Lab. Display and analyze protein structures using Swiss PDB Viewer

Objectives:
　　　1) Display 3D structure of a protein, identify secondary structures, individual residues, H-bonds, and ligands.
　　　2) Export images of protein structures.

Exercise 1) It's small but it has everything – 1IGD (1igd)

　　　This peptide is only 61 amino acids in length, but it has an alpha helix and 4 beta strands. The instructor will demonstrate how to display the beta sheet with H-bonds. The students will then try to display the alpha-helix with H-bonds.

1.1) Download the structure file.
　　　Try google "PDBSUM 1igd". This will leads to a entry in PDBsum website (see Fig 1). Click 'PDBe' on the "links" panel. This will leads to the entry of this structure in the EMBL PDBe server. Click the "Download PDB File", and this will download the file "1IGD.ent" to your computer. You can move the file to the desktop for convenience.
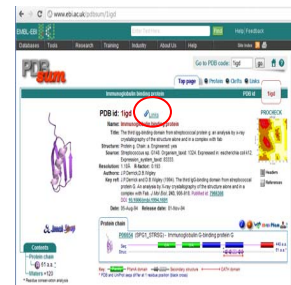
Fig 1. Red circle is "links"

1.2) Open file in SPDBV.
　　　Start SPDV first. Then, choose "File" → "Open PDB file".
　　　Choose "Color"→"by secondary structure". Now, we can see alpha-helix in red, and beta-sheet in yellow.

1.3) Use the control-panel
　　　Click "Wind" → "Control Panel" (see Fig 2). You should be able to see the protein sequence in the "Control panel". Try to click on some amino acid residues to "label" them. You can also choose "v" to show the volume of them, "col" to color them, "ribn" to show them in ribbon-model.
　　　Now, use "Select" →"by secondary structure" and "show" column in the control panel to display only the beta strands. Remove side chains for clarity. Choose "color" →" by CPK".

1.4) Show H-bond in beta-sheet.
　　　"Tools" →"Compute H-bonds". We can also view distance of H-bonds by "Display" →"Show H-bonds distances".
　　　Try "Preference" →"3D rendering" to adjust the quality of the image.

1.5) Save the image.
　　　You can change the background color by "Preference"-> "Color"-> "Background".
　　　You can change the ribbon color in the control panel by "R"->"ribbon", then click 'ribn col'. An example can be seen in Fig 2.
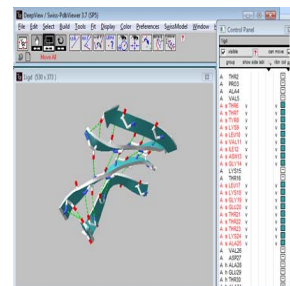　　　To save image, choose 'File'->'Save'->'Image'.

Fig 2. Beta-sheet of 1igd with control panel.

1.6) Show the alpha-helix in ribbon mode with H-bond
　　　Work out this on your own. From the end of the helix, you can see that it looks like a tunnel. Verify that the helix is right-handed.
　　　Save the generated "layer" in a file and save the image in a file. This is part of your lab report.

Exercise 2) The classic – 1MBO (1mbo)

The first protein structure ever solved is myoglobin from sperm whale. It is used in many textbooks. This protein is also once the "molecule of the month" on PDBsum web site. There is a heme ligand in the myoglobin protein. In this exercise, we will learn to use "Layer" and color the ligand and protein differently.

2.1) Download pdb file of 1MBO. (There are multiple source to download the 1MBO pdf files. Try google and your will find alternative sites.)

2.2) Open the PDB file in spdbv. Show only the protein in ribbon mode.

2.3) Use "Layers"

Now, reopen the same file of 1MBO. Click "Window"→"Layers Info". Choose "vis" to see which is the recent layers (see Fig 3). Hide the first layer.

Click the ID on the control panel to jump between layers.

Fig 3. Heme group with 'Layers' and 'Control panel'.

2.4) Show only heme in the second layer (see Fig 3).

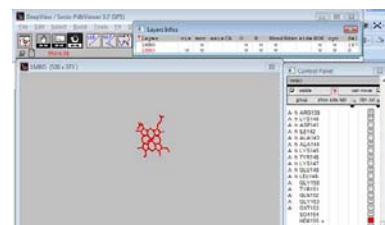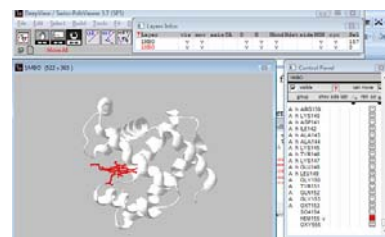2.5) Merge the two images (see Fig 4).

2.6) Save the image.

Lab Report:

Fig 4. Merged layers.

You will be given a protein PDB number. Use SPDBV to generate a picture of this protein in ribbon mode. Color the ligand and protein in different color. Use the picture on the PDBsum website as reference. The closer that your result resembles the picture on the PDBsum website, the better is your score of this assignment.

If you are doing on your own computer, you need to download SPDBV first. The software is available at http://expasy.org/spdbv/ .

Your report must be written in WORD format that contains all of your generated images.

Useful SPDB tips:

Window: It's best to have most of the windows open: **Window/Tool Bar, Control Panel, and Layer Info**.

The atoms in SPDBV are colored as:
C--> gray or white   O --> red   N --> blue S --> yellow
P --> orange H --> cyan   other --> gray.

Assignments

	Name	PDB id
1	Abisola Akinseye	1CHH
2	Ashley M. Hayes	1CHI
3	Ashley M. Lewis	1CHJ
4	Biliesha S. Belvitt	1CIE
5	Blaire C. Spaulding	1CIF
6	Brittainy S. Hoskins	1CIG
7	Camille L. Peeples	1CIH
8	Dominique E. Reeves	1CRG
9	Dorotea J.Hogans-Blaylock	1CRH
10	Ebony M. Mason	1CRI
11	Fabiola S. Breton	1CRJ
12	Isadora M. Porter	1CSU
13	Jada M. Harris	1CSV
14	Kyla L. Greenfield	1CSW
15	Maya G. Welfare	1CSX
16	Melina Y. Zuniga	1CTY
17	Naquasia J. Jones	1CTZ
18	Raynesha L. Grant	1FHB
19	Robin Levy	1IRV
20	Taara A. Avery	1IRW
21	Teneisha R. McDonald	1KYO
22	Tiffany M. Bryan	1LMS
23		1NMI
24		1RAP
25		1RAQ
26		1S6V
27		1U74
28		1YCC
29		1YFC
30		1YIC
31		2B0Z
32		2B10
33		2B11
34		2B12
35		2BCN
36		2GB8
37		2PCC
38		2YCC

Focus: Hydrogen bond in helix, active site, and beta sheet.
Example of helix. Let student work out beta-sheet.

In Willian's textbook, hydrogen bond are mentioned for alpha-helix and beta sheet.
Figure 4-7 for alpha helix and figure 4-9 for beta sheet.

Figure 4-8, 1MBD
Figure 4-10, 3CPA

View the structure of lab 1. Triose and view the broken helices.