**
☐ **Intermolecular ***
☐ **Ligand ***

Clean structure ☐

Protonate protein ☐

Protonate ligands ☐

Preselected ligands ☐

SUBMIT

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.

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.**

Loading a file

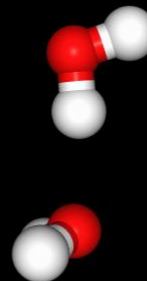
Ready to launch!

A single structure is available.

Remember: you are responsible for the preparation of your system.

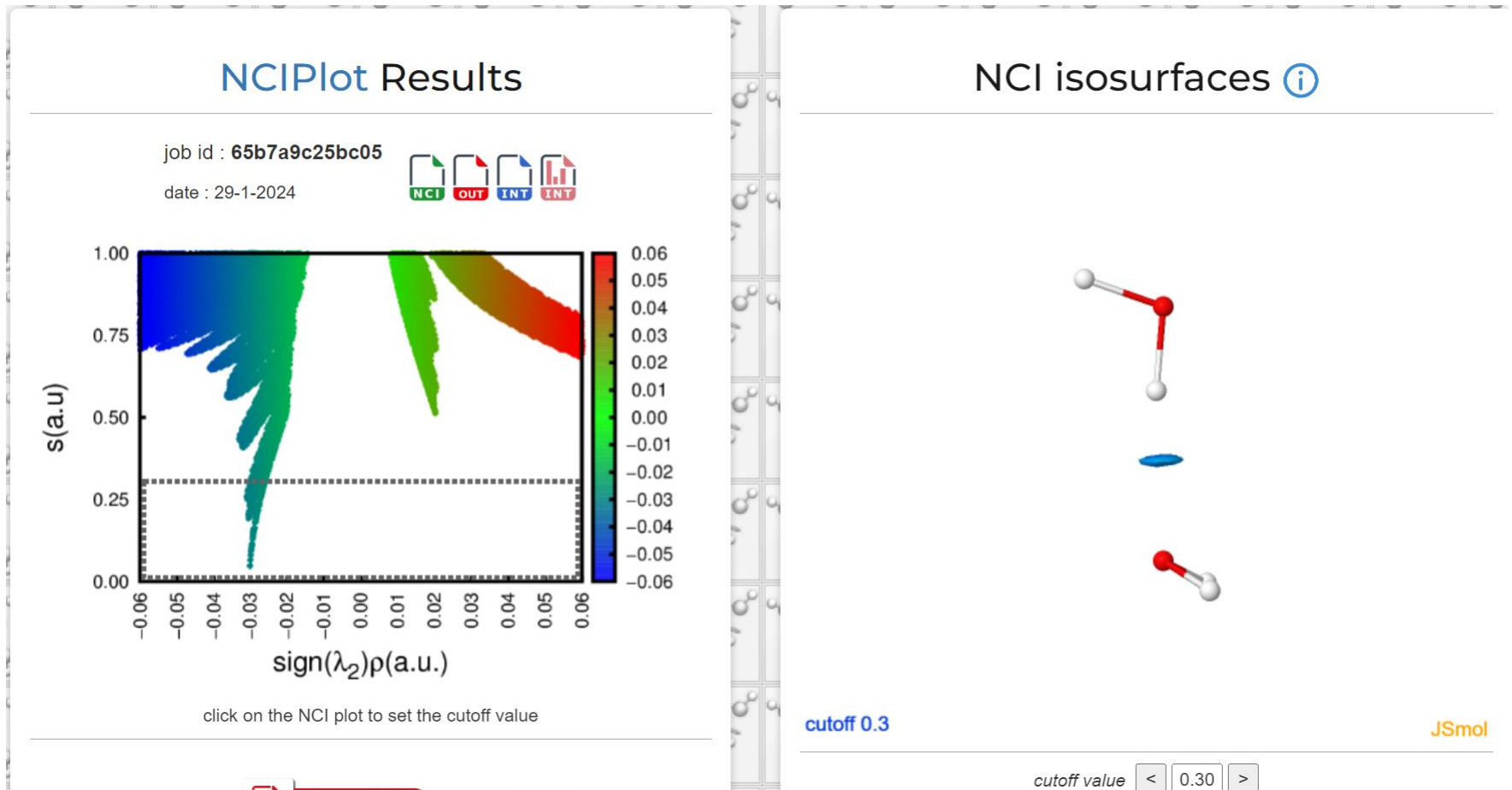
LAUNCH NCI

Visualize your system



Water dimer

- <https://lct-webtools.sorbonne-universite.fr/nciweb/examples/679cd3cebfba4/>



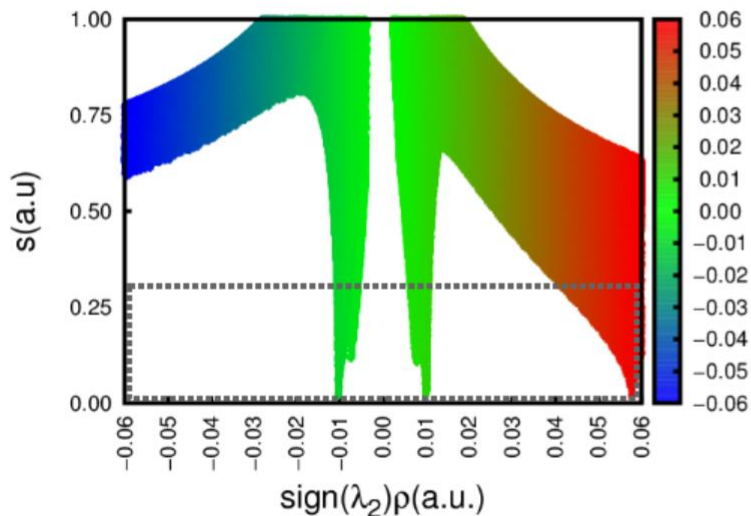
Benzene dimer

- <https://lct-webtools.sorbonne-universite.fr/nciweb/examples/664d9f295f958/>

NCIPlot Results

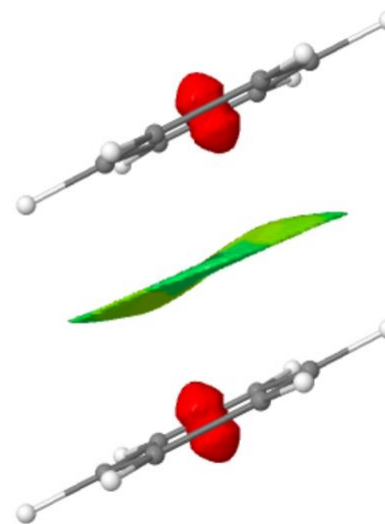
job id : 65b7aa970aedb

date : 29-1-2024



click on the NCI plot to set the cutoff value

NCI isosurfaces



cutoff 0.3

JSmol

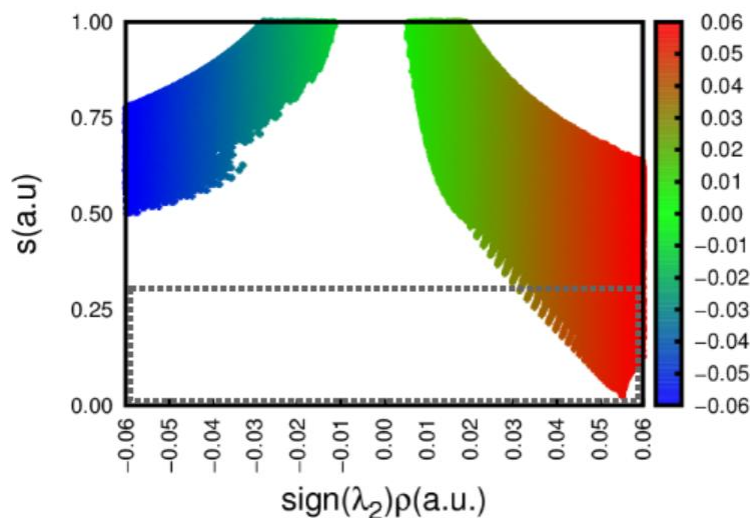
cutoff value 0.30

- <https://lct-webtools.sorbonne-universite.fr/nciweb/examples/679cd49623af1/>

NCIPlot Results

job id : 65b7c758ebec4

date : 29-1-2024



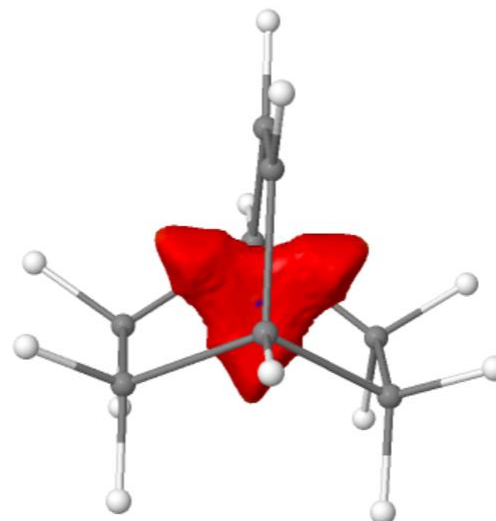
click on the NCI plot to set the cutoff value



Download

15.66 MB

NCI isosurfaces



cutoff 0.3

JSmol

cutoff value 0.30

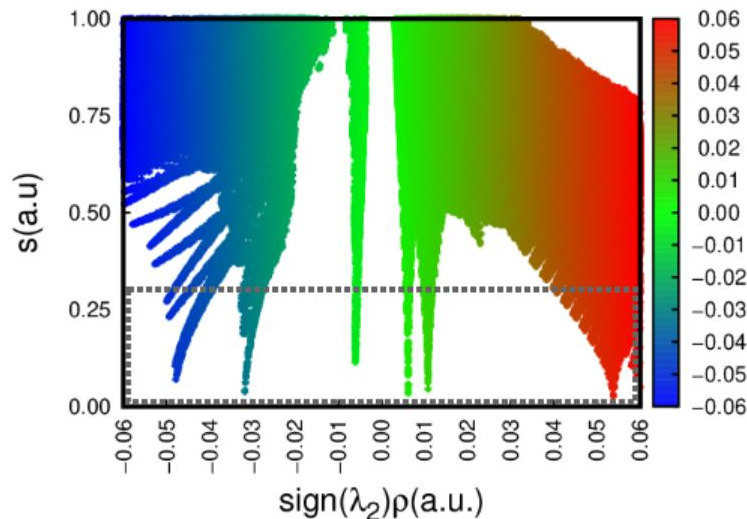
show atoms ☒ | show labels ☐ | b&s sizes

- <https://lct-webtools.sorbonne-universite.fr/nciweb/examples/679cd3ea0080f/>

NCIPlot Results

job id : 679cd3ea0080f

date : 31-1-2025



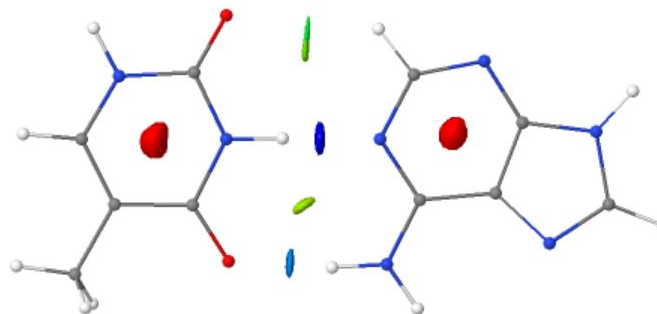
click on the NCI plot to set the cutoff value



Download

23.95 MB

NCI isosurfaces ⓘ



cutoff 0.3

JSmol

cutoff value



0.30



show atoms ☒

| show labels ☐

| b&s sizes

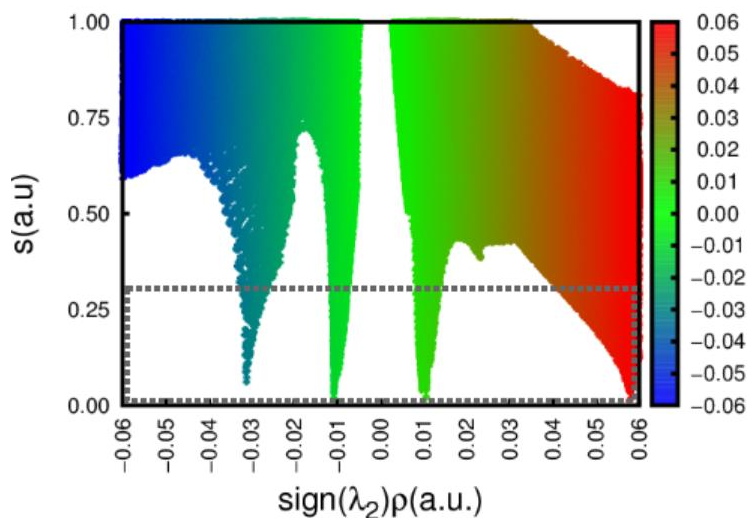


- <https://lct-webtools.sorbonne-universite.fr/nciweb/examples/679cd4d99a655/>

NCIPlot Results

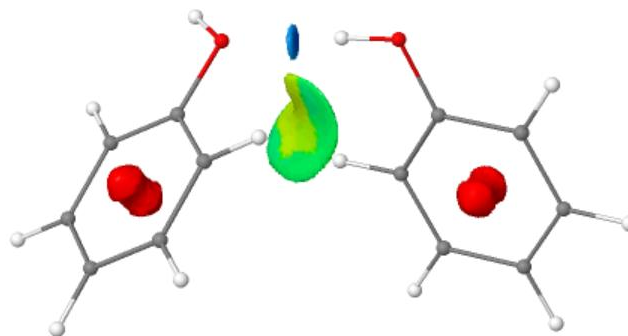
job id : **65b7ca13a2df6**

date : 29-1-2024



click on the NCI plot to set the cutoff value

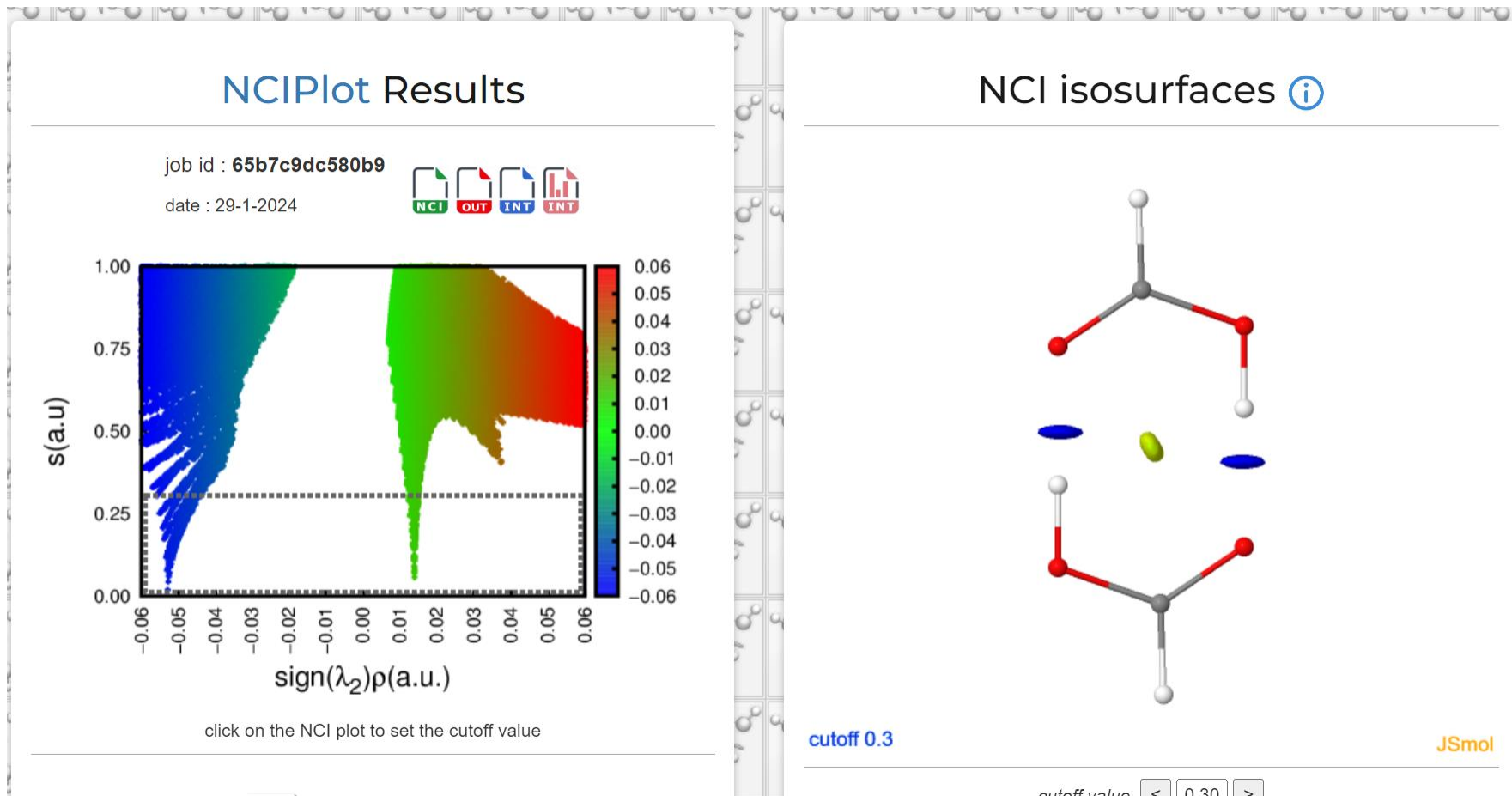
NCI isosurfaces ⓘ



cutoff 0.3

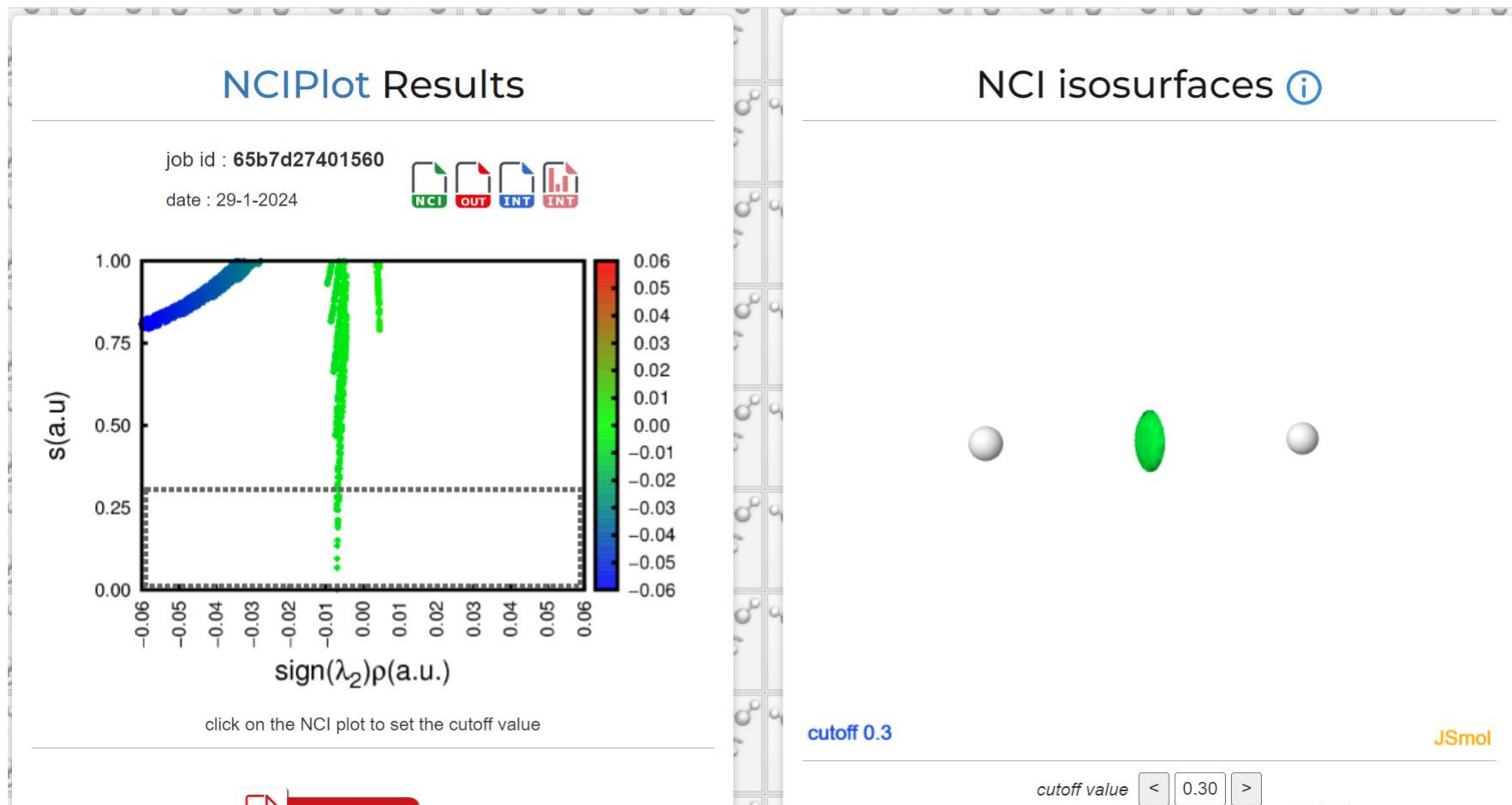
JSmol

- <https://lct-webtools.sorbonne-universite.fr/nciweb/examples/679cd4b4c305b/>



- Exercise 2

- <https://lct-webtools.sorbonne-universite.fr/nciweb/examples/679cd51bbd25b/>

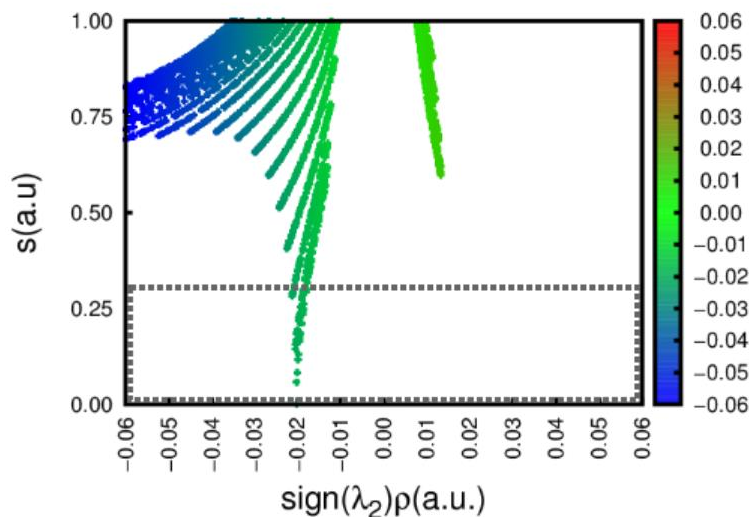


- <https://lct-webtools.sorbonne-universite.fr/nciweb/examples/679cd50b3ce6f/>

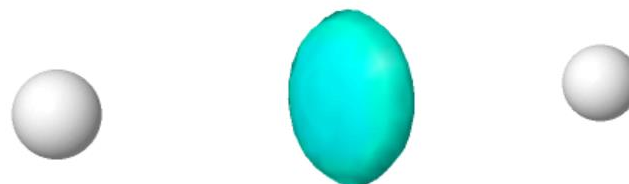
NCIPlot Results

job id : 65b7d28a5bad1

date : 29-1-2024



NCI isosurfaces ⓘ



cutoff 0.3

JSmol

- 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

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.
- 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?

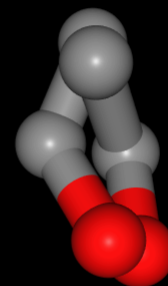
NO

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!

Add Ball & Stick

Toggle rock!

Add Licorice

White background

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!

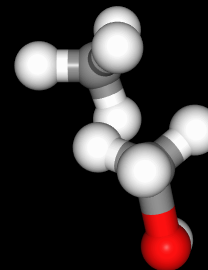
0 elements remaining. **Ready!**

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



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!

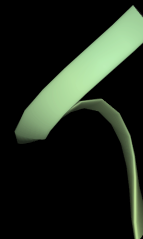
0 elements remaining. **Ready!**

Fragment 1 Fragment 2

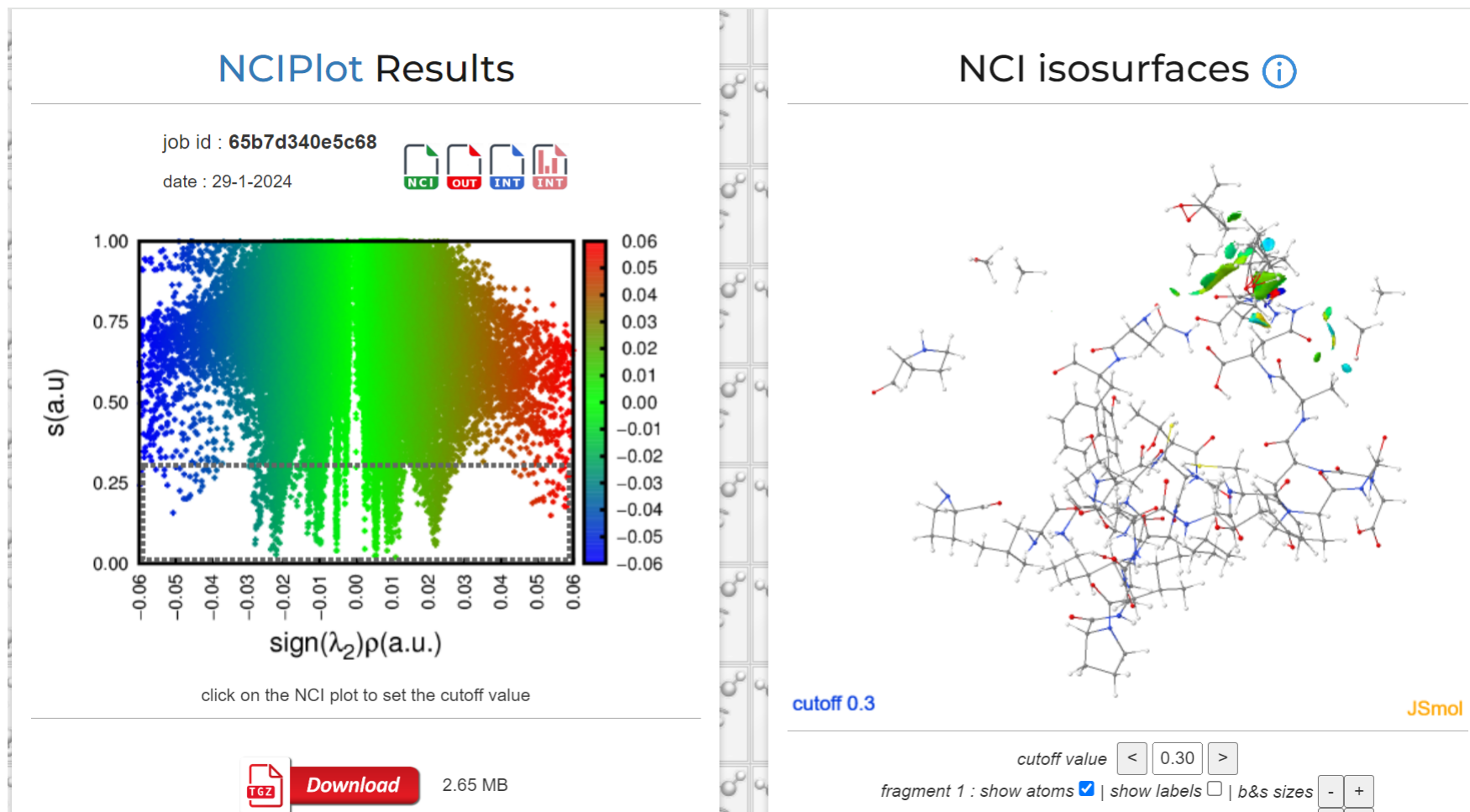
Ligand EOH, number undefined from chain A2001.		☒	☐
Ligand EOH, number undefined from chain A2002.		☒	☐
Ligand EOH, number undefined from chain A2004.		☒	☐
Ligand EOH, number undefined from chain A2003.		☒	☐
Chain A.		☐	☒

APPLY

Visualize your system



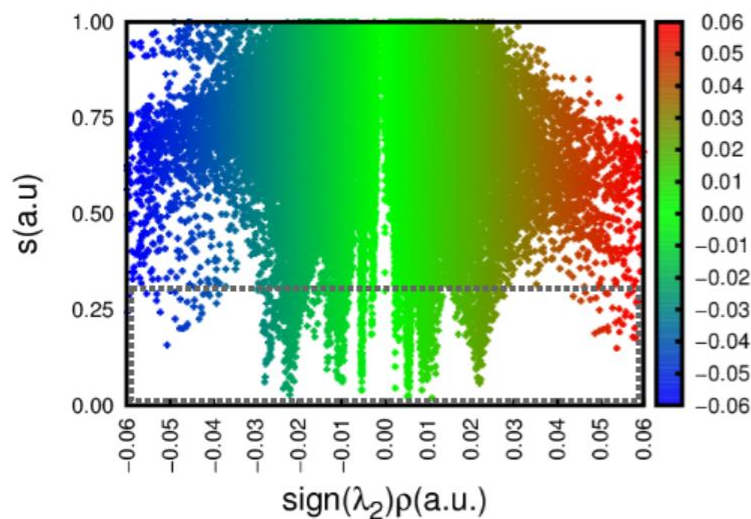
- <https://lct-webtools.sorbonne-universite.fr/nciweb/examples/679ca6dea55d4/>



NCIPlot Results

job id : 65b7d340e5c68

date : 29-1-2024



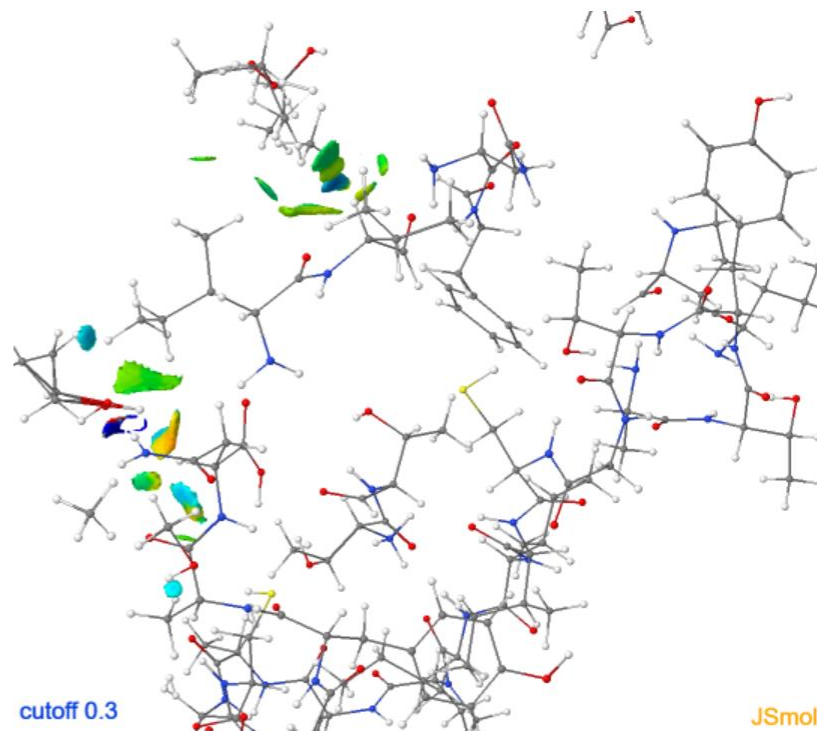
click on the NCI plot to set the cutoff value



Download

2.65 MB

NCI isosurfaces



cutoff value 0.30

fragment 1 : show atoms ☒ | show labels ☐ | b&s sizes