Section for Week 2

PyMol Basics

Visit http://delsci.com/rel/099/ and show the students the download links. Remind students to read the PyMol Tutorial File. You can quickly skim through the tutorial to give the students a sense of its content, i.e. installation instructions, introduction to basic functionality, etc.

GFP Exercise

1. Open GFP pdb file (1EMA.pdb).
2. Show students how to rotate, zoom and translate the molecule.
3. Show GFP as a cartoon diagram.
   1EMA → S → cartoon
4. Highlight the main structural features of the molecule: Beta strands and Barrel Structure.
5. Show side chains on the cartoon.
   1EMA → S → side chain → lines
6. Measure the distance between two atoms.
   Wizard → Measurement
   (select any two atoms to get the distance in angstroms)
7. Show hydrogen bonds.
   1EMA → A → find → Polar Contacts → to any atoms (or any of the options thereof)
8. Chromophore residues are missing in the cartoon diagram. Change the GFP structure to a line diagram.
   1EMA → S → lines
9. Tell students that sidechains inside the barrel react with each other to form the chromophore. Present them with a reaction diagram for GFP chromophore.

Zif268 Exercise

There are lots of protein structure motifs. One of the most famous ones is the "zinc finger" motif, which consists of two antiparallel beta strands and an alpha helix coordinated by a zinc atom. The zinc atom holds these three elements together because they do not have enough inherent hydrophobicity to stay together on their own. The zinc finger motifs are most commonly found on DNA-binding proteins. In this exercise, you will look at the transcription factor Zif268, which contains 3 zinc finger motifs bound to a target DNA sequence.

1. Load Zif268 pdb file (1AAY.pdb)
2. Is the zinc finger motif an example of primary, secondary, tertiary or quaternary structure?
   Answer: Tertiary, since it stipulates an arrangement of strands and helices, which are forms of secondary structure.
3. Modify the field of view.

   In the command prompt, type: "select resi 133-160"
   (selected) → A → rename → "ZincFinger"
   In the command prompt, type: "select chain B"
   (selected) → A → rename → "DNAstrand1"

In the command prompt, type: "select chain C"
(selected) → A → rename → "DNAstrand2"

This creates three objects and renames them.

1AAY → H → everything
ZincFinger → S → cartoon
DNAstrand1 → S → lines
DNAstrand2 → S → lines

Ask students to identify the beta sheet(s) and the alpha helix.

4. Highlight the zinc atom.

   Display → Sequence
   Scroll right on sequence panel and select the middle of three Zinc atoms
   (selected) → A → rename → Zinc
   Zinc → S → As → sphere

5. Highlight Zinc Finger side chains.

   ZincFinger → S → side chains → lines

   Are the main chain atoms or are the side chain atoms responsible for coordination of the zinc atom?

6. Hide the ZincFinger.

   ZincFinger → H → everything

   Does the DNA structure look like a double helix?

7. Can you identify any of the nucleotide pairs?
8. Show the ZincFinger and highlight side chains.

   ZincFinger → S → cartoon
   ZincFinger → S → side chains → lines

9. Identify hydrogen bonds and non-bonded water molecules.

   ZincFinger → A → find → PolarContacts → to any atom
   1AAY → S → non bonded

   How many sequence specific contacts are made by this zinc finger? How many contacts are made to the DNA backbone?

Electronic Figure Submission

This year, the students will have the option of creating and submitting their figures electronically. You should quickly show the students how to download and use Adobe Acrobat, how to label their figures, and how to compress and submit their files. Because of the potential logistical nightmares, please

emphasize how important it will be for the students to name their files correctly and show them the e-mail address to which their files must be submitted.

1. Show the students how to obtain the full version of Adobe Acrobat from http://software.caltech.edu

2. Show the students how to use the comment and markup tools, e.g. the text box tool, to annotate the figures that they create in PyMol. **Stress to the students that EACH FIGURE MUST BE LABELED WITH THE PROBLEM NUMBER, E.G. #3.B. No credit will be given for unlabeled figures!**

3. Show the students how to compress their files into .zip archives.

4. Please also stress to the students the importance of naming their files properly (Format: [SectionNumber]_[LastName].zip) **Misnamed files could cause significant difficulties in the grading process. Therefore, anyone who fails to properly name their file will receive no credit for this portion of the set!**

5. Zip files should be e-mailed to bi1problemset2@gmail.com