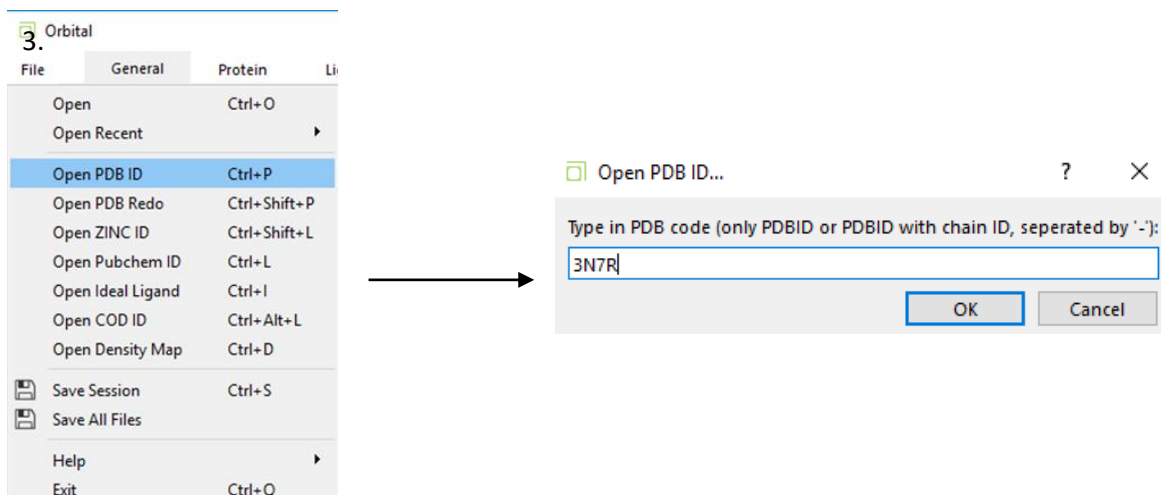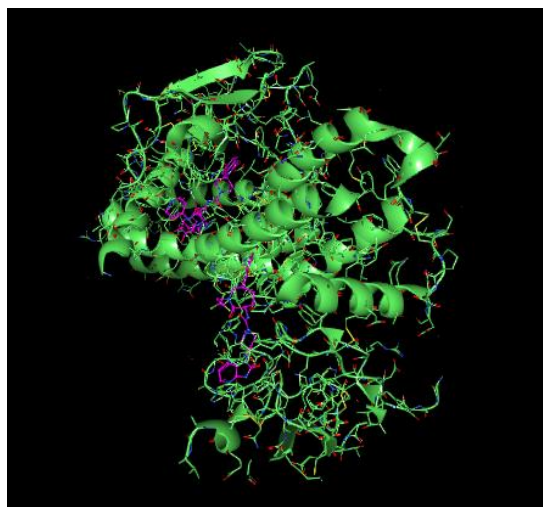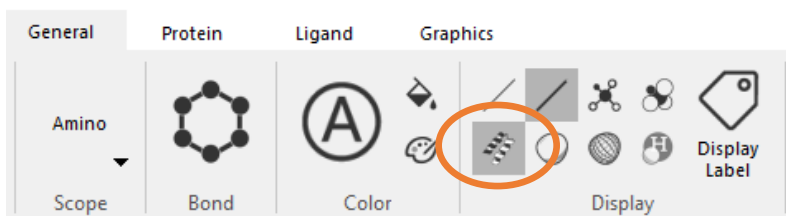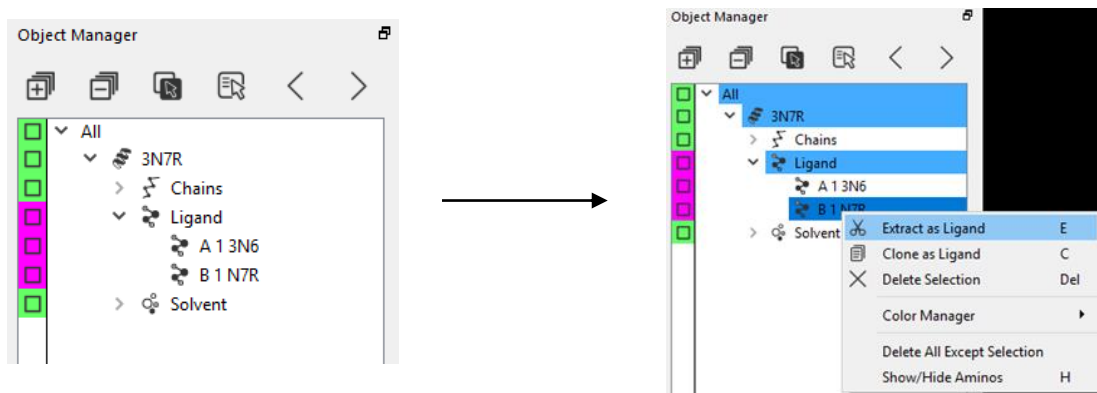# Migraine target: CGRP

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 **3N7R** and select OK in order to open the crystal structure of the CGRP receptor.
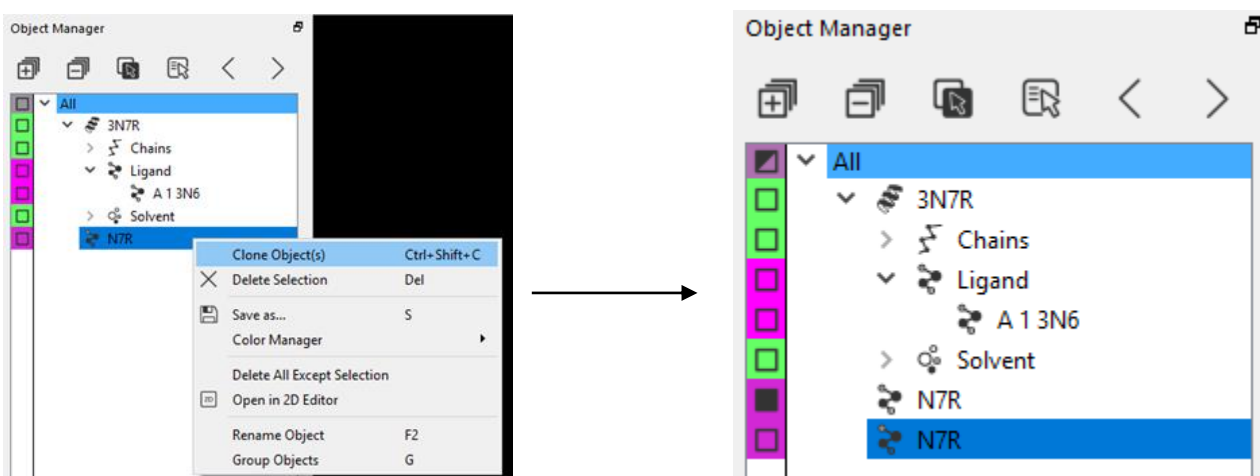
3.

4. Under the **General** tab select the **Cartoon** setting in the **Display** panel in order show the protein in its cartoon structure.
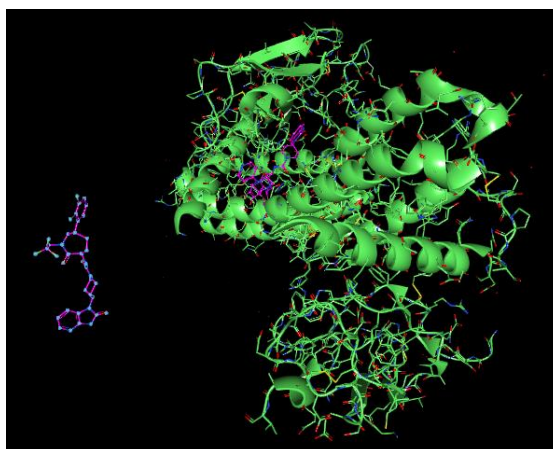
5. Next, open the dropdown menu for 3N7R in the **Object Manager** by selecting the downward facing caret next to the name.

6. Select the ligand tab and right click **B 1 N7R** and select **Extract Ligand** (E).

7. Use the scroll button on the mouse to select the ligand N7R. This will center the ligand in the viewport. Right-click on N7R and select **Clone Object**. Deselect the original ligand and select the clone. Next, the click the highlighted box to the left of the object in order to hide the original ligand.
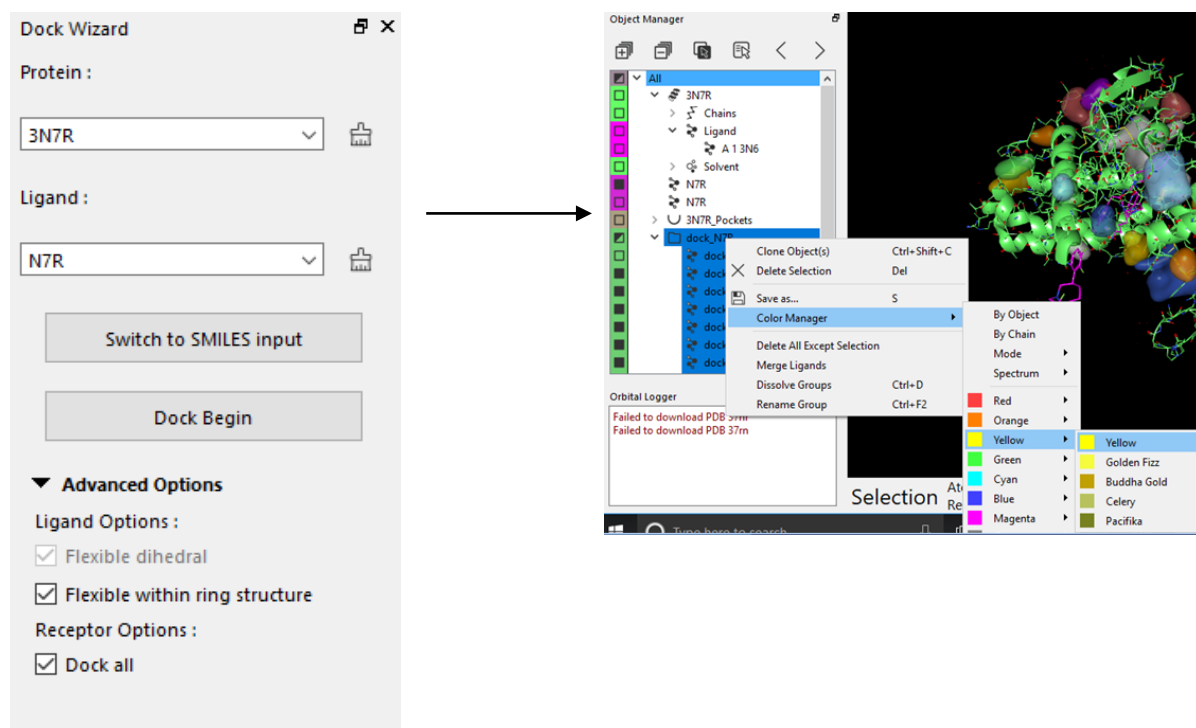

8. In order to zoom in on the ligand click the name in the Object Manager with the scroll button on the mouse. Select the ligand while holding Ctrl + Scroll button on the mouse to move the ligand away from the protein.
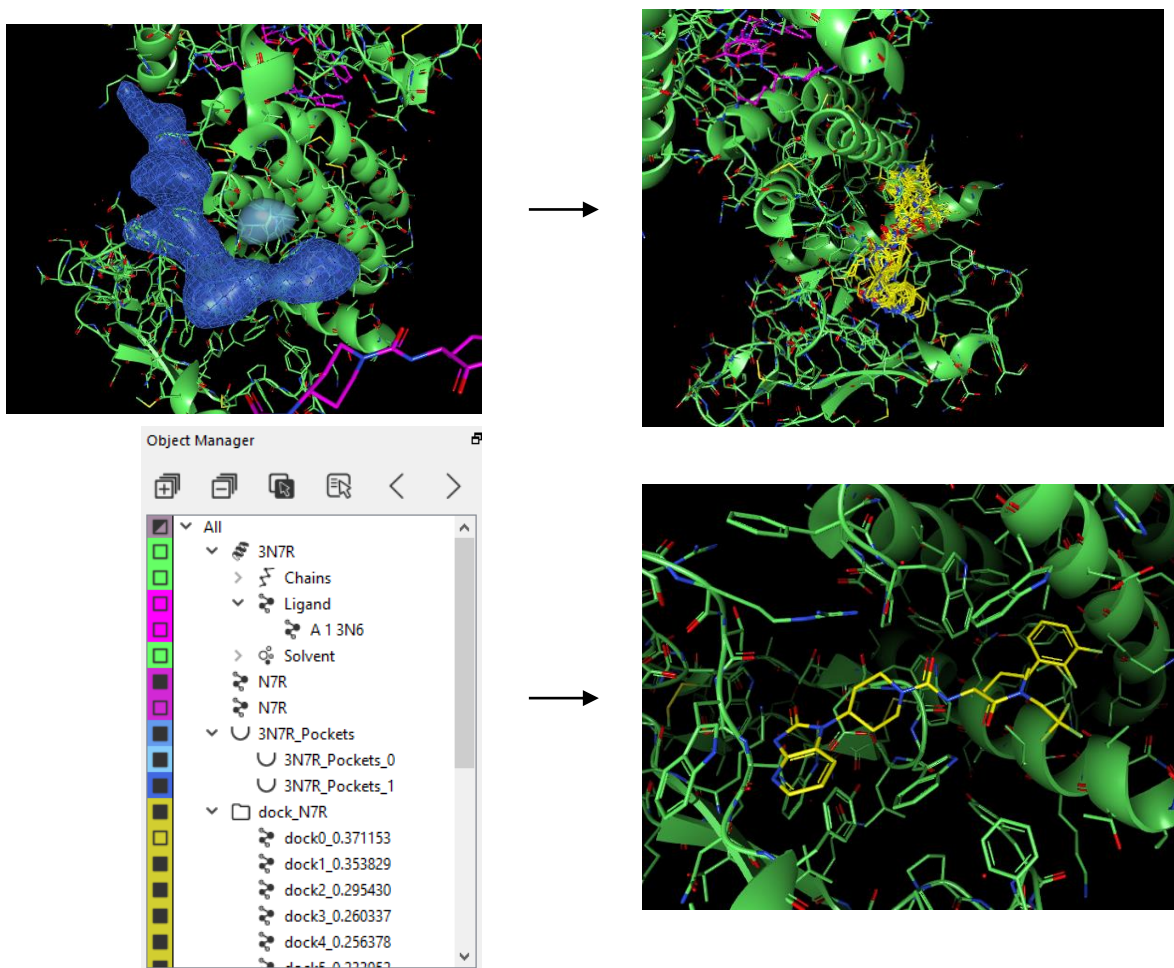
9. In the **Protein** tab select **Show Pockets** under the **Pocket** panel (circled in orange below). Orbital will then assign pockets to the protein surface.
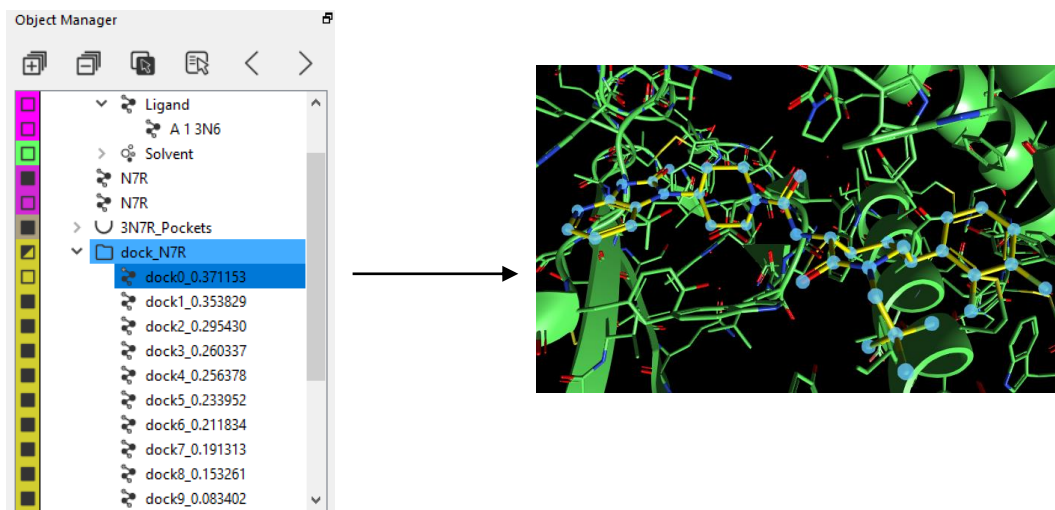

10. In the **Ligand** tab select **Dock Wizard**. The wizard will open a panel on the right side of the screen. Ensure that the flexible dihedral, flexible within ring structure, and dock boxes are checked. When ready, select Dock Begin. A new folder in the Object Manager will be created called dock_N7R under the object 3N7R_Pockets. Right click the highlighted folder and under the Color Manager Dropdown change the color to yellow.
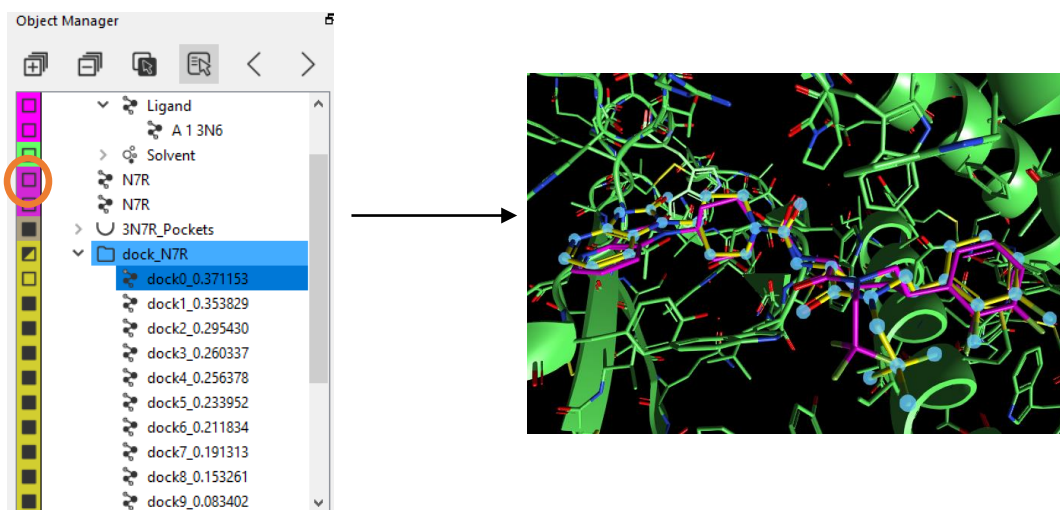
11. In order to dock the selected ligand to a specific pocket, select an amino acid residue and click show pockets in the **Protein** tab. Pockets around that residue will be displayed (blue). Left click on the desired pocket and proceed to dock the ligand as in step 10. All ligands docked will be calculated only for the selected pocket.
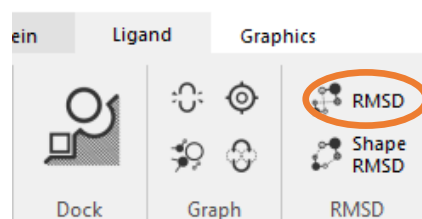

12. Hide the 3N7R_Pockets object in the Object Manager by selecting the square to the left of the name. Then select dock0 with the scroll button to center the object in the view.

13. In the Object Manager, select the black box to the left of the name of the original N7R ligand in order to display it in the screen (in purple below).

14. Select both the first docked ligand and the original ligand N7R. In the **Ligand** tab select **RMSD.** The RMSD will be displayed in the Orbital logger window at the bottom left of the screen.

15. The RMSD of each atom between the structures will also be displayed on the screen.

Matched RMSD between dock0_0.371153 and N7R : 0.79358