PyMol Assignment PharmSci 275

In this assignment, you will make a PyMol movie of your choice and connect it to a topic from the literature and/or your research. This builds on the PyMol tutorial provided earlier in the class.

Background

This assignment assumes you have already installed PyMol and worked through the movie tutorial posted on the course website. If you have not done so you should do so now. Note that the posted PyMol notes/tutorial have links to PyMol, background information, and others, and take you through a variety of other background information.

Don't hesitate to ask with questions, but if you ask something which is already addressed in my PyMol notes, don't be surprised to be pointed back there.

Your assignment

Pick a topic involving functional biomolecules and structural data, from your research, or from your reading of the literature. Make a PyMol movie about the topic, possibly also illustrated with stills and illustrations, and turn it in along with a brief report (0.5-2 page) explaining what I should see, and what I can learn from it. Your report should effectively *narrate* the movie and teach me something scientifically. For example, you might choose to make a movie about HIV protease inhibitors and how they occupy the substrate binding site, identifying key interactions they make with the protease and other important structural features, both with a movie and a set of still images. Again, your report would effectively narrate the movie/stills. (Don't use the HIV protease example since I highlighted it here). Last year, a fair number of people lost points on this assignment because their writeup described the system generally but had no connection to the movie, and/or their movie didn't highlight anything specific about the system. The point of this assignment is *NOT* just to make a nice movie, but to make a nice movie that illustrates something -- for example, **a movie you might use in a talk about your research or someone else's research**.

Your movie should involve, at minimum:

- A morph between at least two views of the molecule (such as a rotation or zoom)
- At least one change of representation

You may also want to use other elements, such as changes in transparency, changes in color, or even changes in what is visible (for example, you could reveal a ligand in a binding site, having it initially invisible). You may also want to highlight hydrogen bonds (PyMol allows this) or measure certain distances to highlight key interactions. Ideally, your movie should focus around some points you want to make based on what you know about the science for the system.

To make your movie, make a script as illustrated in the supplied tutorial, using the Octa-Acid example as a starting point. The final product is up to you -- the point is to understand a scientific point you want to make, and illustrate it using molecular visualization focused on the points you want to make.

You will need to save the movie file. In the Mac version of PyMol, this is as simple as File-> Save Movie As (and you may want to turn on raytracing of frames first) and should be similarly easy in Windows or Linux depending on your installation; if not, see me.

The final grade will be based on whether your movie effectively shows what is going on in the system and on its connection with your written explanation. For full credit, your movie should include the elements noted above, and make several scientific points which you explain clearly in your narrative. You will lose credit if your narrative and movie are disconnected (i.e. if the narrative doesn't explain what I should learn from the movie).

To help with this, you should find a tutorial posted on the course website, as well as some examples and slides.

You can submit your writeup and movie by e-mail if the movie size is small. However, these are often large, and it may be easier to submit your writeup by e-mail and share the movie via Google Drive, Dropbox, Box, or similar. (Note that all UCI Google accounts come with 10 TB of Google Drive storage for free, so you should easily be able to store the file there and share a link with me.)