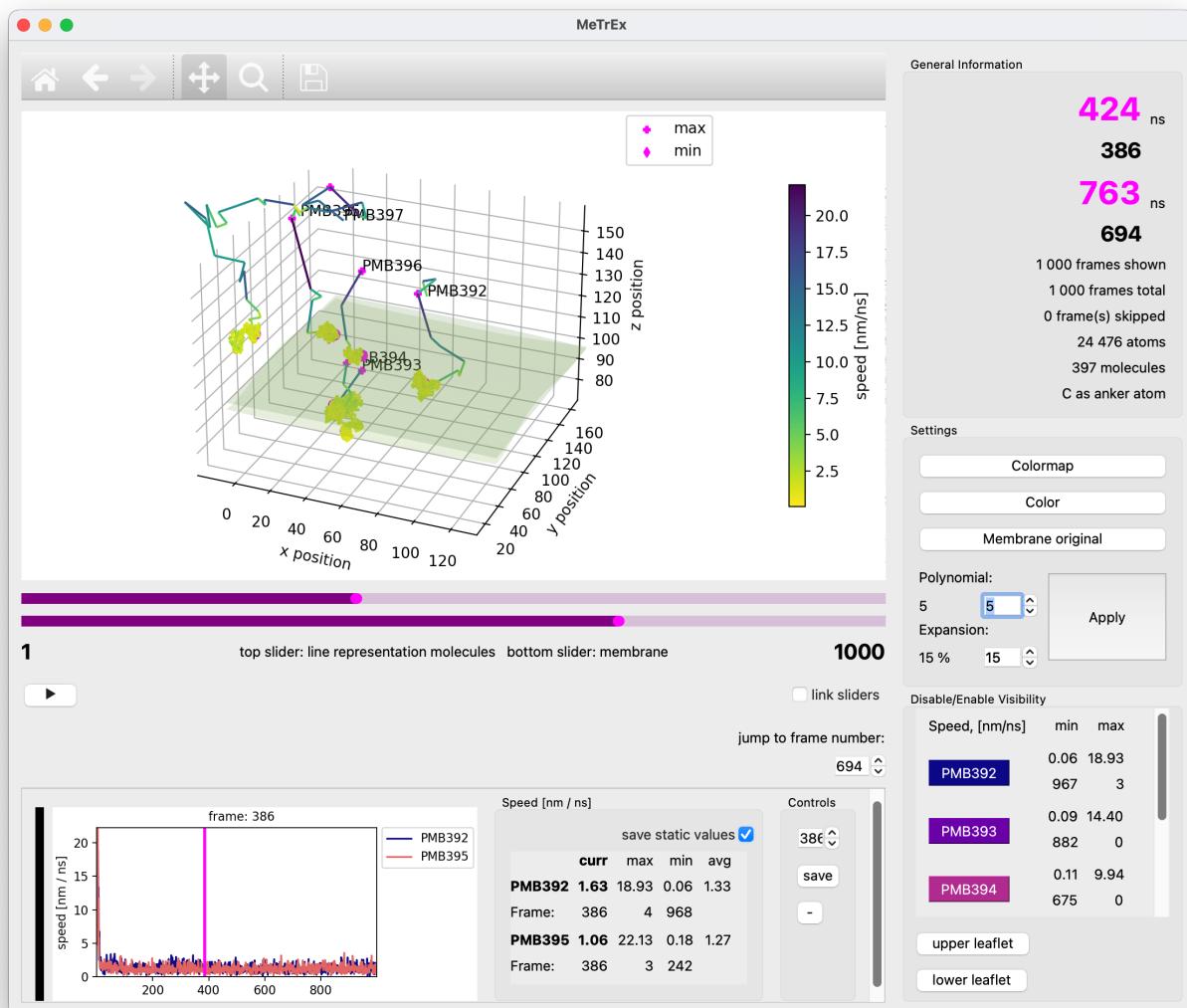
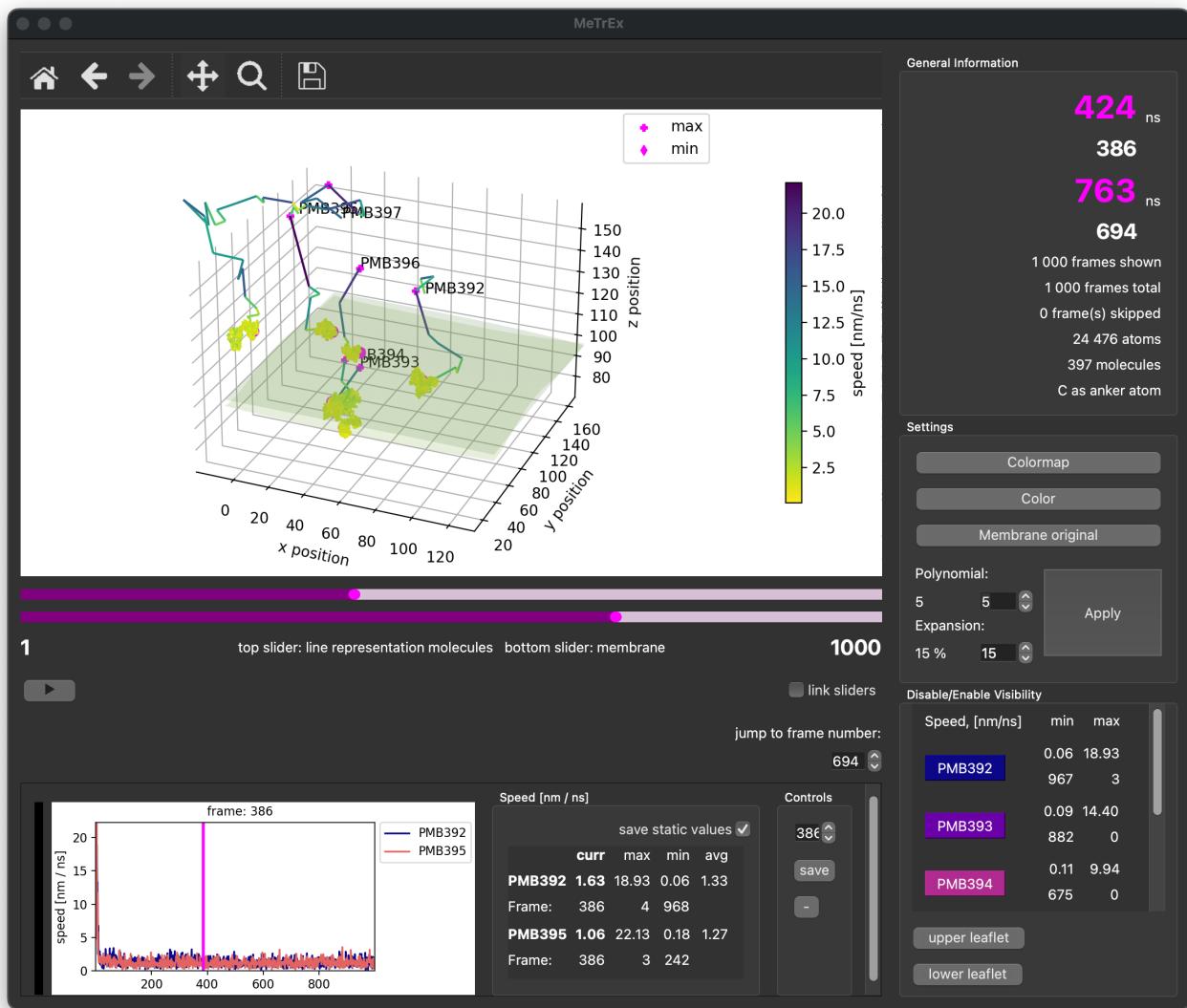


MeTrEx - Membrane Trajectory Exploration

MeTrEx (**M**embrane **T**rajectory **E**xploration) is a python program for the visual exploration of molecular simulation data from membranes interacting with small molecules.

It's main feature is to show an overview of the molecules' course throughout the simulation with an abstract visualisation of the membrane. This overview of the data is shown on the 'main view', which is shown as soon as data is loaded. Different analyses can be mapped onto the main view. These analyses can also be shown in separate plots below the main view, in 'bottom views'. Additionally, you can load other data files in 'sub windows', shown in 'sub plots'. Sliders and information panels give information about the currently shown frame. Exporting data is provided for image, csv and xpdb files.





Availability & Download

See the [Installation](#) section for instructions on download and installation of **MeTrEx**
MeTrEx source code is available from our [GitHub repository](#).

Installation

From Source

Requirements

1. You need python version 3.8 or higher
2. You need [conda](#) package manager installed on your system.

Downloading and Installing MeTrEx

3. Clone the [GitHub repository](#): `git clone https://github.com/sa-ja/MeTrEx`
4. Build the environment with the yml file for your operating system (Windows + MacOS: `metrex.yml`, Linux: `metrex_linux.yml`): ``cd MeTrEx && conda env create -f metrex.yml``
5. Activate the environment: `conda activate MeTrEx`

Run MeTrEx

6. Start MeTrEx from console: `python MeTrEx/main.py`

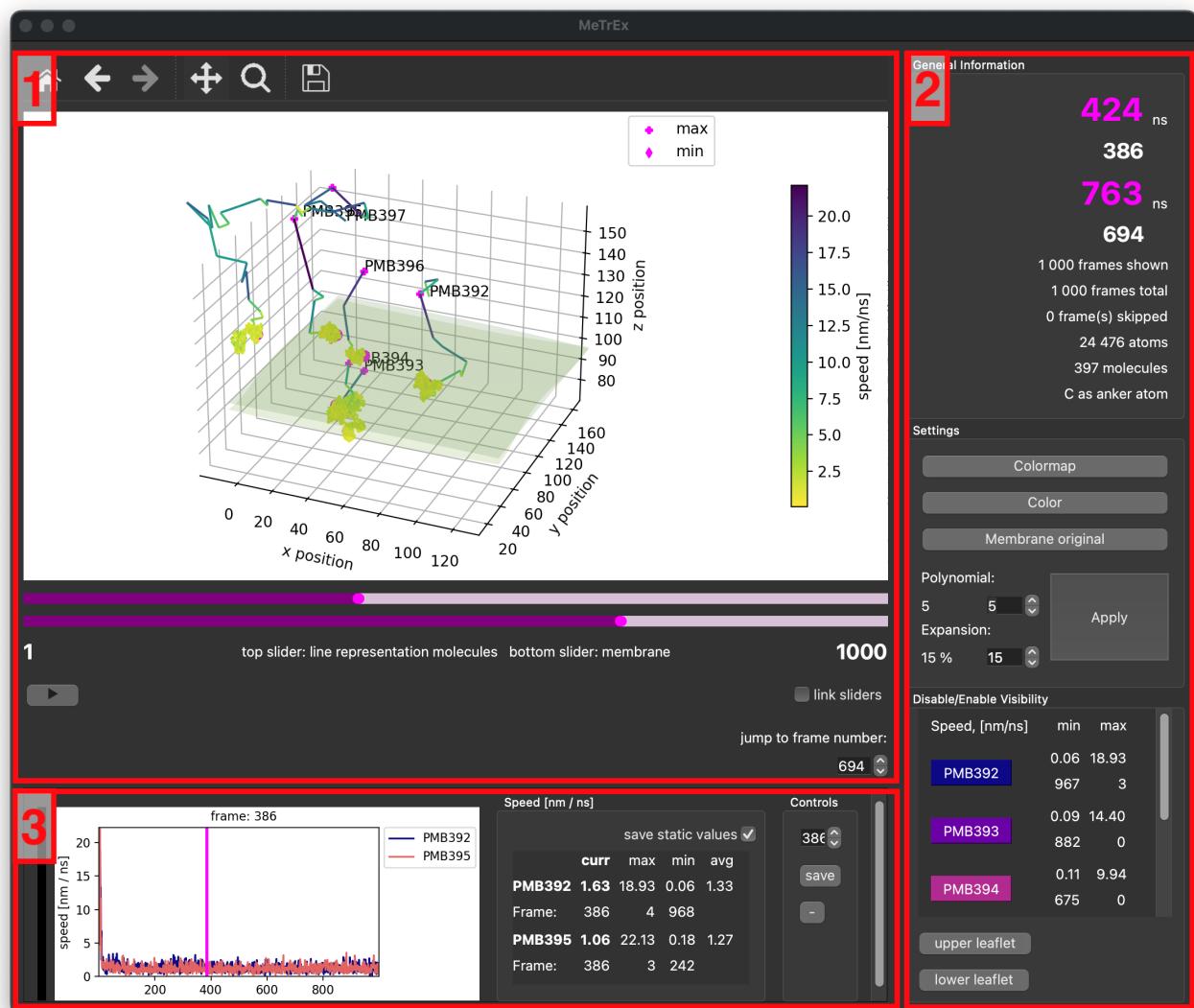
Manual

Main Window

The application window of **MeTrEx** is made up of three parts ([see figure below](#))

1. The main view
2. The information and interaction panel
3. The bottom view(s)

MeTrEx Overview



Load Data

First you need to load two files to perform any analysis with **MeTrEx**.

To do so, you can either navigate to *File > Open* in the menu bar or use the *ctrl+O* shortcut. [See picture](#).

Then, you need to specify a topology file and a file containing simulation data. [See picture](#)

Afterwards an other dialog opens allowing a data reduction by skipping every k-th frame or n frames in the beginning of the data. [See picture](#).

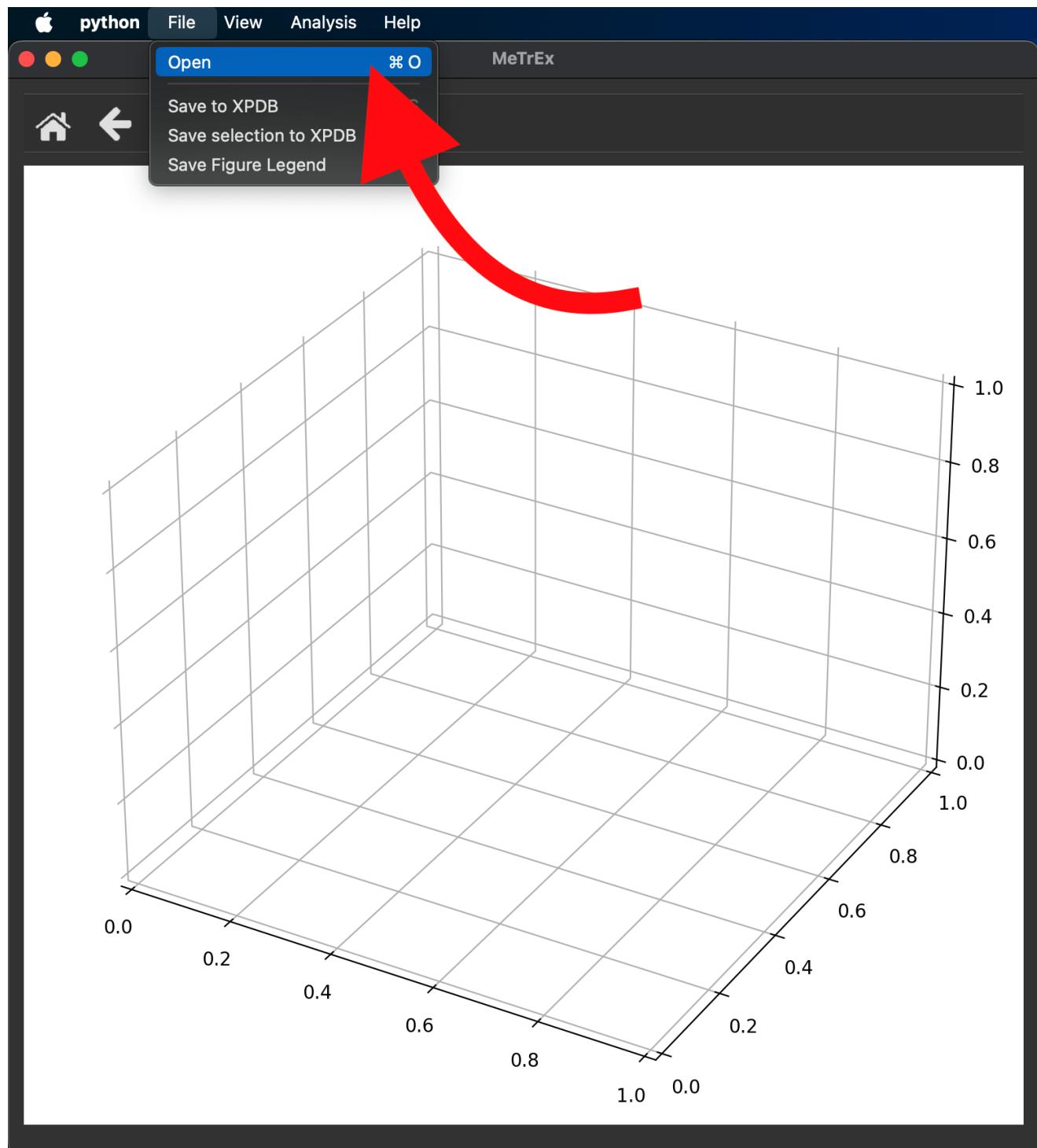
k = select every k-th frame to be shown

n = number of frames to skip at the beginning of the data

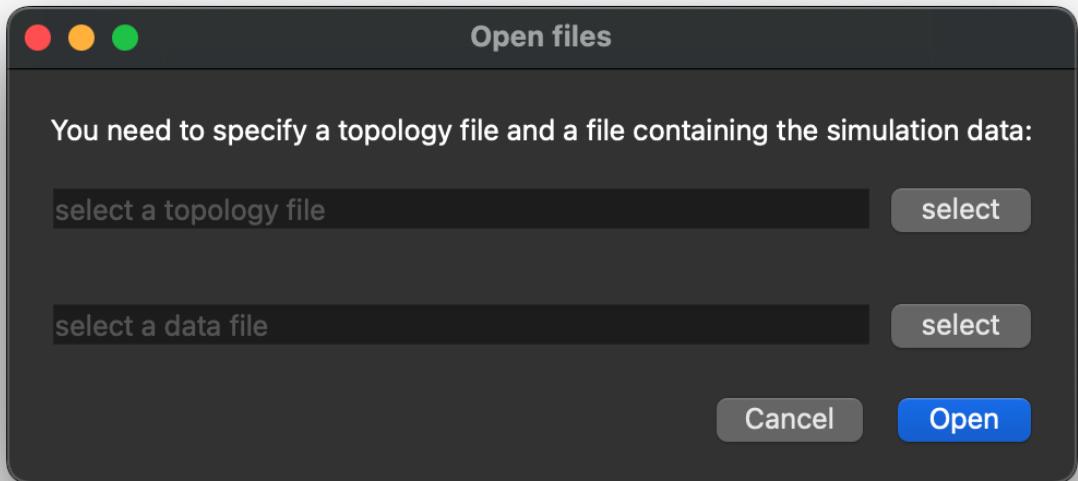
You also need to specify type of molecules that shall be represented by its trajectory line in the line representation. The displayed names are the abbreviations for the molecule types used in the data file. In our example data, PMB is the molecule that should be selected for trajectory line representation. Additionally you can choose to manually select an anker atom which is used for the line representation. Otherwise or in case of an error always C or CA are used.

Once the molecules are chosen and if applicable the anker atom is selected, the view is generated. This can take some time. A rough estimate will be displayed.

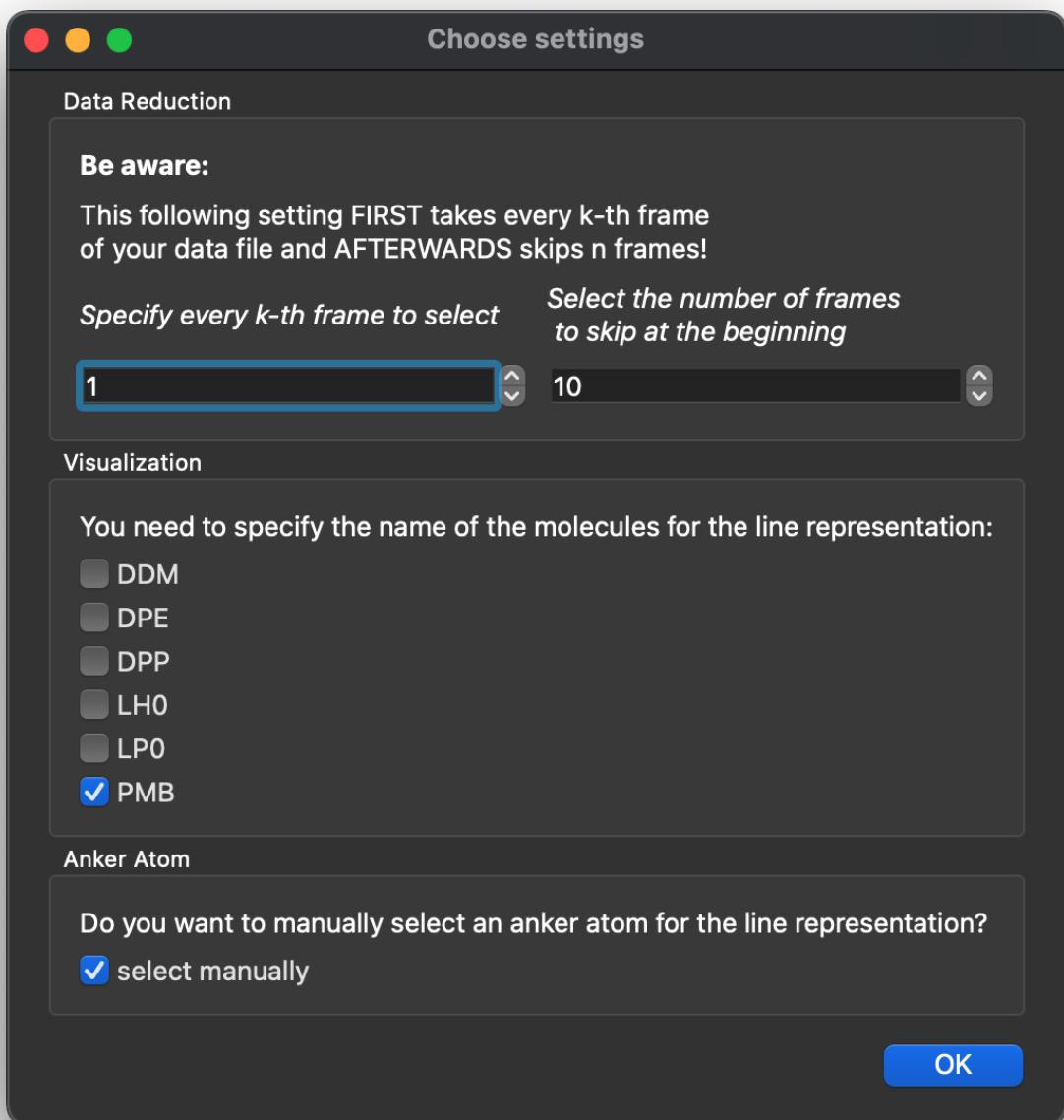
Open File



Select File



Choose Settings



Navigate in Main Graph

There are multiple ways one can interact with the main graph and navigate with it.

By clicking and holding the graph you are able to rotate the graph freely.

On the top left of the main view you can find the control panel with 6 button options. [See picture.](#)

- The house button  is used to reset the main graph to its initial view
- The two arrows buttons   can be used to go back or forward to a previous view setting
- The cross-arrow button  once clicked changes the function of clicking and holding the graph from rotating it to moving and positioning it along the x-, y- and z-axis. This is again deactivated when the cross-arrow button is clicked again or the magnification glass button is selected.
- The magnification glass button  allows you once selected to zoom into the graph.
- The save button  creates a .png file of the current view

Below the graph of the main view are two sliders which can be linked by the checkbox *link sliders*. These sliders allow you to change the graph to a different frame of your simulation data.

The top slider changes the frame of the line representation molecules.

The bottom slider changes the frame of the membrane representation.

Pressing the play button  starts or stops a time laps of the represented data.

The 'jump to frame number' selector can be used to switch to a chosen frame.

Control Panel



Using the interaction panel

The interaction panel consists out of 3 panels: **General Information**, **Settings** and the molecule representation panel (**Disable/Enable Visibility**). [See picture](#).

Inside the **General Information panel** you find information for the position and exact simulation time of the current slider position/frame shown in the main view.

Additional information about the simulation and representation is also displayed here.

The **Settings** panel offers a variety of options:

- Colormap allows you to change the colormap used for the representation of all line representation molecules
- Color lets you pick a specific color for each line representation molecule individually
- Membran original lets you switch between a membrane abstraction and the original membrane representation
- Polynomial and Expansion let's you choose the lipid surface regressions values and recalculate the membrane abstraction. The polynomial can be modified in the range from 3 to 15, membrane expansion from 5% to 30%. Once you set your values, press **Apply** to recalculate. Depending on the data and values this can take some time to compute.

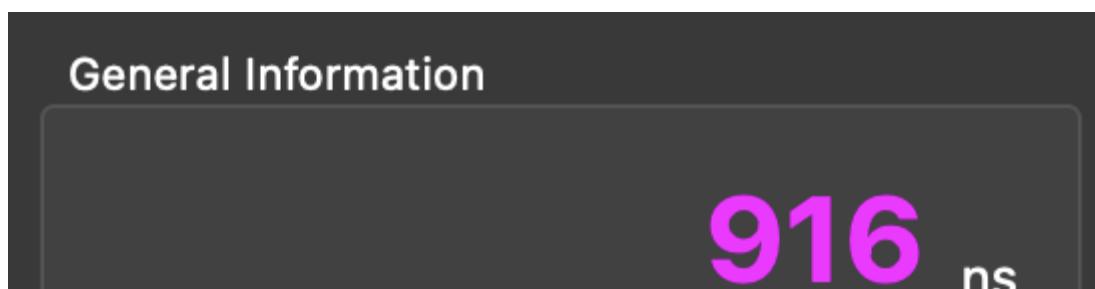
The molecule representation panel (**Disable/Enable Visibility**) depicts the individual molecules which were chosen for representation in [Load Data, see picture](#).

If one of the three mapping methods of [Change View](#) is chosen, the respective minimum and maximum is displayed next together with the associated frame number.

By clicking the molecule name you can disable or enable individual molecule representations.

The buttons **upper leaflet** and **lower leaflet** disable or enable the corresponding membrane representation.

Interaction Panel



417

916 ns

417

500 frames shown

1 000 frames total

0 frame(s) skipped

24 476 atoms

397 molecules

CA0 as anker atom

Settings

Colormap

Color

Membrane original

Polynomial:

15

15



Apply

Expansion:

30 %

5



Disable/Enable Visibility

Speed, [nm/ns]	min	max
PMB392	0.06	10.02
	233	2
PMB393	0.05	7.47
	346	0
PMB394	0.07	6.23
	229	0
PMB395	0.07	12.46
	203	1
PMB396	0.05	13.29
	132	0

upper leaflet

lower leaflet

Change View

To modify and further analyse the data multiple options to change the view and provide further graphs are available. All these options are found in the menu bar under ['View'](#).

Modify Main View

The following methods provide an overview of different mapping functions inside the main view.

Select frame range

To select a specific range of frames go to *View > Select frames* and select a range of frames you want the data to be reduced to. If you want to return to the original main view with all frames use *View > Reset*.

Show frame position

If you want to see the chronological position of the molecule in the trajectories indicated by a color gradient use *View > Map Position*. To reset the main view to its original state use *View > Reset*.

Show intramolecular distances

To visualise the changes of the intramolecular distance [\AA] between exact two different atoms of the representative molecules over time as a color gradient use *View > Map intramolecular distance*. A [dialog](#) will appear in which you have to select a pair of atoms for each representative molecule. Add the selection to the final selection by pressing + or remove an incorrect selection by pressing – to fix the incorrect entry.

The molecule representation panel in the interaction panel will show the minimal and maximal intermolecular distance value as well as the corresponding frame number.

To reset the main view to its original state use *View > Reset*.

Show molecular speed

To visualise the progression of the speed [nm/ns] of the representative molecules go to *View > Map Speed*. The speed progression is displayed as a color gradient.

The molecule representation panel in the interaction panel will show the minimal and maximal molecular speed value as well as the corresponding frame number.

To reset the main view to its original state use *View > Reset*.

Reset view

To reset the main view to its original state use *View > Reset*.

Add and Modify Bottom View

The bottom view provides a more in depth analysis and visualisation of the mapping methods described in [Modify Main View](#).

Each bottom view panel has three areas, the graphical display, the statistical display and a control panel; [see picture \[3\]](#).

The control panel has the option to select a specific frame for this bottom view. To save the graph of the bottom view use the `save` button. When the check box in the statistical display is activated a .CSV file of the in the overview shown data is saved, too. Use the – button to remove this instance of the bottom view.

Additionally in single instance view you can press `s/h` to show or hide minimum and maximum labels.

Show molecular speeds in bottom view

To show the progression of the speed [nm/ns] of the representative molecules or their single atoms in the bottom view you can go to *View > Show below > Speed* to display one instance in a single graph or *View > Show below > Multiple Speed* to display multiple instances in one graph.

Show molecular distances in bottom view

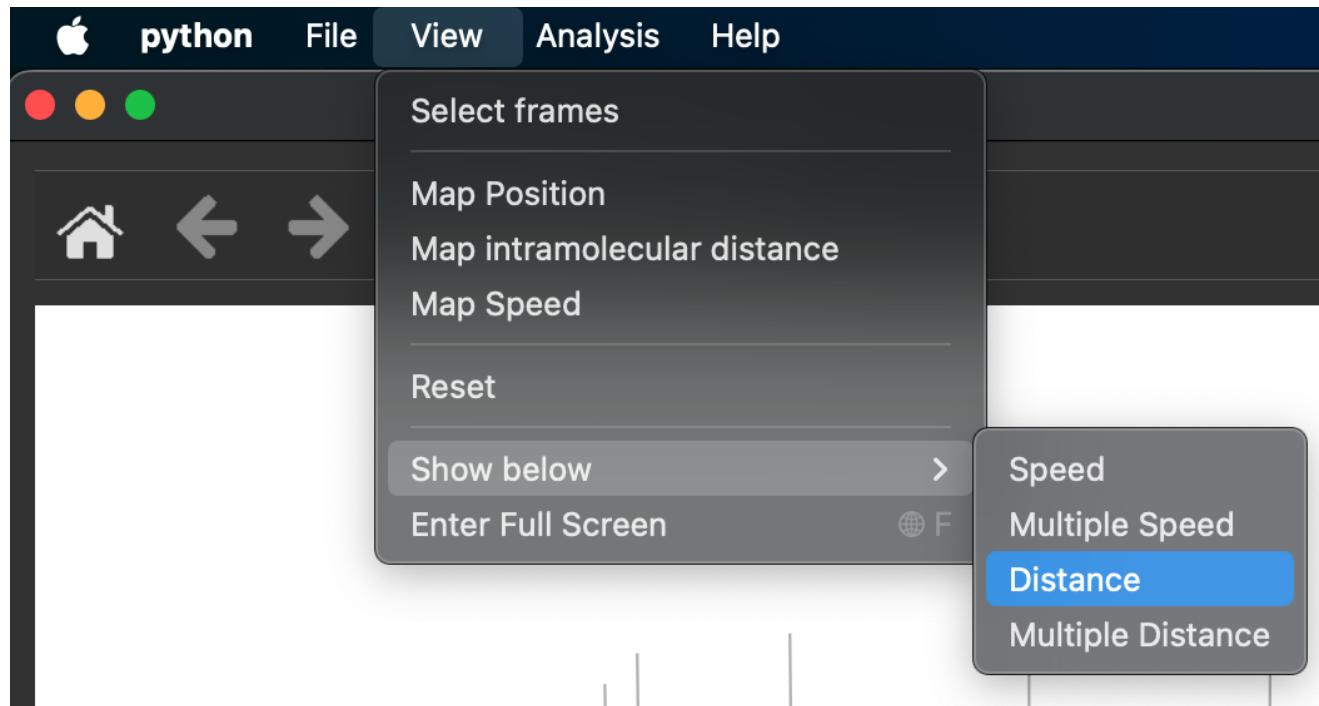
To show the changes of the intramolecular distance [\AA] between exact two different atoms of the representative molecules or all other molecules of the simulation in the bottom view you can go to *View > Show below > Distance*

to display one instance in a single graph or *View > Show below > Multiple Distance* to display multiple instances in one graph.

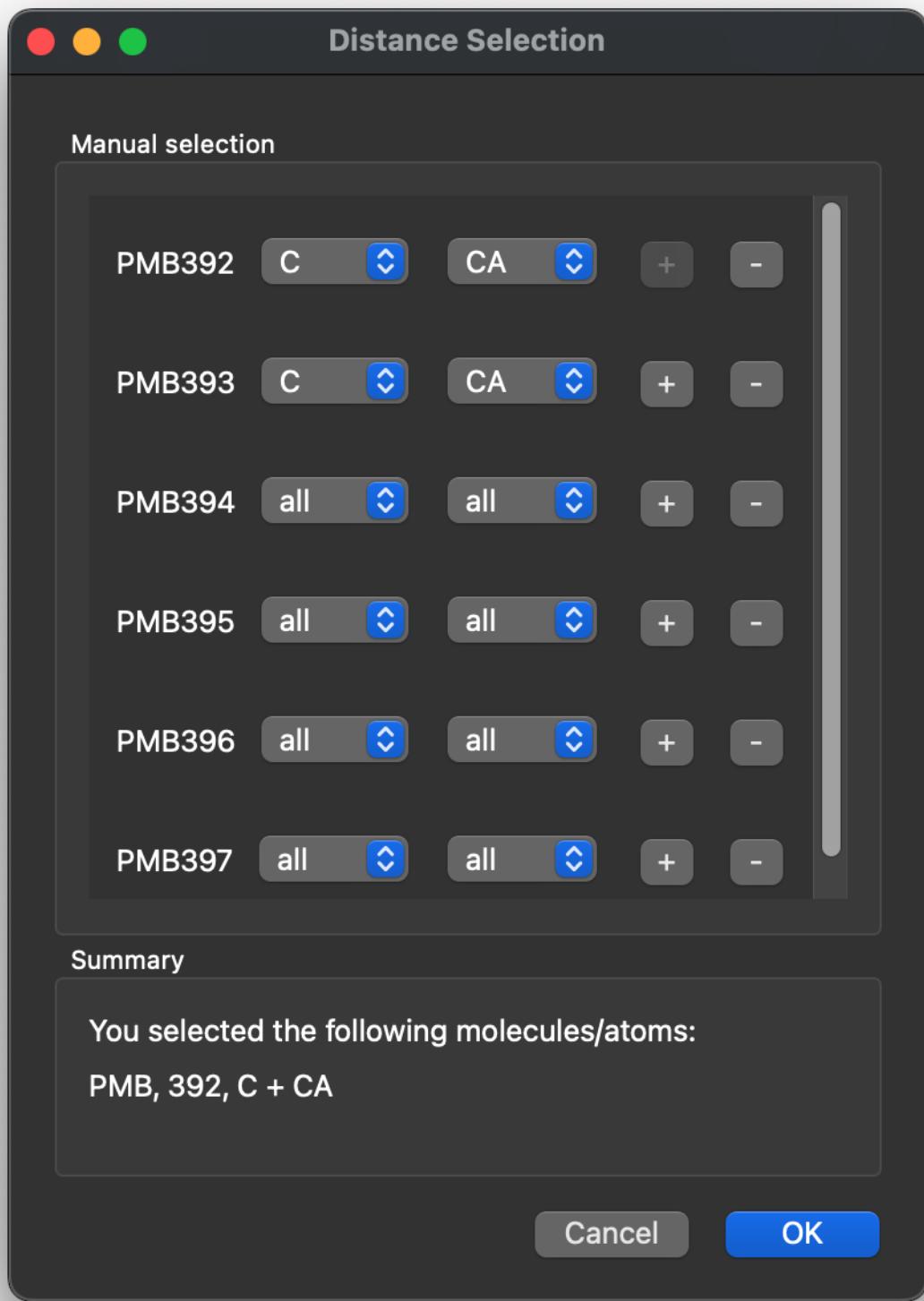
Full Screen Mode

To switch to full screen mode go to *View > Enter Full Screen* or use the shortcut `ctrl + F`.

Change View Path



Distance Selection



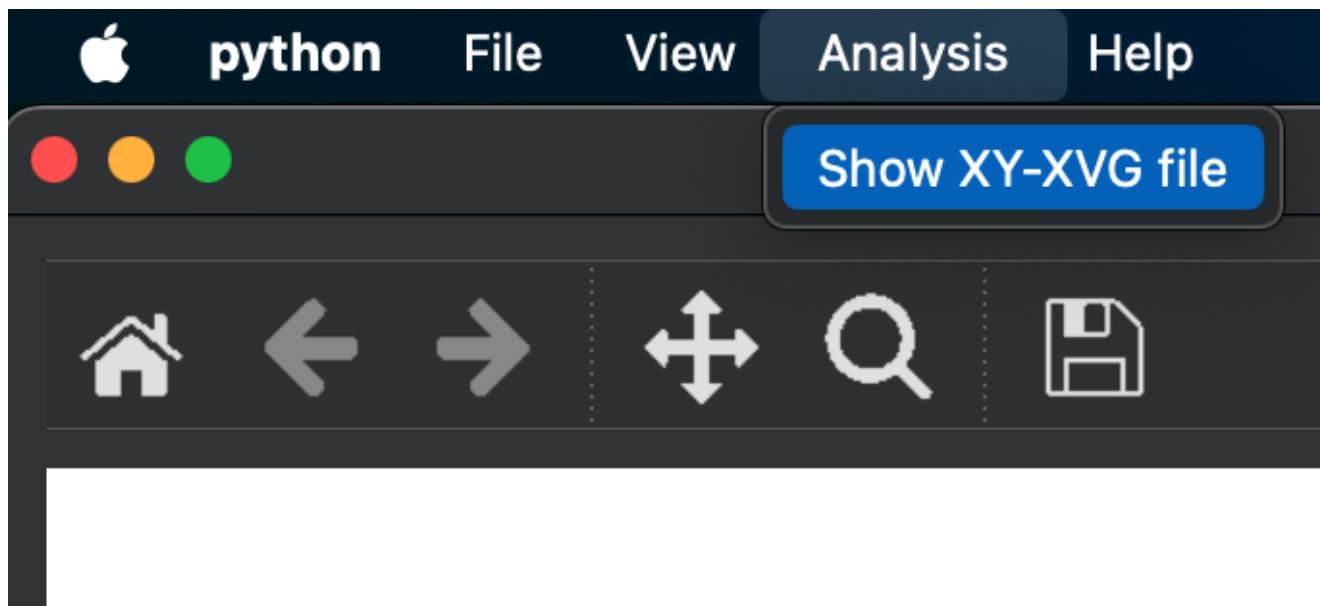
Further Analysis

To display data from an .XVG file go to *Analysis > Show XY-XVG file* ([see picture](#)). You need to provide a file and must at least select one representative molecule ([see picture](#)).

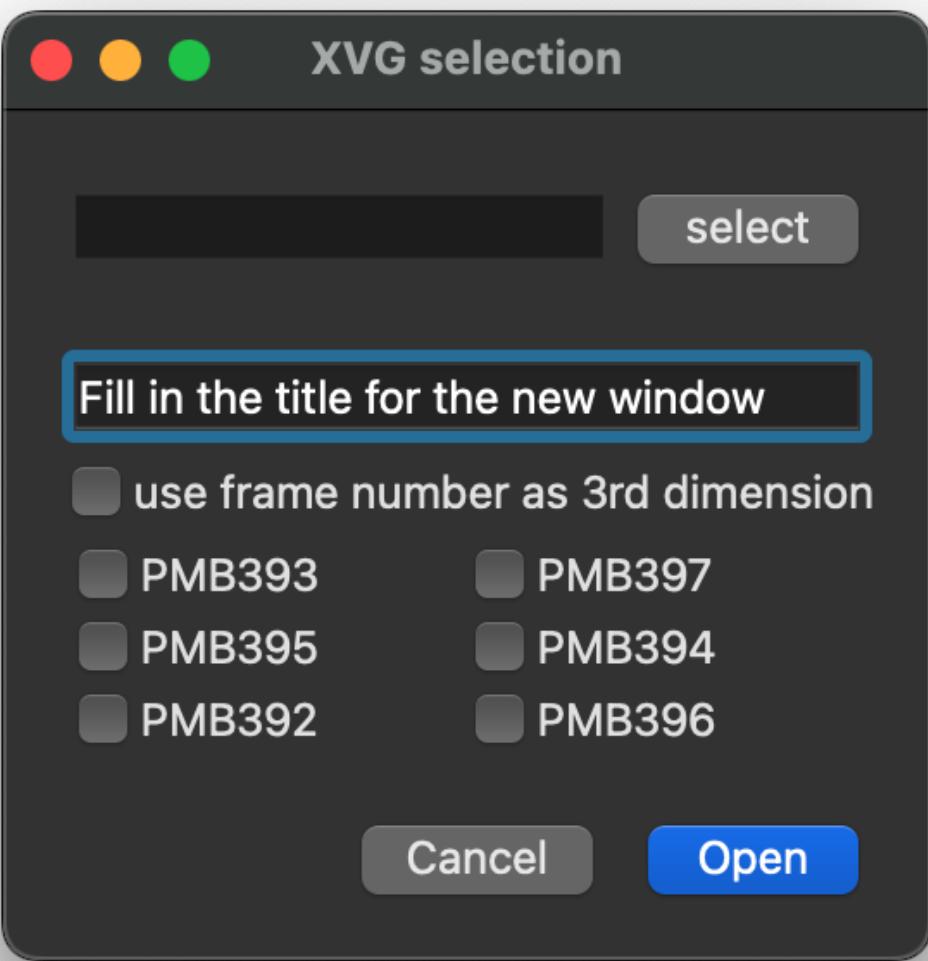
An additional window will open ([see picture](#)) You can use the slider to show the changes over the time scale or use the `jump to frame number` to highlight a specific frame. Pressing the play button starts or stops a time laps of the represented data.

The options of the side bar provide the options to change the colours of the graph, modify the legend and hide the sphere which indicates the current selected frame. The `save` button will save the graph as a .png file.

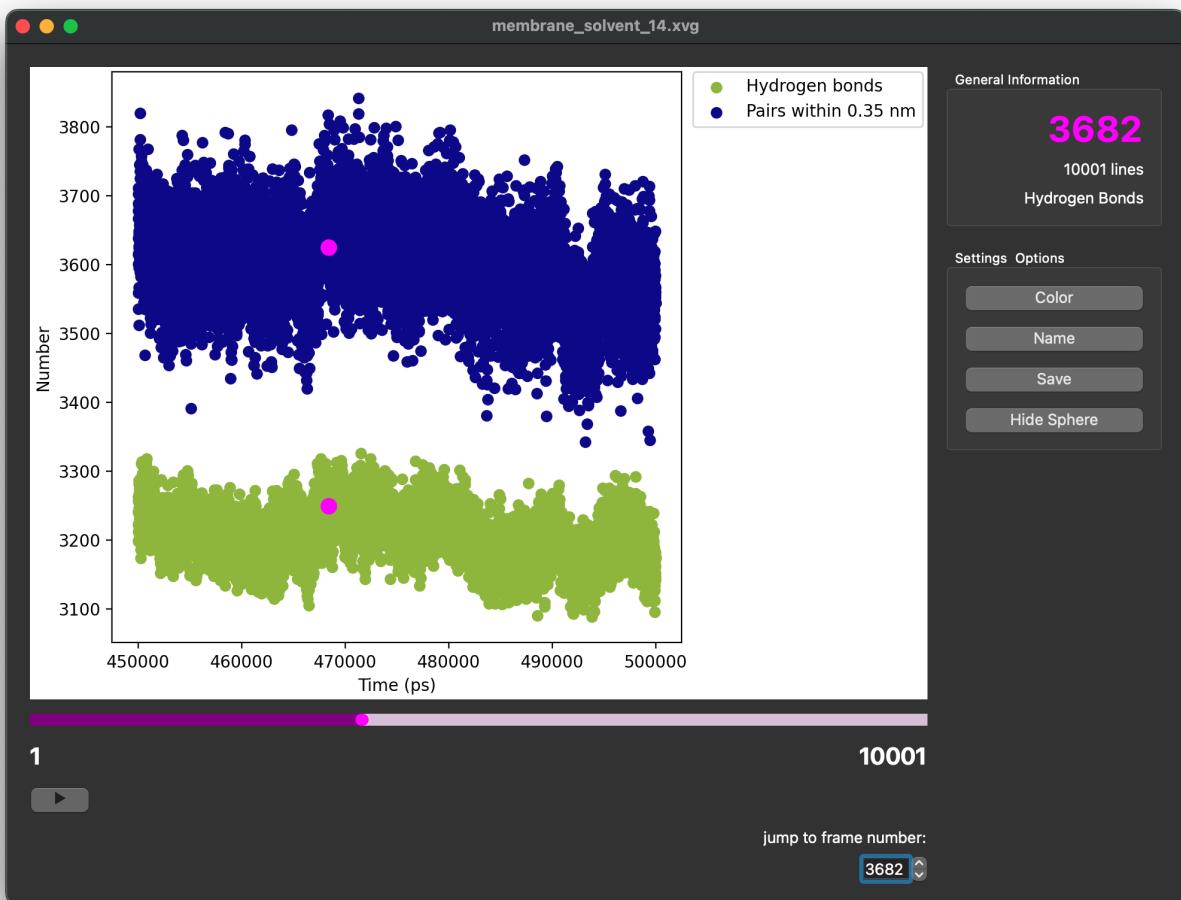
Show Analysis



XVG Selection



Sub-Window



Save File

There are different options to save your analysis or visualisations.

Save PDB file

In the menubar you can use *File > Save to XPDB* to save interesting structures as .PDB file.
Use *File > Save selection to XPDB* to save only selected molecules as .PDB file.

Save image

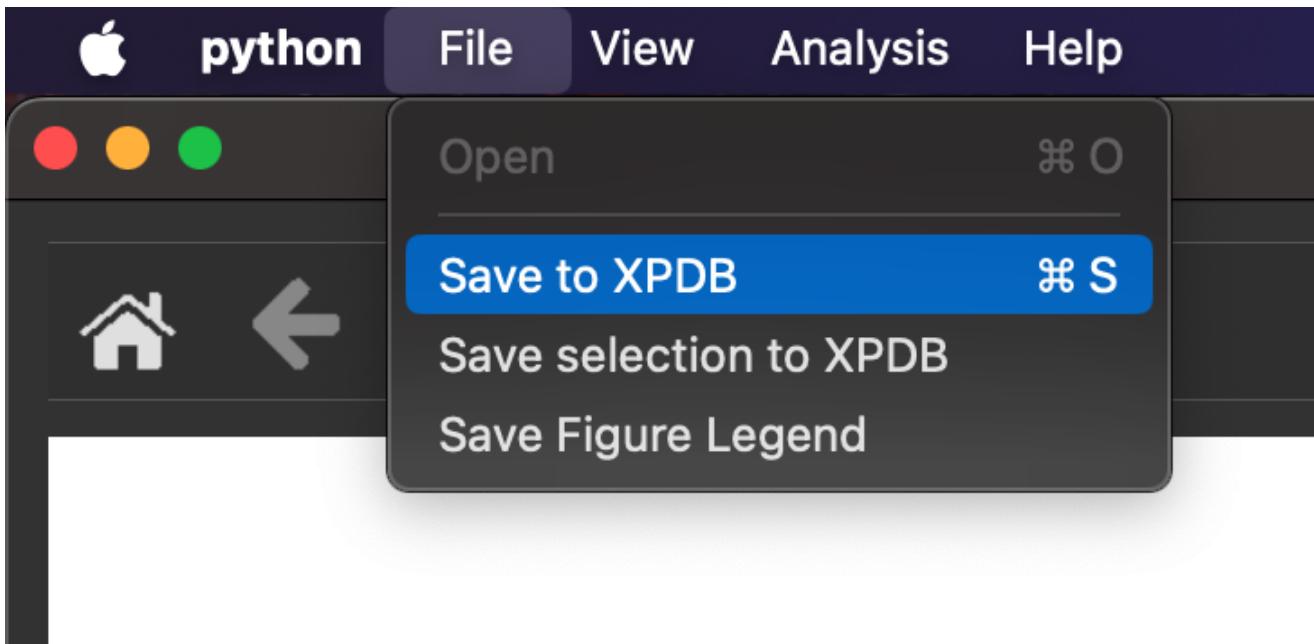
If you want to save the view and all legends use the *save button* on top of the main view as described in [Navigate in Main Graph](#).

To save only the legend of the main view use *File > Save Figure Legend* ([see picture](#)).

To save the graph of the bottom view use the *save* button on the right side of the graph. When the check box in the analysis-overview-box is activated a .CSV file of the in the overview shown data is saved, too.

When working in an separate analysis window you can save the corresponding image with the *save* button on the right side of the additional window.

Saving



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Cite

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When using MeTrEx, please cite: