FORECASTER Platform Tutorial

Self and Cross Docking using FITTED

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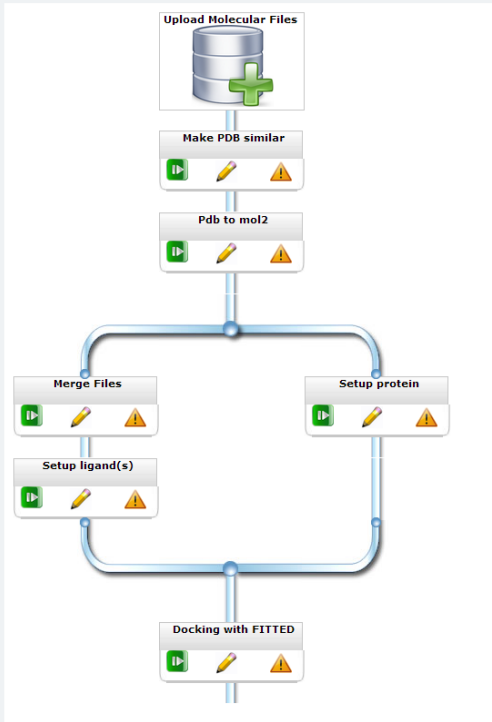
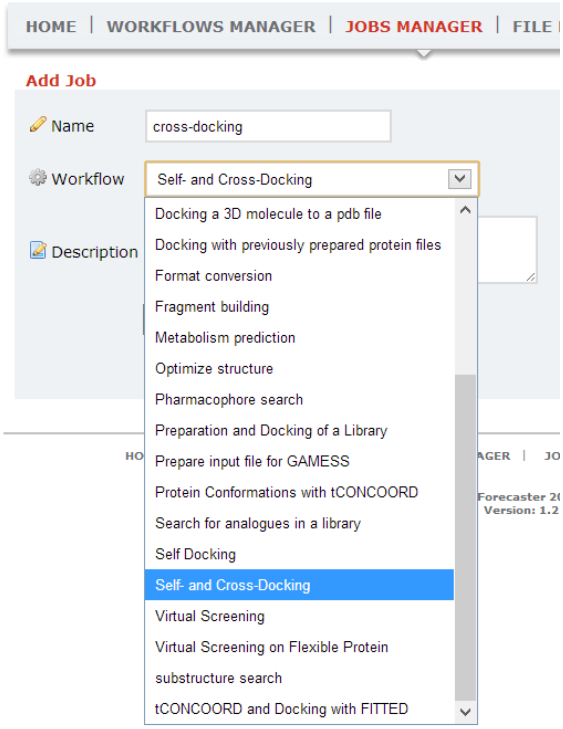
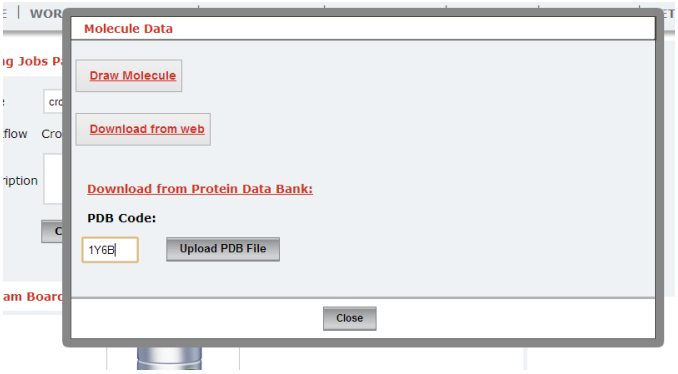
In this tutorial, we will use 3 PDB files: 1Y6B, 2P2H, 2P2I. A **cross docking** in a **rigid protein** docking mode will be done. The same workflow can be used to run a cross docking in flexible protein docking mode

1. Create a new job and select the “Self and Cross-Docking” workflow (If the workflow doesn’t exist already, contact us or create it from the workflow manager).

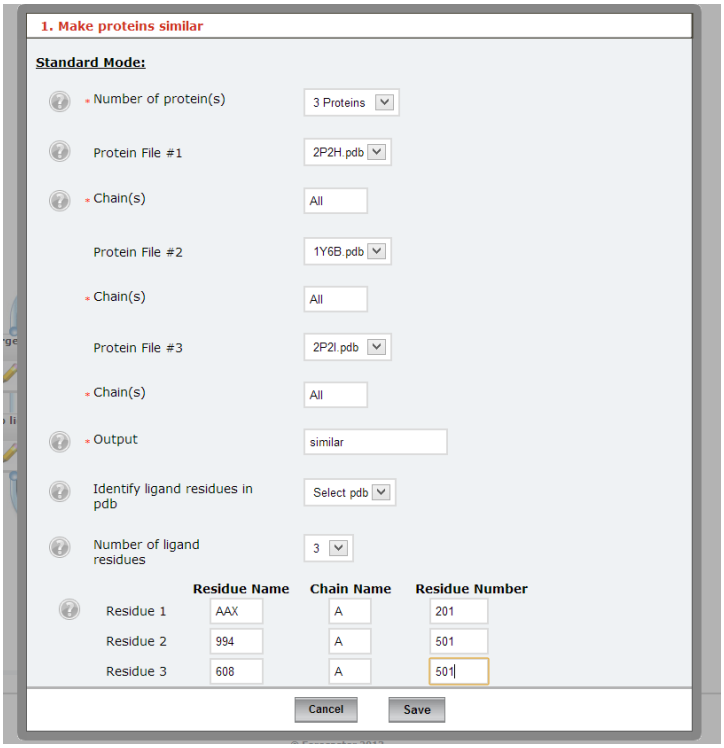




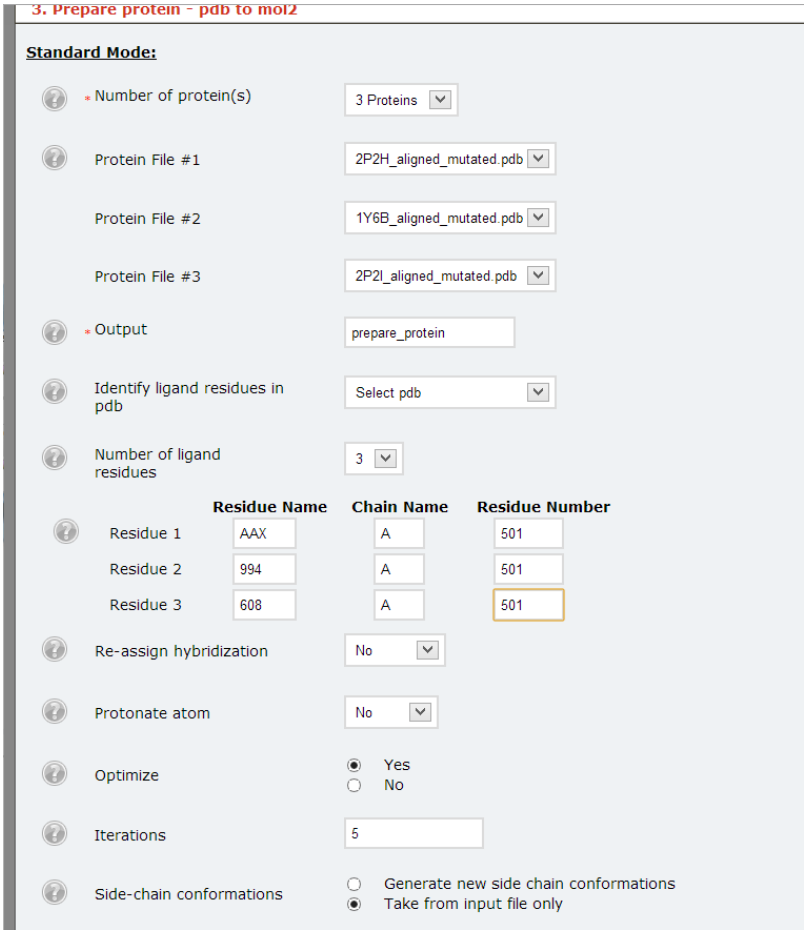
2. Upload the PDB files by clicking on the cylinder “Upload Molecular Files”.



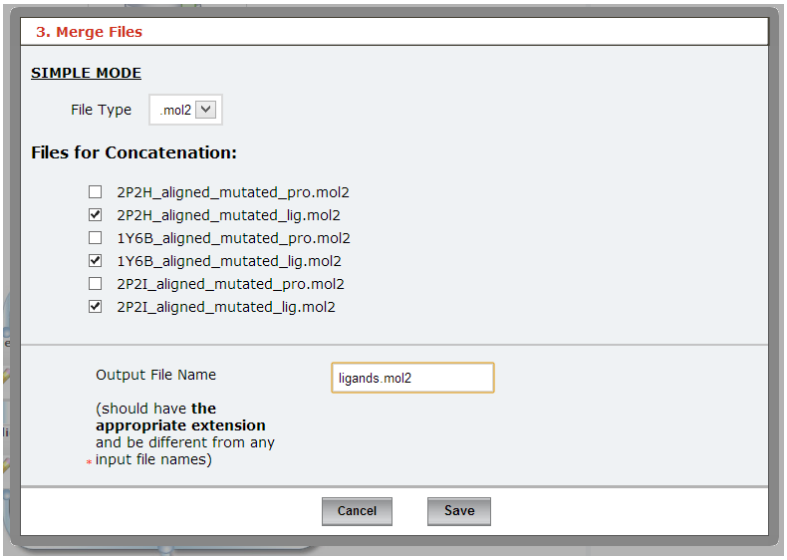
3. In the “Make PDB similar” box, fill in the required settings. Then click save.



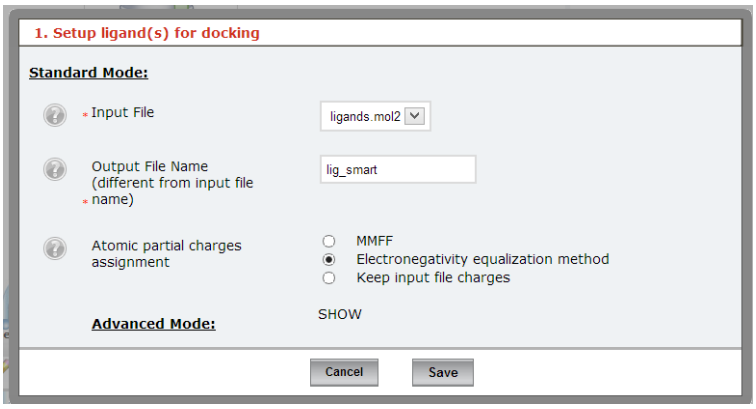
4. In the “PDB to mol2” box, fill in the aligned_mutated proteins and residues. Leave all other settings as default. Then click save.



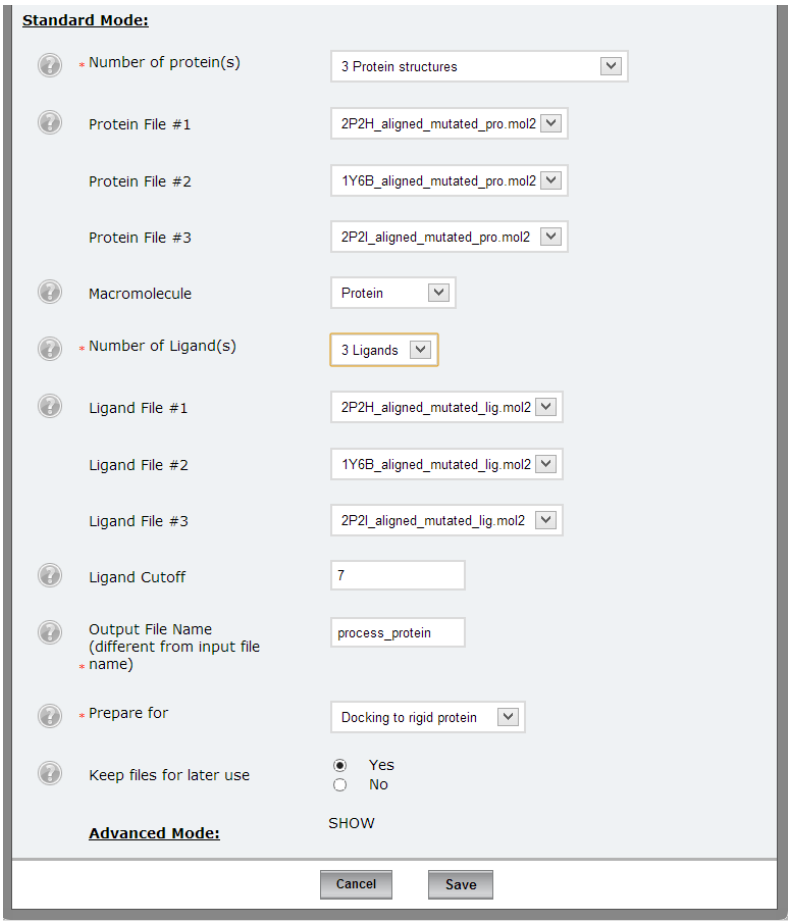
5. In the “Merge Files” box, merge the ligand files to create a single multi-mol2 file. Don’t forget the “.mol2” extension.



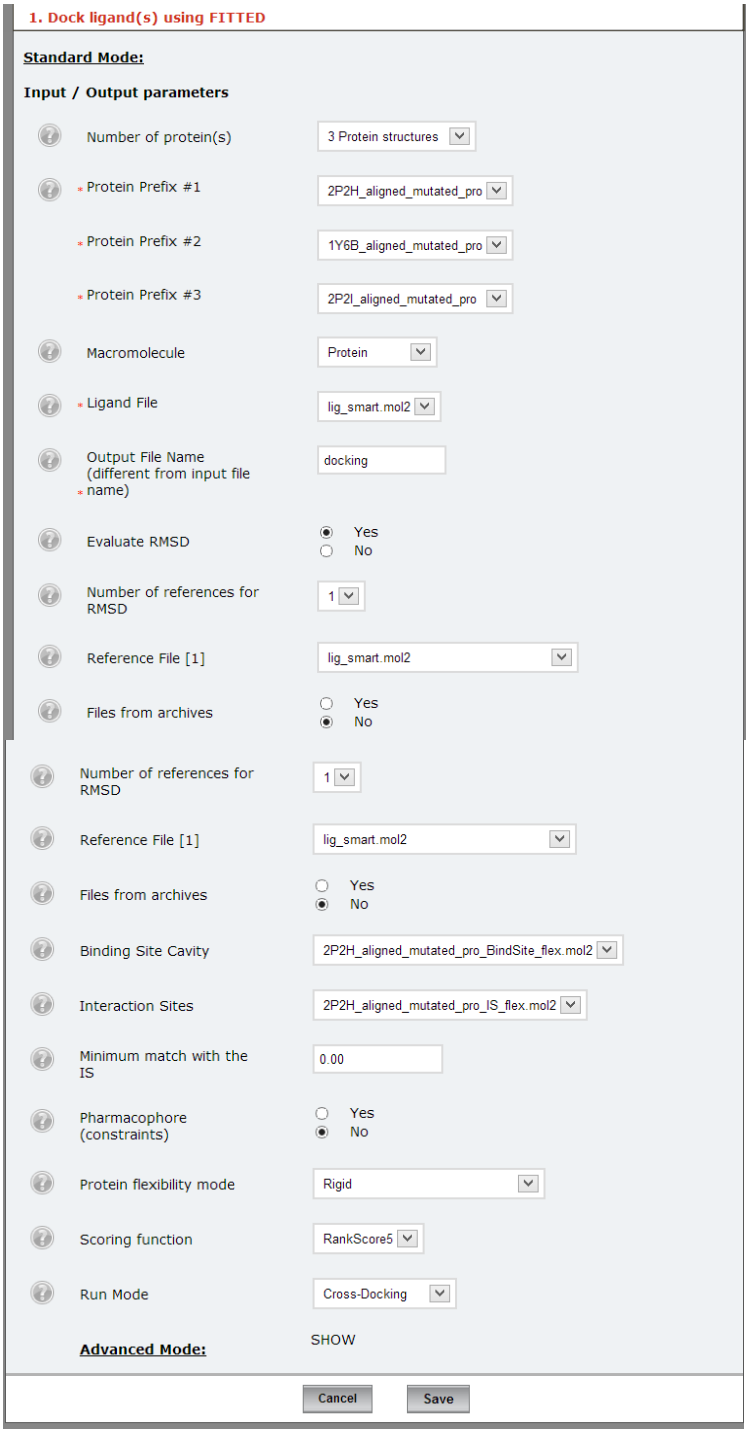
6. Prepare the ligands within the “Setup Ligands” box.



7. Prepare the proteins within the “Setup Proteins” box. Choose Docking to rigid protein.



8. Fill in the settings for the “Docking with FITTED” box. Pay attention to selecting “Evaluate RMSD”, the proper flexibility mode “Rigid” and set the Run Mode to “Cross Docking”.



9. Once the docking is complete, the complete results can be found in docking-results.txt and the docking.sdf contains the docked poses.