Workshop on
Bioinformatics Approach in Enzymology: Molecular Structure and Data Analysis
Dokuz Eylül Üniversitesi, 2 to 6 June 2014

Student assignment

(This may be your mini-project, or you may do something more ellaborate if you want.)

We will first agree with each student what protein he/she will be working with, based on your personal interest or on random assignment.

Tasks to perform:

1. Load from PDB the structure of the chosen or assigned enzyme-ligand complex into Jmol.

2. Save a copy of that file to your local disk, using the PDB ID code in its name.

3. Render the protein as a cartoon, colored by order of residue in the sequence (N-terminal blue to C-terminal red). The ligand of interest should be in ball and stick with CPK color. Other ligand should be rendered as sticks only with white color. Water should be hidden.
Save a PNGJ file ("file number 3") of that state of the model.

4. Now render the protein as a thin smooth line (trace), colored by secondary structure (magenta for alpha helix, yellow-orange for beta sheet, white for random coil, blue for turns). Render the ligand of interest as ball and stick, with CPK color. Hide the other ligands but display the water as 20% Van der Waals spheres. Set the orientation and zoom of the model so that it displays a close view of the ligand (even if not all the protein is seen).
Save a PNGJ file ("file number 4") of that state of the model.

5. Distances:
Start with file number 4. Then render as sticks the whole residues that have some atoms within 3.5 Å of the ligand of interest. Those neighbourings atoms should also be rendered as small spheres (e.g. 23% VdW). Make a close view of the ligand site.
Save a PNGJ file ("file number 5") of that state of the model.

6. Surfaces:
Make a molecular surface of the whole protein, colored opaque. Render the ligand of interest as full spacefill while the other ligands as sticks only. Color each ligand in a different color.
Save a PNGJ file ("file number 6") of that state of the model.

7. Surfaces (advanced):
Render the protein as cartoon only, colored by sequence (blue to red rainbow). Make a surface for the pockets in the protein and color it in some light shade of blue, translucent. Render all ligands as ball and stick. Add a translucent surface just for the ligand of interest (in a different color).
Save a PNGJ file ("file number 7") of that state of the model.

8. Contacts (advanced):.
From the protein, show only the full residues that are closer than 4 Å from the ligand of interest, as sticks. Among the ligands, show only the ligand of interest, as ball and stick. Among the water molecules, show only those that are within 4 Å from the ligand of interest, as balls. Use the "contact" command to display circular patches for the VdW contacts (red hot-spots) between ligand and protein and also for the hydrogen bond contacts.
Save a PNGJ file ("file number 8") of that state of the model.

On Friday, you will make your presentation by sequentially loading each of those files into Jmol and briefly explaining what each one allows to observe regarding the interaction between the enzyme and the ligand. You can prepare some written notes for talking about each "moleular scene".
Additionally, you should briefly explain what is the biological function of that enzyme.