SINAPs V1 - Documentation

Current version: V1

➔ SINAPs requirements

Operating software:

- SINAPs analysis component:
  - Linux (tested under Ubuntu 18.04 LTS and 20.04 LTS)
  - Can work under Windows and Mac using Anaconda (not tested yet)
- SINAPs visualization plugin:
  - Linux (tested under Ubuntu 18.04 LTS & Ubuntu 20.04 LTS)
  - Windows (tested under Windows 10)
  - Mac (tested under MacOS Catalina)

Python:

- Python 3 version: Python 3.7
- Required Python 3 packages: Pytraj via ambermd, Biopython

UCSF Chimera:

- No specific version required
- A recent build is recommended (1.14 or 1.15)

➔ Installation

SINAPs analyzer - via conda (recommended installation):

```
cd ..installation_path../
conda create --name SINAPs python=3.7
source activate SINAPs
conda install -c ambermd pytraj
conda install biopython
```

It is possible to add a command in the .bashrc file. If the command in the .bashrc is set, simply launch SINAPs analysis component with the “SINAPs” command.

```
alias SINAPs="source activate SINAPs ; python3 ..installation_path../SINAPs.py"
```

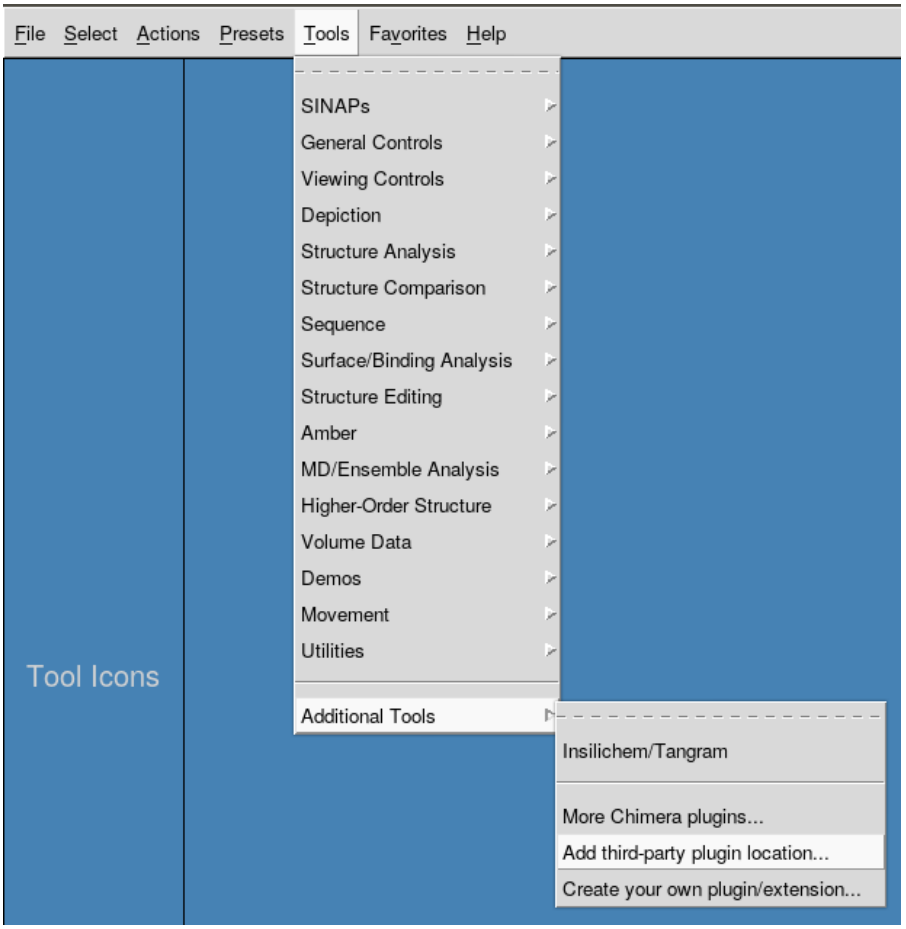
If the command in the .bashrc is not set, activate the SINAPs conda environment before launching the SINAPs analysis component:

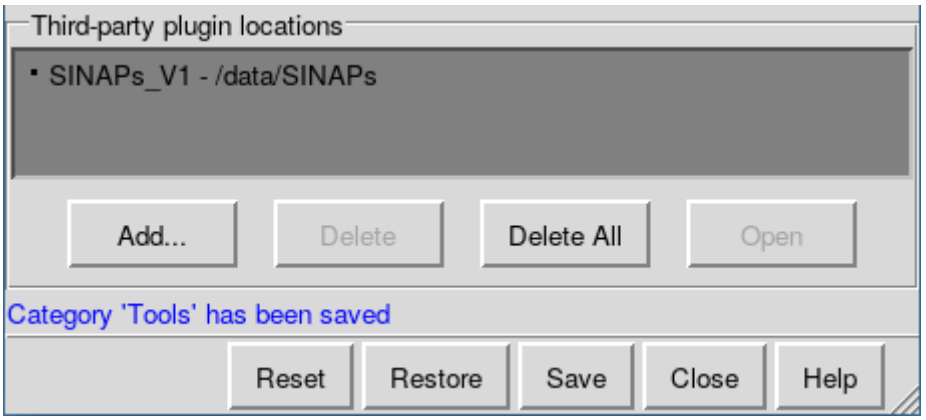
```
source activate SINAPs
python3 ..installation_path../SINAPs.py
```

SINAPs visualization plugin - UCSF Chimera:

In UCSF Chimera :

- Tools >> Additional Tools >> Add third-party plugin location >> Add..
- Specify the main directory of SINAPs (/!\ Do not specify the SINAPs_Visualizer folder, but the previous one /!\)


File
Select
Actions
Presets
Tools
Favorites
Help
SINAPs
General Controls
Viewing Controls
Depiction
Structure Analysis
Structure Comparison
Sequence
Surface/Binding Analysis
Structure Editing
Amber
MD/Ensemble Analysis
Higher-Order Structure
Volume Data
Demos
Movement
Utilities
Additional Tools
Tool Icons
Insilichem/Tangram
More Chimera plugins...
Add third-party plugin location...
Create your own plugin/extension...


Third-party plugin locations
SINAPs_V1 - /data/SINAPs
Add...
Delete
Delete All
Open
Category 'Tools' has been saved
Reset
Restore
Save
Close
Help

➔ Tested input files

- **AMBER trajectories:**
  - Topology .parm7 ; Trajectory .nc
  - Other formats are tolerated
- **GROMACS trajectories:**
  - Topology .pdb ; Trajectory .xtc
  - Topology .top ; Trajectory .trr (with the addition of all .itp files in the input directory, as well as a copy of the forcefield directory used)
  - Current issue: If you use multi-chain structures, please verify that all chains have an identifier
- **PDB files:**
  - PDB trajectories
  - PDB files

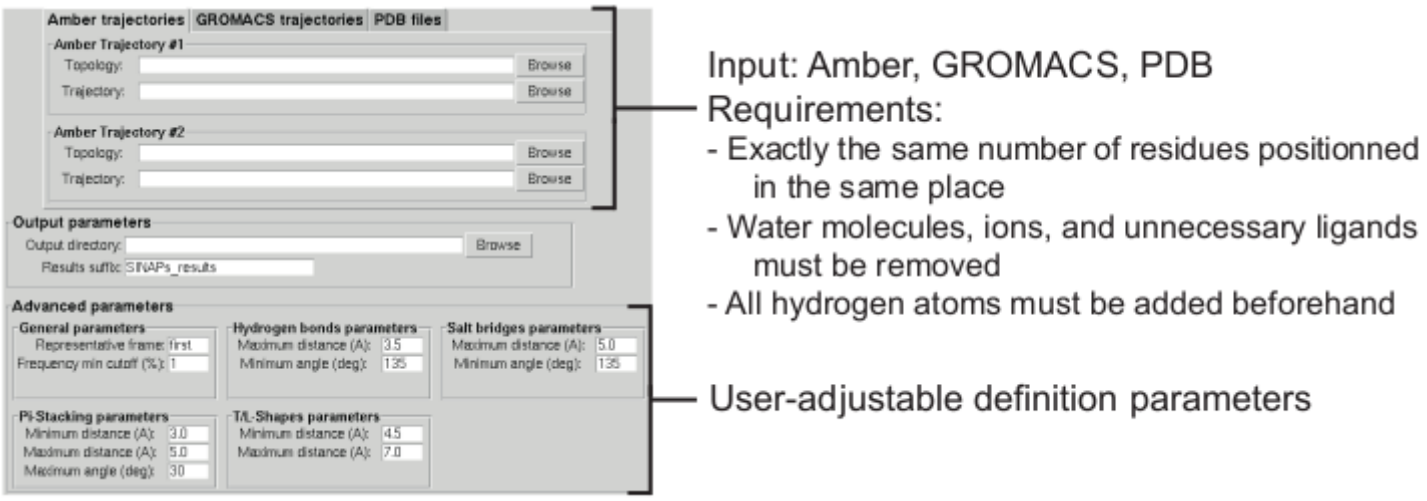
➔ Requirements

- Add all hydrogen atoms.
- Remove all water molecules, ions, and unnecessary ligands.
- The structures must have exactly the same number of amino acids positioned in the same place (the type of the amino acids is not important). In case of difference, it is mandatory to remove all amino acids without correspondence.
- Only the 20 proteinogenic amino acids were tested.

➔ Using SINAPs

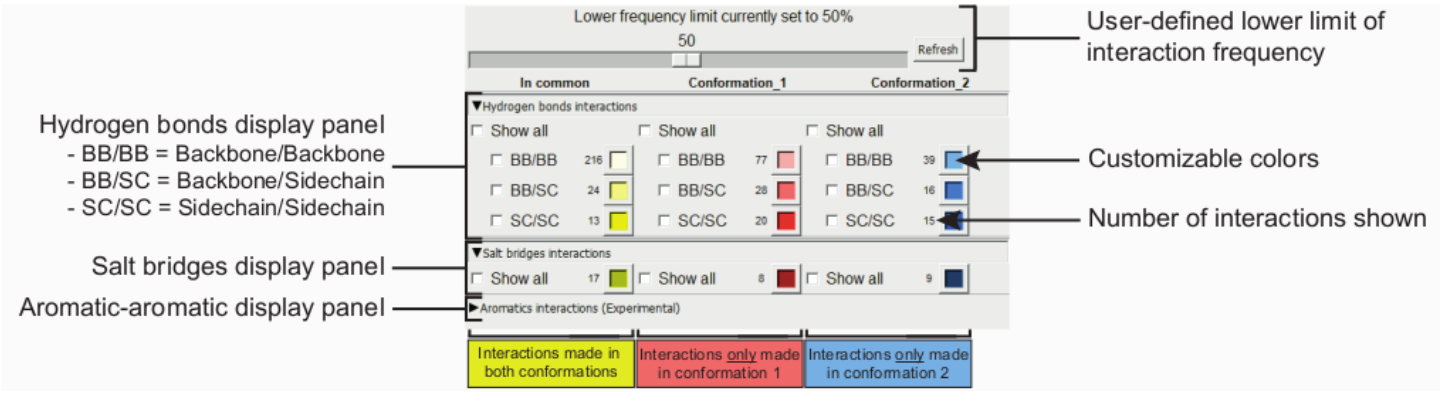
SINAPs analysis component:

- Information to be specified:
  - Input files
  - Output folder created beforehand (an option to create the output folder automatically will be added in the future).
- The output folder must be unique for each analysis.
- The representative frame can take "first", "last", or the key frame number as an argument.
- "Frequency min cutoff (%)" allows you to only keep in the output the interactions with a frequency greater than or equal to the argument. However, it is not recommended to change it.
- It is possible to study interaction networks in a single simulation/structure by specifying the same file twice. The observation in UCSF Chimera allows highlighting the main interactions realized in this single case, without comparison.



SINAPs visualization plugin:

- Tools >> SINAPs >> SINAPs Visualizer
- Specify the folder containing the output files, then load data
- The frequency bar allows you to display only the bonds with a frequency greater than or equal to the chosen cutoff
- For the moment, only the backbone can be displayed (to simplify the representation as much as possible). However, it is possible to overcome this choice by manually loading a PDB structure with side chains, and aligning it to the structures opened by SINAPs.



➔ Current issues

SINAPs analysis component:

- No error messages in the graphical interface: check directly in the terminal if the program runs correctly.
- Crash when using structures with ions: please remove all ions beforehand.
- GROMACS: If you use multi-chain structures, please verify that all chains have an identifier.

SINAPs visualization plugin:

- Interactions within the hydrogen bonds and salt bridges categories are represented as hydrogen bonds instead of salt bridges when the two graphical options are selected.
- Native “Save image” Chimera function does not keep the same bond width as represented in the graphical interface.