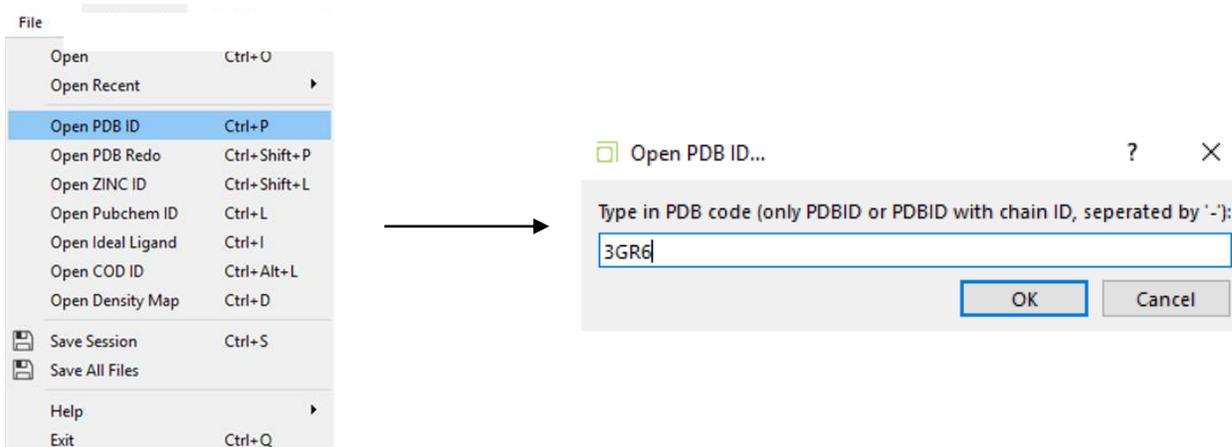
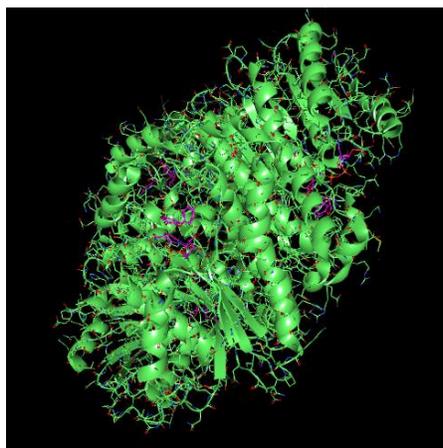
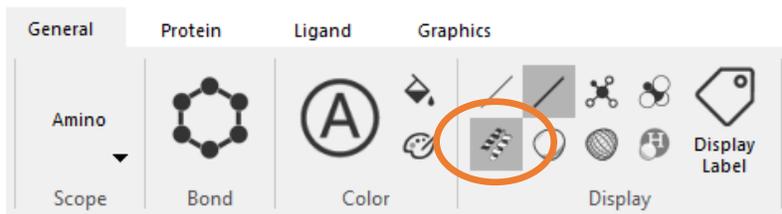


Conformational errors of deposited high resolution crystal structure of chemical compound identified by Accutar docking platform.

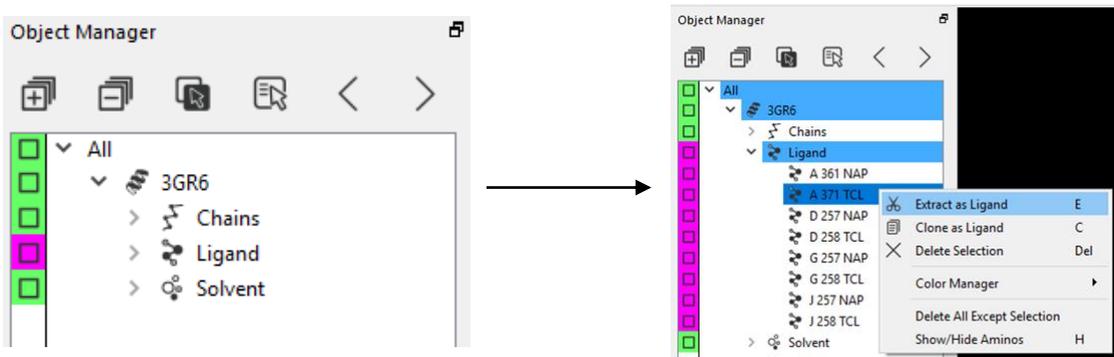
1. **Open** Orbital from the desktop. In the **File** dropdown menu, select **Open PDB ID** (Ctrl+P).
2. In the Open PDB ID popup window, enter the PDB ID **3GR6** and select OK in order to open the Crystal structure of the staphylococcus aureus enoyl-acyl carrier protein reductase (fabI) in complex with NADP and triclosan.



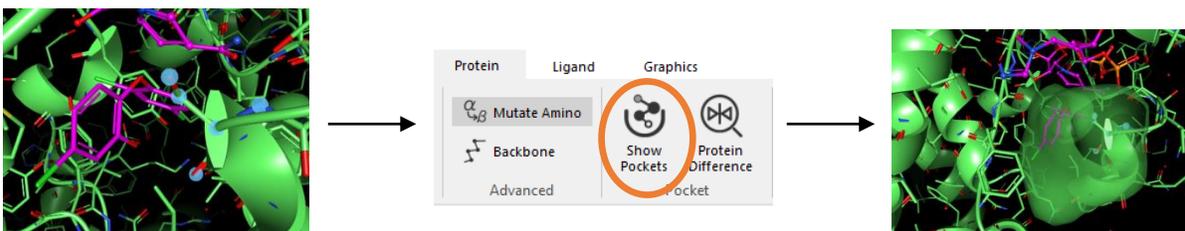
3. Under the **General** tab select the **Cartoon** setting in the **Display** panel in order show the protein in its cartoon structure.



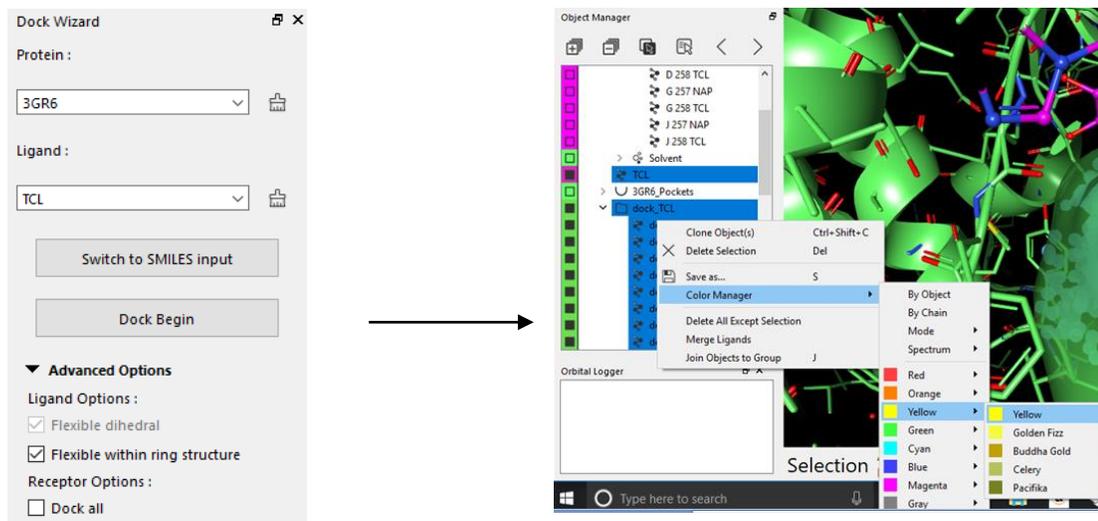
- Next, open the dropdown menu for 3GR6 in the **Object Manager** by selecting the downward facing caret next to the name.
- Select the ligand tab and right click **A 371 TCL** and select **Extract Ligand (E)**.



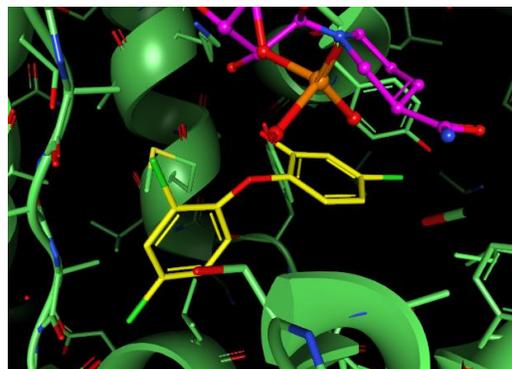
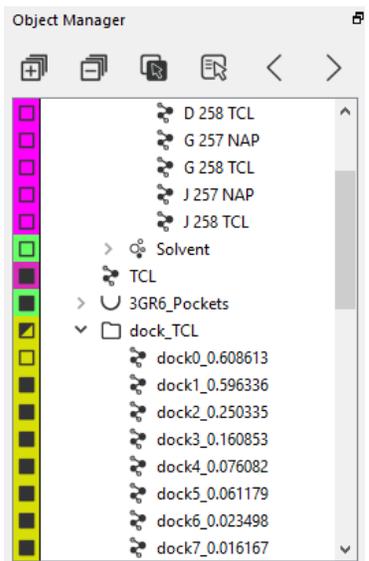
- Use the scroll button on the mouse to select the ligand TCL. This will center the ligand in the viewport. Left-click to select the amino acid adjacent to the ligand (selected below). Then, in the Protein panel select show pockets and the pocket surrounding that residue will be displayed. Select the pocket in the viewing screen before docking.



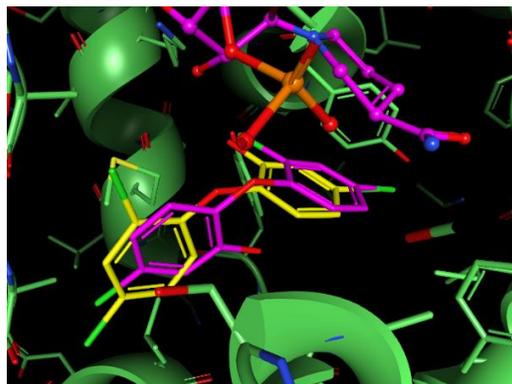
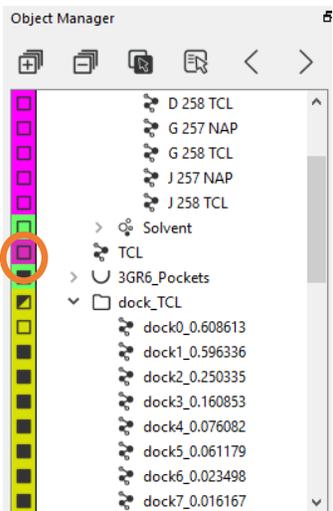
- In the **Ligand** tab select **Dock Wizard**. The wizard will open a panel on the right side of the screen. Ensure that the flexible dihedral, flexible within ring structure, and dock boxes are checked. When ready, select Dock Begin. A new folder in the Object Manager will be created called dock_TCL under the object 3GR6_Pockets. Right click the highlighted folder and under the Color Manager Dropdown change the color to yellow.



8. Hide the 3GR6_Pockets object in the Object Manager by selecting the square to the left of the name. Then select dock0 with the scroll button to center the object in the view.



9. In the Object Manager, select the black box to the left of the name of the original TCL ligand in order to display it in the screen (in purple below).



10. In the **File** dropdown menu select **Open Density Map** and enter 3GR6.

