Pymol tutorial

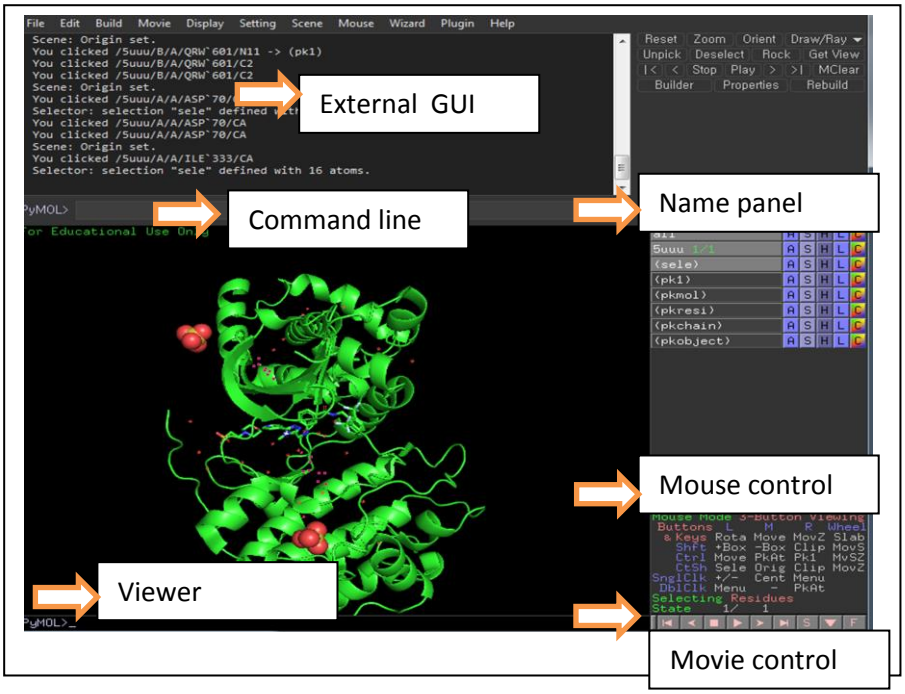
Download Pymol:

Download Site: pymol.org
License file: https://pymol.org/edu/?q=educational/

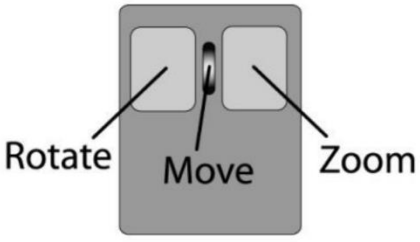
The pymol interface:

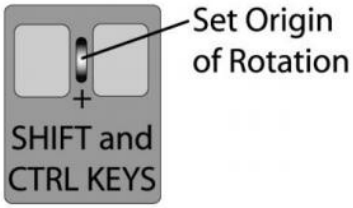
1. **How to download PDB via Pymol**
    a. Go to **File** >> **Get PDB**
    b. Enter the PDB ID as **5UUU**
    c. Click **Download**

2. **The interface**
    a. External GUI
    b. Internal GUI
    c. Name panel
    d. Viewer
    e. Sequence bar



3. **Mouse control**





4. **Representations: lines, sticks, ribbon, cartoon, surface etc.**
    a. Go to name panel
    b. Click **H > Everything** (this will hide everything)
    c. Click **S > lines**
5. **Remove water:**
    a. Go to the **name panel**: Click All > A> Remove water
6. **Saving sessions:**
    a. **File** > **save session**

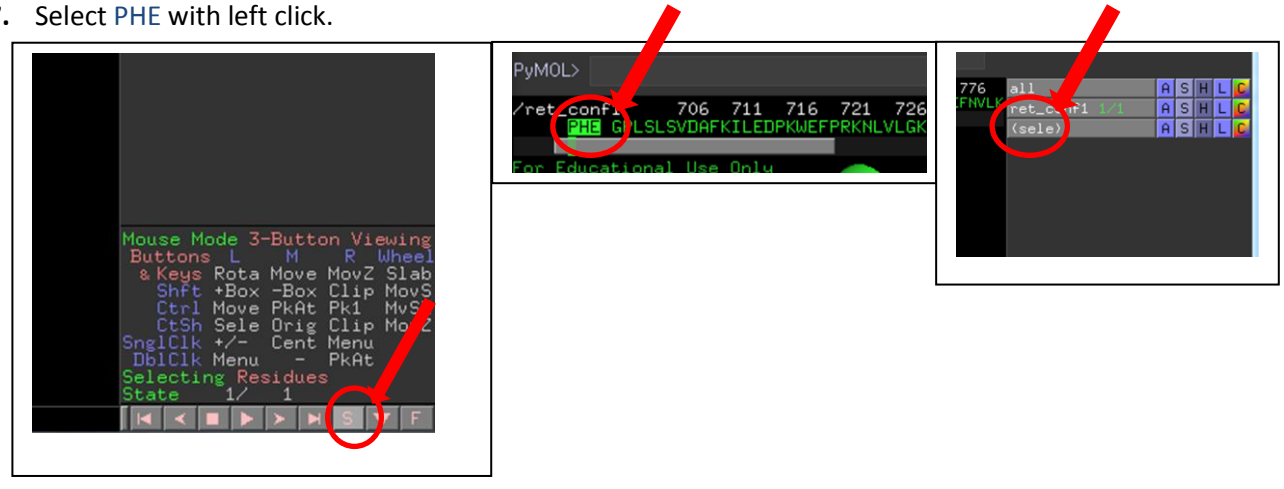
7. **Exporting molecules from pymol**
    a. Left click on the molecule (ligand) in the viewer
    b. Go to the **name panel** on the left: **<sele>** > **A** > **rename selection**
    c. Type in "**ligand**" and hit **Enter**
    d. Go to **File** > **Export molecule** > set **Selection** to **ligand**

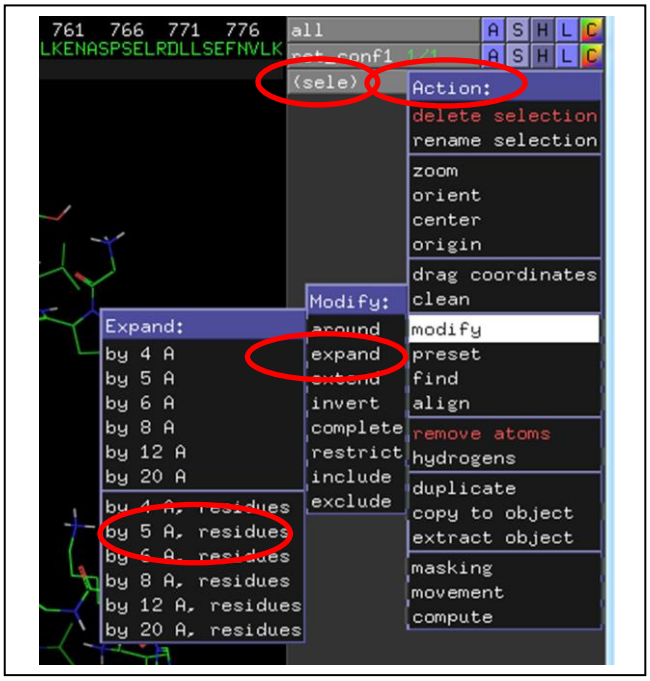
Protein Ligand Interaction:

1. Open the PDB file that has the Protein-Ligand complex (i.e the output of Autodock run)
2. Rename the object:
    i. Go to name panel and click the '**A'** corresponding to the object to rename: **(object)>A> rename object**
    ii. rename object to "ret_conf1"

Creating a New Object: This object will consists of the ligand and all residues that are at 5 A^{o} from the Ligand.

3. Go to Name panel: **Left click all > H> everything**
    Left click all > S> lines
4. Display the "sequence panel".
5. Left click on the label "S" at the **right-bottom** of the interface (refer picture).
6. Notice the PHE that is separated from the rest of the sequence.
7. Select PHE with left click.



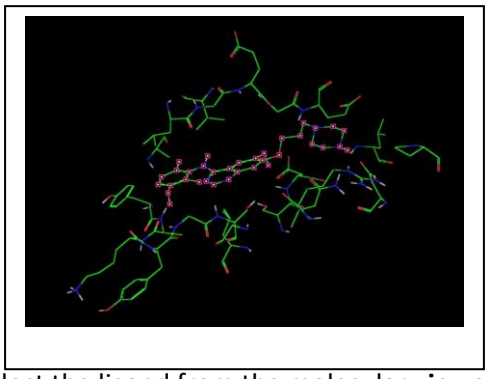


8. Select the residues:

9. <sele> > A > modify> Expand > by 5 A, residues

10. <sele>> A>copy to object> new

11. Go to **name panel**: Unselect all objects except obj1.



12. select the ligand from the molecular **viewer.**

13. Left click on the Ligand. (figure 5)

14. Change the ligand representation to **'stick'**

- **a. <sele> > H >everything**
- **b. <sele> > S> stick**

15. Show all H-bonds

16. <sele> >A > find > polar contacts> to others excluding solvent

17. Label all residues that forms H-bond with the ligand

- a. Single-left-click on all the residues that forms H-bond with the ligand.
- b. <sele> > L> residues

18. Show all residues that forms H-bond with the ligand in 'stick' representation:

- a. Single-left-click on all the residues that forms H-bond with the ligand.
- **b. <sele> > S> stick**

19. Finally, remove the 'stick' representations: **<obj1> > H > stick**
<obj1> > S > cartoon

20. Render the image and save it:
    - i. Go to the pymol command line and enter: **ray 2000**
    - ii. **File > Export Image as > PNG**

21. Save your work : File > Save session as > **pymol_RET_ligand_interaction**