

Bioc 565--Deep View (Swiss-PDB Viewer) molecular graphics program tutorial tips
Aug 27, 2008

- For understanding and analyzing protein structures, it is critical that you become familiar with **molecular graphics** programs. There are many freeware programs that are available on the web. In this class we will learn just one, called **Deep View**, which is also sometimes called **Swiss-PDB Viewer**.
- To learn how to use the program we are using **Gale Rhodes' online tutorial** at <http://www.usm.maine.edu/~rhodes/SPVTut/index.html>. You should note that this is **not the same** as the Swiss-PdbViewer tutorial available on the Swiss-PdbViewer website at <http://ca.expasy.org/spdbv/text/tutorial.htm>. These are two **different** tutorials. The Rhodes tutorial is accessible via a link from this site, however.
- We would like you to do **Sections 1-8** of the Rhodes tutorial on your own by next Wednesday, Sep 3.
- I personally find it easier to work from a hard copy of the tutorial, since you can then save the screen space for running the program itself as you follow the tutorial from the hard copy. 5 hard copies will be found in the BSW 243 Computer Lab in maroon binders on the shelf by the door. (don't remove these from the room).
- We encourage you to use the Computer Lab for the DeepView tutorial and associated problem sets. It will be open anytime the building is open, although certain classes have times during the day reserved. However, if you wish, you can download your own copy of DeepView for free (available for many platforms at <http://ca.expasy.org/spdbv/>) onto your own computer. The caveat is that if you are using your own computer and something doesn't work, we may not be able/willing to help you.
- To work the tutorial you will need the PDB file named **1HEW**. Download the PDB file from the PDB home page (<http://www.rcsb.org/pdb>) by typing the PDB identifier (e.g. 1HEW) in the site search window at the top of the home page, then clicking on the arrow next to Download Files in the left column, then clicking on "PDB text". It should then download automatically to your computer, or ask you if you want to save it to disk (you want to save it in your folder under the U drive). After downloading, open up DeepView and open the PDB file from within the application using **File:Open PDB File** in the program menus. I think this will be easier and better than following the download instructions listed in the tutorial.
- On the next page are a few specific tips that will make the tutorial work better on Windows on the computers in BSW 243.

Bioc 565: Specific tips on getting the Deep View tutorial to go smoothly:

1. Preferences: Loading Protein

To work well, the tutorial as written depends on what is done with the protein after loading it (i.e. what atoms/residues does it load and display). This may vary depending on how the last user had the preferences set. So, before you load 1HEW into Deep View, go under Preferences: Loading Protein and make sure the following things are set correctly:

Options to apply: Detect secondary structures should be checked. Nothing else should be.

Default appearance: Backbone and side chains. Check show hydrogens (if any) and uncheck show solvent (if loaded).

Default color: CPK

Apply default settings to: check.

Ignore solvent: check.

Note that the 1HEW file actually does contain solvent molecules (waters), but I don't believe the tutorial ever uses/shows them, so it's best to ignore (not load) them here. However, if you want to see them, you can reload the protein later with the "ignore solvent" box unchecked.

2. Centering and sizing the model:

The tutorial repeatedly has you center and size the model around the displayed residues. The button on the left-hand side of the toolbar works to do this on all platforms. The "help" key obviously doesn't exist on the keyboard for the PC, and the = key on the number pad doesn't work for Windows either. Interestingly, neither does right clicking, which is what the tutorial says you should use for Windows! What DOES work on Windows is the "insert" key on the number pad!

3. Left, right and both mouse buttons:

On the machines in 243, moving the mouse in the display window while holding down the LEFT MOUSE BUTTON ROTATES the model. Doing the same while holding down the RIGHT MOUSE BUTTON TRANSLATES the model. Doing the same while holding down BOTH MOUSE BUTTONS ZOOMS IN/OUT. This is an additional way of toggling between these three functions (though I usually use the TAB key as mentioned in the tutorial).

4. "Return" in the tutorial obviously equals "enter" on the nonnumeric portion of your keyboard.

