Task #2

Designing a 3D Protein with Jmol!

Due: Friday, September 22nd

Before attempting to design a protein in Jmol, take a few minutes to explore the
Protein Data Bank website http://www.rcsb.org/pdb/home/home.do

- Once you are on the website, type in the search bar: Zinc Finger (or try any other well-known protein, like hemoglobin or insulin). Notice how many hits you get! … A lot! Let's narrow the search…
- Click on the black "PDB 101" tab near the upper left. Once there, type in Zinc Finger again. Read article within the first link that comes up (Feel free to explore more on this site, like the "Molecule of the Month" and various activities under the "Learn" tab).
- Throughout the article, various PDB files are referenced in blue. Find the very last one (1zaa). You can either click on that link, or go back to the main PDB page and search for 1zaa.
- Under the Structure Summary, and Literature, you'll find the title and abstract of an article. This article is known as the "Primary Citation"… or the main paper that describes that structure. If you were going to model this protein, you'd need to read that article.
- More information about the Protein Data Bank and how to use it to download and model proteins can be found in our Jmol Training Guide at:
  http://cbm.msoe.edu/smartTeams/smartTeamsLocal.php
- Click on the Sequence tab. Scroll down and look at the sequence information. You should be able to find a diagram that shows the key features of the protein, like the alpha helices, beta sheets, and binding sites for any attached ligands (in this case, Zinc, or ZN).

Answer this question:

1) According to the sequence diagram for 1zaa, what are the 4 binding sites (amino acid name and number) for ZN C 201?

- How do Scientists determine these structures? Go to this website and check out the "Intro to X-ray Crystallography" video: http://pdb101.rcsb.org/teach/biomolecular-structures-and-models/learning-materials

Answer these questions:

2) In 5 sentences or less, summarize how scientists purify proteins.
3) In 5 sentences or less, summarize how scientists crystallize proteins.

Next, let's explore the **Jmol Training Guide** at http://cbm.msoe.edu/smartTeams/smartTeamsLocal.php

Jmol Training Guide Questions

- Create a folder on your desktop and download a copy of **Jmol version <mark>14.15.3</mark>** into that folder.

- Read sections 3-7 in the training guide, and answer the following:

    4) What commands would you use to remove the cartoon backbone and display an alpha carbon backbone?
    5) What color is carbon, hydrogen, oxygen and nitrogen in CPK coloring?
    6) How do you save the model you are working on for later editing?
    7) What command is used to get rid of water molecules displayed in the file?
    8) Identify the commands used to highlight beta sheets and color them purple.
    9) What set of commands is used to add hydrogen bonds to the beta sheets only?
    10) What commands are used to add the residue glutamic acid 10 with a "clean backbone" and colored in red?
    11) List the commands to correctly calculate and add struts to a model design.

- Now, practice designing a Zinc Finger (1zaa): In the Protein Data Bank site, bring up the pdb file **1zaa**. Click on the drop down tab of **"Download Files"** (located on the right) and choose **"PDB Format"**. Place the pdb file into the desktop folder you created for your model designs; the same folder where you downloaded Jmol.
- Go to this website: http://cbm.msoe.edu/teachingResources/images/jmolTraining/zincFingerCommands.pdf , and follow the commands (enter in Jmol) to practice designing a zinc finger.
    12) Save your model as a jpg and include it with the answers to your questions above.

This task will be marked as complete on the progress bar when your team emails the correct answers (#1-12) to Judy (birschbach@msoe.edu) no later than

Friday, September 22nd

First, second and third place WILL be awarded for Task #2!