



## STEP 10 RANKING OF MODELS

Now, when you know how to generate models with PyRy3D and how to use basic features of the program you can wonder:

OK, but what if I have a set of alternative models e.g. from docking and I want to check which one fits best to data from experiments including distance restraints and/or an electron density map? Will PyRy3D help me here?

The answer is YES!

PyRy3D Extension offers **Ranking of Models** – an option to rank models based on experimental data such as distance restraints or quality of fit between complex structure and corresponding electron density map.

1. Close UCSF Chimera and open new session again.
2. To use **Ranking of models** a first step is to achieve a set of alternative models. You can get them by any other docking method e.g.

GRAMM (<http://vakser.bioinformatics.ku.edu/resources/gramm/grammx/>),

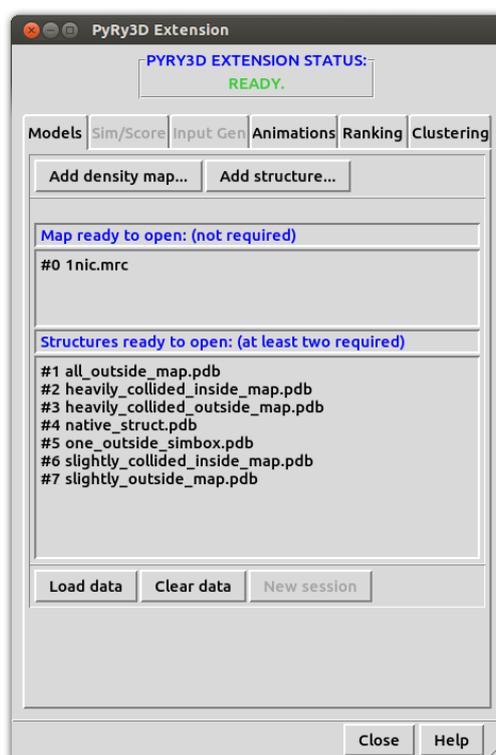
PATCHDOCK (<http://bioinfo3d.cs.tau.ac.il/PatchDock/>).

Usually as a result of such approaches a user receives a set of models. However, the missing information is which model fulfills best other (not used in docking) experimental data e.g. from chemical cross-linking, footprinting, electron microscopy? Here for the workshop we have already prepared a dataset of alternative models for you (**create\_ranking**).

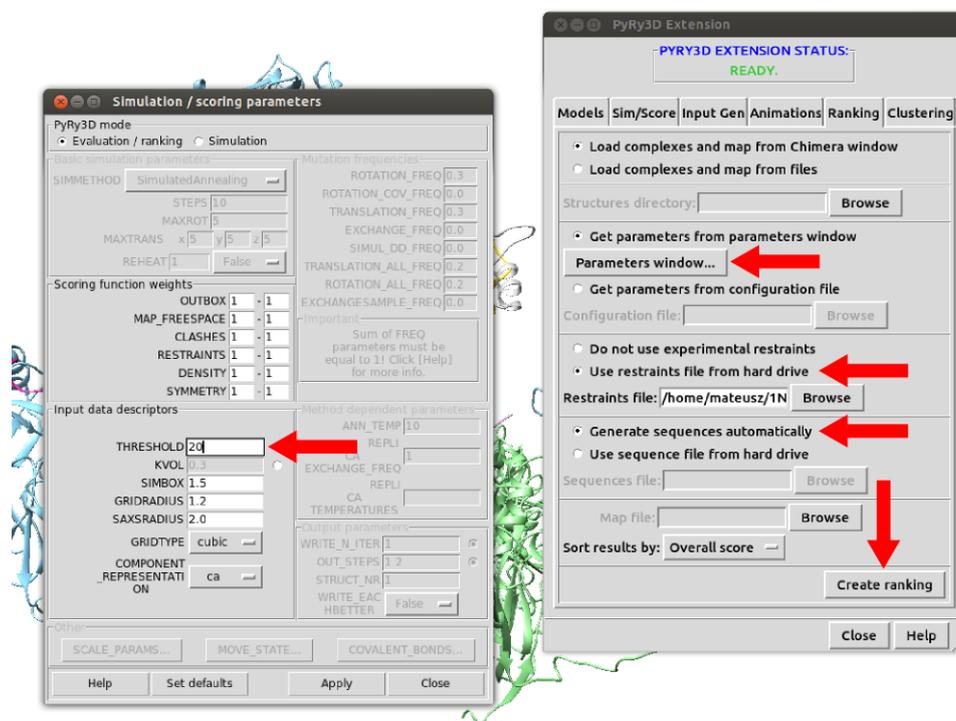
3. The files used in your ranking might also be the results of previously performed PyRy3D simulations.
4. There are two ways you can provide input complexes for ranking. You can generate a set of .tar files (standard input format for the program), using PyRy3D Chimera Extension's input generator, and provide a path to the directory containing generated packages. The other way, which is described in this tutorial, is simply by loading the PDB files into Chimera via the extension. You have to remember about several things while preparing your models:
  - The models' coordinates must be saved relative to the density map
  - Each model must be one separate PDB file (with as many chains as there are components)
  - There can be only one model per PDB file



- To load your density map and structures into Chimera, go to the Extension's **Models** tab and load the files the same way you'd load separate components of one complex (except now, instead of single chains, the pdb files must contain whole complexes). Add your density map, add your structures and click **Load data**.



- Go to the extension's fourth tab, called "**Ranking**". There, go to parameters window and change the density map's threshold to 20. Also, in order to include spatial restraints in your ranking, provide restraints file using "Use **restraints file from hard drive**" option. Select "**Generate sequences automatically**", and click "**Create ranking**" to start the evaluation.



- After a while (the time depends on the number of structures in your ranking, configuration parameters and complexity of your complexes) a table with the full ranking is displayed, where you can see how each complex was scored. You can change the way the structures are sorted using the menu on the bottom of the ranking window. You can also save your ranking to a text file. The models in ranking are named after their model numbers in Chimera's window - you can use the **Model Panel** tool to check which file corresponds to each position in the ranking. As you can see in our example, the highest scored model was model number 4, which corresponds to the 1NIC's native structure.

