Lab 6 and 7: Turning a 2D figure into a 3D scene for a Proteopedia page

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Lab 6: This week, we will do a "dry" experiment, i.e. work at the computer. The beginning question will be "How can we transform a published 2D-picture of a protein into an interactive 3D-object showing the same features?"

The software we will use is called Jmol. It is used on the Proteopedia site to render structures in three dimensions and is used in other web pages as well. We will first learn some basic commands by working through some examples in the manual (page 14-22 in Cohlberg's Jmol manual, http://web.csulb.edu/~cohlberg/Jmolmanual.html), and then move on to our question.

The figures we will try to turn into 3D are from a paper we already discussed in class: "Interconversion of the specificities of human lysosomal by enzymes associated with Fabry and Schindler diseases." by Tomasic IB, Metcalf MC, Guce AI, Clark NE, and Garman SC.

One of the authors, Dr. Scott Garman, is an expert in protein structure and will give us some feedback on our 3D figures before we post them on Proteopedia.

Each group will do a different figure. Choices are:

- Fig 1B: structure of alpha GAL
- Fig 1C: structure of alpha NAGAL
- Fig 2A: structure of alpha GAL-SA bound to GalNAc
- Fig 2B: structure of alpha GAL-SA bound to Gal
- Fig 2C: structure of alpha GAL-SA, "empty" active site
- Fig 2D+E: superposition of structures

After locating the relevant structures in the Protein Data Bank (www.pdb.org), you will recreate your figure in Jmol (https://chemapps.stolaf.edu/jmol/jsmol/simple.htm) and save the script. The goal is to have the same representation, colors and view of the molecule.

Deliverables: Please save the image as a .pngj file (this is a file format that can be loaded into Jmol to recreate the 3D rendering but is also interpreted as image by browsers and applications) and submit it on our learning management system. With your submission, state which features of the published figure you still have to add (labels, surfaces, superpositions, electron density)

Lab 7: For the second portion of this hands-on lesson, we will discuss feedback from Dr. Garman and work together on implementing the missing features. Depending on the figure you are working with, you might have to learn specific commands and techniques to implement surface representations, different kinds of labels, electron density representations, etc.). If you have extra time, you will use it for starting to write the text that introduces your figure, and to write the figure caption.

Deliverables: Jmol script of the figure, and figure caption and introduction to figure.