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## STEP 9 PREPARING INPUT FILES FOR THE MAIN COMMAND-LINE PROGRAM AND SERVER

It usually happens that a user will find a nice-looking tool dedicated to solve a particular task. However to run it a lots of requirements are necessarily and additionally input files for the program must be prepared in very specific (often very complicated) format. This is why we developed **Input Generator** tool which prepares files in format required by command-line PyRy3D. Having files generated automatically from the Chimera Window, user just needs to run a program with no additional modifications ☺

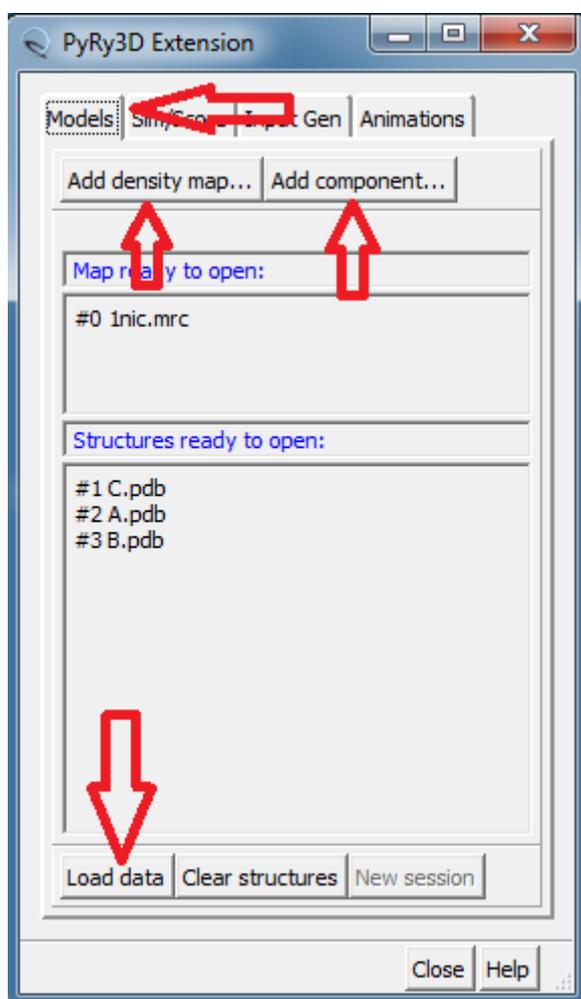
PyRy3D UCSF Chimera Extension offers a possibility to quickly and easily generate input files in particular format required by command-line software. Particularly you can obtain:

- **\*.tar archive with structures** saved straight from the screen (all modifications you will perform like rotations, translations will be included)
- **\*.fasta sequences** generated automatically from structures
- **\*.map electron density map** will be saved from the viewer (here simple coping, no modifications including threshold change are saves)
- **\*.txt configuration file** with parameters you chose in **Parameter Window**

The only input file that is **\*yet not possible\*** to create via PyRy3D Extension is a file with restraints. You have to prepare it alone following the rules described here: <http://filtrest3d.genesilico.pl/readme.html/> OR use server to prepare these files: <http://filtrest3d.genesilico.pl/filtrest3d/help.html/> (please bear in mind that a server does not support Boolean operators). **Good news!** The restraints generator will be added in next version of PyRy3D extension.

Having all input files created automatically via PyRy3D Extension you can easily use them to run local version of the program. No further modifications of files are required, just run the program and wait for models! As easy as that ☺

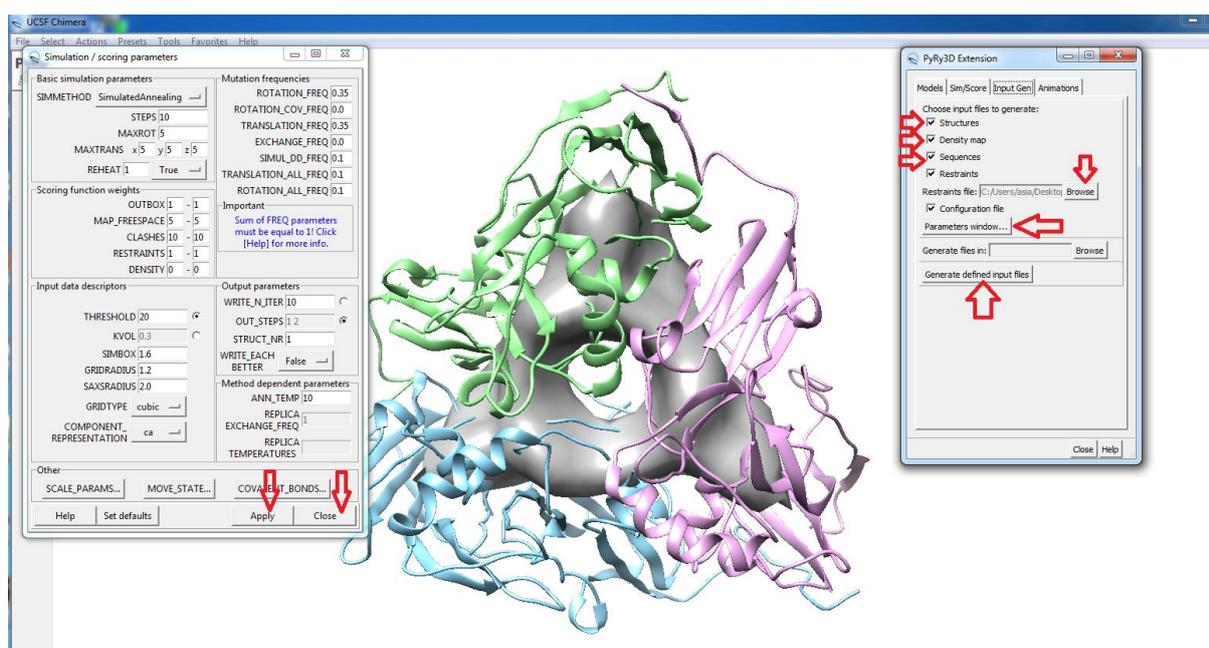
1. Close Chimera and open a new session of the viewer.
2. Using the **PyRy3D Extension**'s interface, load all structures of 1NIC complex components (**A.pdb**, **B.pdb**, **C.pdb**) and the electron density map (**1nic.mrc**) into the Chimera's graphics window (see **STEP 4**)



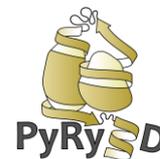
3. Go to **Input Gen bookmark** of the Plugin's interface to generate following input files:
  - a. **Structures** - if checked, the program generates a proper .tar archive that contains PDB files ready to be used in PyRy3D software. The PDB files are generated based on the structures that are currently displayed in the UCSF Chimera viewer (orientation according to the electron density map is also saved).
  - b. **Density map** - an electron density map from the screen is copied into the output folder (simple copy of whole file, the chosen threshold value is not considered).
  - c. **Sequences** - a multi FASTA file is generated based on the structures opened in the viewer. **ATTENTION:** Sequences in a FASTA file will be identical with

those in PDB files. If structures lack any residues (e.g. due to disorder) please load FASTA file from your hard drive.

- d. **Restraints** - a file with spatial restraints is copied to the common directory. Check restraints and select **1nic.restr.txt**. **ATTENTION:** PyRy3D uses Filtrest3D format to describe interactions between complex components. The file can be prepared automatically by the filtrest3D server: <http://filtrest3d.genesilico.pl/filtrest3d/index.html/>
- e. **Configuration file** - to set the parameters values, use the "**Parameters Window**" (it's the same window that you use before performing evaluations and simulations). All changes you will introduce will be included in file prepared by the extension. Select 10 000 steps this time.



- f. After you select all data to generate by the PyRy3D Extension, just select a folder where you want to store files (**Generate files in, Browse**) and click **Generate defined input files**
- g. In **Outfolder** you should have:
  - **input.tar** – archive with structures shown on the screen
  - **sequences.fasta** – sequences of components from input.tar folder
  - **config.txt** – file with parameters chosen
  - **restraints.txt** – copy of file you provided



- **1nic.mrc** – copy of file with electron density map
4. Now try to run PyRy3D server with those files: <http://pyry3d.icm.edu.pl>. Compare results with one obtained with the GUI. The model should be much more accurate, isn't it?