

## Week 8: Introduction to Proteopedia.

**Experiment Summary:** To learn the basic structure of Proteopedia and begin to construct a Proteopedia page.

### **Introduction:**

For the second half of the semester, we will spend the majority of the laboratory time working on constructing and presenting Proteopedia pages about your G-protein coupled receptors (G-PCRs). Proteopedia is the Wikipedia for proteins that connects the protein data bank (PDB) entry for a protein with short descriptions and tutorials about that protein (1,2). The big benefit to Proteopedia is that while reading about a protein, you can also view the discussed portions of the protein structure in three-dimensional format using Jmol. So in addition to a written discussion of your structure and topic, you will also need to design protein structure visualization exercises in Jmol to accompany your summary. These structural visualizations will need to directly connect to the material listed in your summary and clearly depict the important structural information.

### **Introduction: Reading Assignment:**

1. E. Hodis, J. Prilusky, J. L. Sussman (2010) Proteopedia: A collaborative, virtual 3D web-resource for protein and biomolecule structure and function, *Biochem. Mol. Biol. Educ.* **38**, 341-342.
2. J. Prilusky, et al. (2011) Proteopedia: a status report on the collaborative, 3D web-encyclopedia of proteins and other biomolecules, *J. Struct. Biol.* **175**, 244-252.

### **Experimental Procedure:**

**Locate the Proteopedia Video Guide:** at the Proteopedia Main Page ([www.proteopedia.org](http://www.proteopedia.org)), find the link near the top left of the page entitled "Video Guide" (watch the Proteopedia VideoGuide modules 1-2)

### **Examine some Example Proteopedia Pages**

- 1) Look at the following three Proteopedia pages, all of which were constructed by Butler University undergraduate students in previous CH462 classes, then answer **Q1**:  
[http://www.proteopedia.org/wiki/index.php/Dipeptidyl\\_peptidase\\_IV](http://www.proteopedia.org/wiki/index.php/Dipeptidyl_peptidase_IV)  
[http://proteopedia.org/wiki/index.php/Fatty\\_acid\\_amide\\_hydrolase](http://proteopedia.org/wiki/index.php/Fatty_acid_amide_hydrolase)  
[http://www.proteopedia.org/wiki/index.php/Palmitoyl\\_protein\\_thioesterase](http://www.proteopedia.org/wiki/index.php/Palmitoyl_protein_thioesterase)

**Q1**

**Locate an automatically seeded page that corresponds to the PDB code for your protein** (watch the Proteopedia VideoGuide module 3, then complete the following tasks and answer **Q2**)

- 2) Use the search box at Proteopedia's main Page to locate an automatically seeded Proteopedia page for your protein by entering a 4-character PDB ID code for your protein. Examine the page. **Q2**

### Constructing your own personal Sandbox:

- 3) Login to Proteopedia using the login that was provided to you. Click on your name at the top of the page.
- 4) Click on the tab “edit this page” at the top.
- 5) Suppose that your name (and your account login name) is *Your Name*. In the wikitext box, add the following: **\*[[User:Your Name/Sandbox 1]]** (Don't type "Your Name"! Type your own real login name! Make sure there are no spaces before the above line. It should begin at the left edge of the wikitext box.)
- 6) Click the *Save Page* button near the bottom of the page.
- 7) Now you should see this in your page: [User:Your Name/Sandbox 1](#) (The underline will not appear until you touch the **red** link with your mouse.) The link is **red** because your *Sandbox 1* page does not yet exist.
- 8) Click the **red** link.
- 9) You should now be at a page titled *Editing User:Your Name/Sandbox 1*.
- 10) You now have a protected Sandbox, and you are ready to type content into it, and use the Scene Authoring Tools. After you have saved your new Sandbox 1 page, if you go to your personal User page, and click your browser's Reload/Refresh button (or click it on the View menu), the link to your new page should turn **blue**: [User:Your Name/Sandbox 1](#) The change in color of the link from **red** to **blue** is a convention in wikis that means the page now exists (has been saved).

### Adding Text to Your Sandbox:

(watch Proteopedia's VideoGuide 4, then perform the following tasks and answer **Q3**)

- 11) Create a descriptive heading: such as the name of your protein and the name of the organism it is found in. Change the 1<sup>st</sup> Heading in the sandbox page by typing your desired text to replace “Your Heading Here (maybe something like 'Structure')” inside the == == wikitext markup characters. You can view the text and the resulting Proteopedia page by hitting the *Show preview* button in the middle of the page.
- 12) You can edit the properties of the text like italics or bold by using the click boxes above the textbox. Change the text naming your organism to italics. Preview the changes.
- 13) Another key feature of your text will be the insertion of additional headers to your document. Insert headers by putting your text between “== text ==”. You can also make subheadings under these by putting in “=== text ===”.
- 14) Try inserting multiple headers/subheaders into the document and preview your results. **Q3**

### Adding an Image to Your Sandbox:

(watch Proteopedia's VideoGuide 5, then perform the following tasks and answer **Q4**)

- 15) Find an image of your protein, either...
  - ...use one of your own custom designed pictures of your protein that you previously made in PyMol
  - or
  - ...get a premade picture from the PDB: the default rainbow-colored cartoon picture that is displayed in the upper right portion of the PDB front page for your protein should allow you to download a picture by clicking on the “more images” link and

then right clicking on an image on the resulting page. Save the image to your H drive. (For your actual Proteopedia page when we publish them onto the web, you will need to be careful with the permissions on your images and insure that you have the rights to publish them. We can discuss this more as you work on your pages. For now since these pages are private to your account, this will not matter so choose any image.)

- 16) Go to the left side of the Proteopedia page under “toolbox” and select “Upload File”. (You will see a similar warning to the one above). Upload the image that you downloaded and copy the file name for the image.
  - 17) Go back to your Sandbox page and click insert image from the top. Delete the “example.jpg” portion of the text that was inserted and replace it with the name of your uploaded file that you just copied. Click on the *Show Preview* button.
  - 18) Now go back to your text box and we are going to change some features about the file.
  - 19) After the name of your file, but still within the double brackets, enter the following terms with each separated by a pipe character (|): |100 px|left|thumb|Figure Legend
- #### Q4

### Adding a 3D Structure to Your Sandbox

(watch Proteopedia’s VideoGuide 6, then perform the following tasks)

- 20) Get your cursor to the left edge of a blank line in the Sandbox editing window.
- 21) Hit the 3D icon at the top of the page to add in an applet, which results in the appearance of the following text:

```
<Structure load='Insert PDB code or filename here' size='350'  
frame='true' align='right' caption='Insert caption here'  
scene='Insert optional scene name here' />
```
- 22) Replace the blue highlighted text, **Insert PDB code or filename here**, with the 4-character PDB ID code for your protein. Preview the results (*Show preview* button).
- 23) Change the figure caption to the name of our protein by replacing the **Insert caption here** text. Preview the results (*Show preview* button).
- 24) You should have now had an interactive applet appear on your page. Convince yourself that you can move, rotate, and zoom the protein structure shown in this applet. If you right click on the applet, you will also get a menu with different choices of variables to change about the display of the protein.

### Adding Scenes (Green Links) to Your Sandbox

(watch Proteopedia’s VideoGuide 7, then perform the following tasks)

- 25) Instead of using the aforementioned menu within the Java applet, we are going to use the “Scene Authoring Tools” to change the appearance of the starting scene. Click on the blue [\[Show\]](#) link immediately following “Scene Authoring Tools”. Click on the tab titled, “Load Molecule”. Enter your protein’s 4-character PDB ID code into the box for “By PDB Code.” Hit Load. You should see the same picture of your protein show up in the small box to the right.
- 26) Click on the tab titled “selections”. Hit “All protein”. Hit “Replace Selection”.
- 27) Click on the tab titled “representations”. Try out the different type of representations. Hit “Set Representation” between each different type. Choose the representation that you like best for the entire protein.

- 28) Click on the tab titled "colors". In addition to the monotone color choices, you can also color your protein based on different properties of your protein. Try coloring by charge and then by polarity. Set the final coloration as "N->C rainbow (named chain)". Choose a background color other than white.
- 29) Go back to the "selections" tab. Enter a range of residue numbers of your choice (this could be an individual helix in your protein, or a cluster of binding site residues or even simply a random sampling) into "Limit to residue numbers". Hit "Replace selection". Go back to the "representation" tab and choose "spacefill". Go to the color tab and color this section white.
- 30) Zoom in on the selected amino acid(s) and choose a view that best highlights this selection.
- 31) Click on the tab labeled Save scene. Enter a name for your scene. Click the *Save current scene* box. Copy the scene name at the bottom in the wikitext and paste into your text box.
- 32) Copy the name of your scene (the text within the single parentheses) and paste into the "Structure Load" at the very end where it says "scene". Keep the single parentheses. Hit "Show preview". If this works correctly, the initial applet screen should look like the scene that you just created.
- 33) Go back to your scene in the Scene Authoring Tools and reload your scene.
- 34) Reorient the protein (zoom, rotate, move) and then resave the scene. Use the same name and it will give it a new number (2) for the second version of this scene.
- 35) Copy the Wikitext into your editing page. Remove the words "Texttobedisplayed" and replace with a descriptive name for your scene.
- 36) Hit "Show preview". You should now have a green link displayed on your page with the text that you entered into the scene name. Click on this green link. What happens to the scene shown?
- 37) You have completed the basic introduction to Proteopedia. Feel free to keep playing around and learning more functionality. When you are complete, follow the instructions in #37.
- 38)** Once you have completed these steps on your Sandbox, you should then take a screen shot of the completed Sandbox and add this image to your assignment document. **Q5**

Name(s) \_\_\_\_\_

### Assignment: Proteopedia Introduction

- 1) What features did all three of these example Proteopedia pages contain? What features were different among the three pages? Were there any details that stuck out to you about the pages?
  
- 2) Knowing your protein as well as you now do, identify at least one useful feature that is present on the automatically seeded page. Identify at least one potentially useful feature that is missing from the automatically seeded page (*i.e.* something you featured in your oral presentation).
  
- 3) What gets added to the page after you put in multiple header 2 texts?
  
- 4) What did each of these terms do to the image? Why might they each be helpful in designing your Proteopedia page? What would happen if we changed it to 300 px or to right?
  
- 5) Paste the screen shot of your final Proteopedia page from today. It should contain the following in order to get full credit:
  - Heading(s) and sub heading(s) text
  - A 2D image of your protein
  - A 3D applet of your protein
  - At least one Green Link in text that recalls a particular scene in the 3D applet, in which selected individual residues of the protein are displayed differently from the bulk of the protein

- I. Overall Appearance (2 pts)
  - a. Logical and well organized layout
  - b. Visually appealing
  - c. Proper use of color
  - d. Sections of the page well labeled
- II. Story (3 pts)
  - a. Complete at the level of the primary articles featured
  - b. Coherent connection of the key features of the protein between written sections and three-dimensional structure links
  - c. Highlights key biological or chemical features of the protein and connects them to the structure
  - d. Does not solely focus on minor structural details about the protein
- III. Written Text (3 pts)
  - a. Properly formatted
  - b. Properly displays in Proteopedia
  - c. Clear introduction to structure
  - d. Clear explanation of important features in the structure
  - e. Puts the importance of the protein and its biological function in context
  - f. Clarity of writing
  - g. Lack of grammatical errors
- IV. Two Dimensional Picture(s) - at least two (2 pts)
  - a. Quality and formatting
  - b. Visually appealing
  - c. Proper use of color
  - d. Highlights an important part of the story
  - e. Different from 3D figure(s)
- V. Three Dimensional Structure(s) (6 pts)
  - a. Quality and formatting
  - b. Visually appealing
  - c. Proper use of color
  - d. Highlights an important part of structure
  - e. At least six different green links to the structure in the text
  - f. Variety in the representations for the six different structures
  - g. Different from 2D picture(s)
  - h. Informative captions
- VI. References (2 pts)
  - a. Includes at least five pertinent reference citations (high quality primary articles in peer-reviewed journals)
  - b. Consistent and appropriate formatting
- VII. External Resources or Links (2 pts)
  - a. Includes pertinent external/internal links
  - b. Proper formatting

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 Total =

20 points

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|--|----------|
| I. Overall Appearance  | (5 pts)  |
| a. Logical and well organized layout   |          |
| b. Visually appealing  |          |
| c. Proper use of color   |          |
| d. Sections of the page well labeled   |          |
| II. Story  | (10 pts) |
| a. Complete at the level of the primary article featured   |          |
| b. Coherent connection of the key features of the protein between written sections and three-dimensional structure links |          |
| c. Highlights key biological or chemical features of the protein and connects them to the structure                      |          |
| d. Does not solely focus on minor structural details about the protein   |          |
| III. Written Text  | (8 pts)  |
| a. Properly formatted  |          |
| b. Properly displays in Proteopedia  |          |
| c. Clear introduction to structure   |          |
| d. Clear explanation of important features in the structure  |          |
| e. Puts the importance of the protein and its biological function in context   |          |
| f. Clarity of writing  |          |
| g. Lack of grammatical errors  |          |
| IV. Two Dimensional Picture(s) - at least two  | (5 pts)  |
| a. Quality and formatting  |          |
| b. Visually appealing  |          |
| c. Proper use of color   |          |
| d. Highlights an important part of the story   |          |
| e. Different from 3D figure(s)   |          |
| V. Three Dimensional Structure(s)  | (12 pts) |
| a. Quality and formatting  |          |
| b. Visually appealing  |          |
| c. Proper use of color   |          |
| d. Highlights an important part of structure   |          |
| e. At least six different green links to the structure in the text   |          |
| f. Variety in the representations for the six different structures   |          |
| g. Different from 2D picture(s)  |          |
| h. Informative captions  |          |
| VI. References   | (5 pts)  |
| a. Includes at least five pertinent reference citations<br>(high quality primary articles in peer-reviewed journals)     |          |
| b. Consistent and appropriate formatting   |          |
| VII. External Resources or Links   | (5 pts)  |
| a. Includes pertinent external/internal links  |          |
| b. Proper formatting   |          |

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Total =  
(each day late = -2 points)

50 points