BIOC351: Proteins

PyMOL Laboratory #1

Installing and Using

Information and figures for this handout was obtained from the following sources:

Introduction to PyMOL (2009) DeLano Scientific LLC.

Installing

PyMOL will run on Macs (10.4+), Windows (XP to 7), and many flavors of Linux.   To install PyMOL on your machine please do the following:

Mac: Place the binary (MacPyMOL-v1.3r1.tar.bz2) on your desktop and double click it. It will automatically unpackage it and leave it on your Desktop.

PC: Place the 32bit binary (PyMOL-v1.3r1-Win32.msi) on your desktop unless you are sure you are running the 64bit version of Windows 7 (PyMOL-v1.3r1-Win64.msi). Double click it and it will automatically install in your Programs.

Linux: Place the binary on your desktop (pymol-v1.3r1-Linux-x86-TclTk8.5.tar.bz2). To install it type: tar -zxvf -v1.3r1-Linux-x86-TclTk8.5.tar.bz2
            ./setup.sh

Regardless of the version you are using, PyMOL functions the best with a 3-button (2-button, scroll wheel) mouse.

Windows of PyMOL

Upon starting PyMOL you will be faced with the following windows:
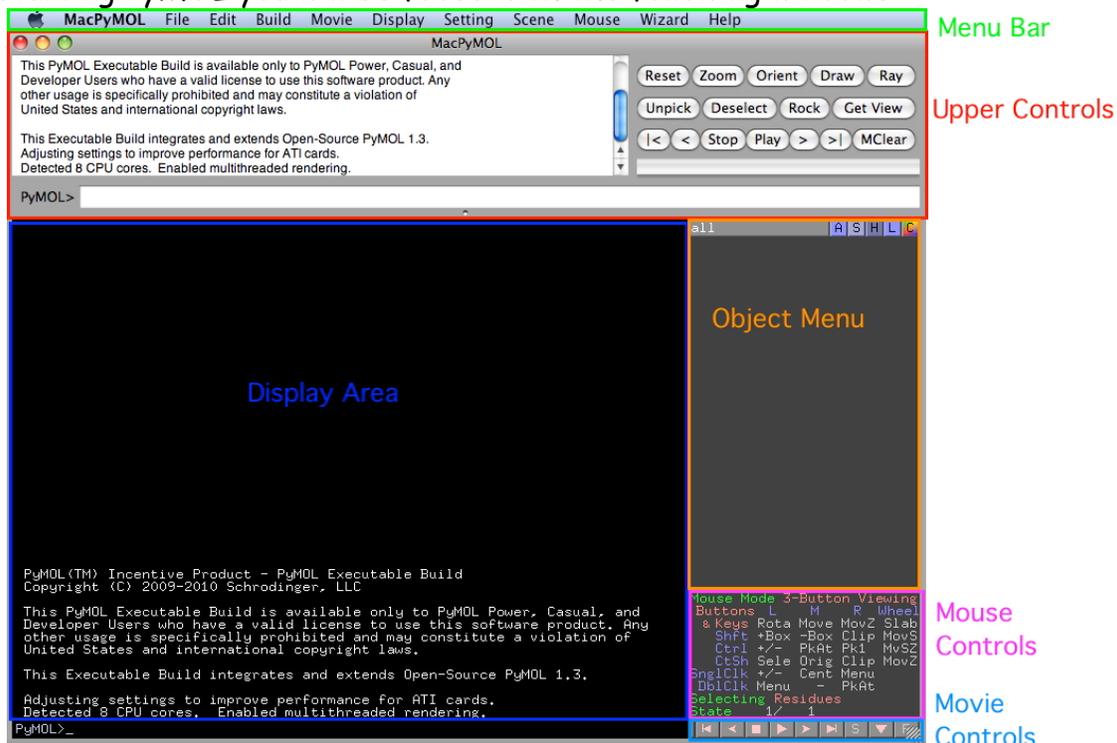
<u>Menu Bar</u>: Just like a menu bar in any other program, this one will allow you to do many things that I will show you can be done other ways.

<u>Upper Controls</u>: Basically the left-hand side of this window shows you exactly what PyMOL is doing and any errors if they appear. Very handy for when things aren't working. On the right-hand side of the window are handy quick action buttons. The lower part of the window represents a command line where you can directly interact with PyMOL.

<u>Display Area</u>: Where your molecules will appear. As we learn about objects and selections they will also appear here.

<u>Object Menu</u>: Allows you to control individual objects or selections. This will be discussed further on the next page.

<u>Mouse Controls</u>: PyMOL has multiple mouse modes (set from Mouse on the menu bar). This area defines what the various button/key combinations do.

<u>Movie Controls</u>: These controls allow you to set through a movie.

Loading a structure

Basically PyMOL has two ways of loading a structure. The first is to use **File** → Open which will read in a PDB file that you have locally saved on your machine. The second method is to **fetch** a molecule. To use this feature you must know the PDB ID (1A8E, 1SDD, etc) for the structure you what to visualize. To fetch a structure, use the following command:
          fetch your favorite PDB ID
in the command line area of the Upper Control window.

<u>Exercise A</u>
          Go to PDB and find a molecule that you would like to examine more closely. Download its coordinates to your Desktop. To download the coordinates, click on Download Files. It will reveal a window allowing you

Where to download PDB files at: http://www.rcsb.orgPDB Downloads.

several options for saving the file. Please click on PDB File (Text) and it will save the file to your machine (either the Desktop of Download folder depending on how you have configured the browser).

Download options at PDB.

Now search for a second structure you would be interested in viewing—record its PDB ID here _____.
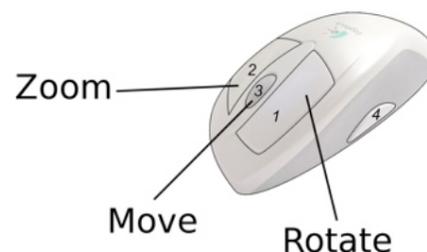
Now open your first file in PyMOL.
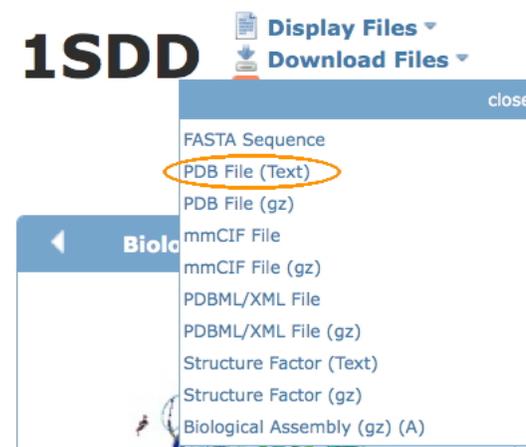
Orienting a structure

PyMOL works with a trackpad, though I find it extremely cumbersome. Therefore I recommend you use a 3-button mouse. When the mouse is set for 3-button viewing mode the mouse behaves as shown in the figure. If you roll the scroll wheel towards you it will "slab" the molecule.

Basic mouse functions in PyMOL.

If you every get lost (zoomed to far or can't find your molecule) just hit Reset in Upper Controls window and it will re-center your view to the middle of your structure(s).

Exercise B

Spend a few minutes moving the molecule around. Zoom up close—what happens when you click on an atom? Can you identify it? The answer is yes, look up at the left side of the Upper Controls window. You should see something like this:

Selector: selection "sele" defined with 10 atoms.
You clicked /1sdd//A/SER`92/O
Which defines: /PDB ID//Chain ID/Amino Acid Number/Atom
Please identify everything in your structure that is NOT an amino acid (non green backbone)

You will notice that all your clicking around has caused a lot of things to have ugly pink squares around them. If you click on Deselect button in the Upper Control Panel these will all be removed.

Before we begin the next section I encourage you to view the built in PyMOL demos (***Wizard*** → Demo). Click on each of them (the menu appears beneath the Object Menu Panel) to see what kind of images you could be making!

Object Menu Panel

This panel allows you complete control over the objects you have loaded (the structure in your case). Each of the letters following the object generate large lists of options that are very handy.

Example Object Menu Panel. All controls everything below it. 1cll and 1ggz are objects. (sele) is a disabled selection. –kinases is a group of 5 proteins (kinases1-5), though kinase2 has been disabled. We will discuss creating objects, selections and groups later.
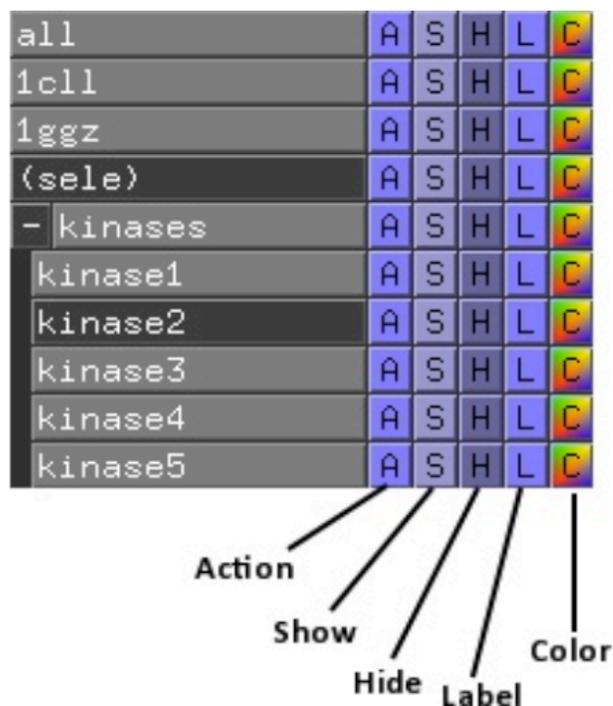
A (Action): Allows you to **orient** your object, **align** it to something, use a **preset** display mode, **generate** symmetry molecules to examine packing, **find** hydrogen bonds, **generate** protein contacts, or compute **hydrogen** positions (if not an NMR structure).

S (Show): Allows you to format the display of your object. Your choices include: **lines**, **sticks**, **ribbon**, **cartoon**, **spheres**, **surface**.

H (Hide): Allows you to hide the formatting of any object that you have previously shown.

L (Label): Allows you to label different parts of your objects, including: **residues**, **chains**, **elements**, **b-factors**, and **occupancies**. Generally this menu is more useful when you have created objects which don't encompass an entire molecule.

C (Color): Probably the handiest of all the Object Menu tools. This allows you to color **by element**, **by chain**, and **by ss** (secondary structure). In addition it shows you the entire color pallet available to you.

Color chains, delete selections, find potential hydrogen bonds. Hide that structure (click on its object name) and fetch your other structure in (fetch pdb_ID_code), center on it. Change its colors, change its view- what is the difference between ribbon and cartoon?

Menu Buttons

As with any program, the Menu buttons provide many essential tools. Today I will just share a few of them with you but as we continue to explore PyMOL I will introduce more to you.

File

Save Session

> PyMOL has the ability to "save state"—in other words it can return to exactly to the orientations, colors, displays, etc. that you had when you saved the session.

Reinitialize

> When you need to delete everything and return it to the baseline state.

Display

Background

> Allows you to change the background color from black to white or grey.

Exercise D:

Lets reinitialize PyMOL and fetch your other structure.

Explore the structure for a few minutes to get familiar with it. Identify the number of chains, anything that is not an amino acid, etc.

Display you molecule in a cartoon (if multiple chains make each chain a different color). Now put an electrostatic surface on it.

Now lets change the transparency of the surface (**Settings** → Transparency → Surface → 60%) to allow what is beneath to be seen. Ray trace it and see how it looks (click on the Ray button in the Upper Control menu). You should change the background color to make the image more striking (**Display** → Background).

Save your session so we can continue on Wednesday.