Lab sheet#8
Structure visualization using jmol

Objectives:

- Download protein sequence as PDB format.
- To be familiar with structure visualization program (Jmol).
- Display 3D structure of a protein, change its view, color and select motifs by writing commands.

Use Jmol program to perform the following:

Jmol is a free molecular viewer, used to create and view three dimensional structures of proteins.

Exercise .1:

1. Open Protein Data Bank (**PDB**) website, Search for **1B0U** protein; which is the PDB ID of ATP-binding subunit of the histidine permease from salmonella typhimurium.
2. Download the protein sequence as **PDB format**.
3. Open Jmol program and open the protein sequence file. (file➔get PDB).
4. Change Style display from Atom style to **Cartoon** scheme style.
   (Click right ➔style➔scheme➔cartoon).
5. Open the console window, change the **color** of the whole structure to **grey**.
   (Click right ➔ console➔type: select all➔ press enter➔ type: color grey➔ press enter).
6. Open the protein page in protein database (NCBI) to know the different motifs of the protein and their location.
7. Select the **Walker A/P-loop motif** (39-46), and color it by blue.
   (type: select 39-46 ➔press enter➔ type: color blue➔ press enter).
8. Select the **ABC transporter signature motif** 154-163, and color it to green.
   (type: select 154-163 ➔ press enter➔ type: color green ➔ press enter).
9. Select **Walker B motif** 174-179, and color red.
   (type: select 174-179 ➔ press enter➔ type: color red ➔press enter).
10. Show the ATP **ligand** as **Ball and stick** scheme style.
    (type: select ligand ➔ click right ➔style➔scheme➔ ball and stick).
11. Show which one is closest to **Walker A/P-loop motif** and measure the **distance** between them. (toolbar➔ click the ruler icon)
12. Change the measurement unit from **nm to Angstroms**.
    (click right ➔measurements➔distance unites angstroms)
13. Save the protein structure as a picture. (toolbar➔ click the camera icon)

Exercise .2:

1. Open Protein Data Bank (**PDB**) website, Search for **1TRZ** protein; which is the PDB ID of Human Insulin hexamer.
2. Go down to the molecule description to see how many polymers and chains does insulin have.
3. Download the protein sequence as **PDB format**.
4. Open Jmol program and open the protein sequence file.
5. Change Style display from Atom style to **Cartoon** scheme style.
6. Change Style display to **Backbone 1.5** scheme style.

   (Click right ➔console➔type: Backbone 1.5➔press enter).
7. Turn cartoon style off. (type: cartoon off➔press enter)
8. Select sheets and color orange.

   (type: select sheets ➔ press enter➔ type: color orange ➔press enter)
9. Select helix and color yellow.

   (type: select helix ➔ press enter➔ type: color yellow➔press enter)
10. Show cysteins (Sulfur) that forms disulphide bridges "showing how the polypeptides hold together throw S-S bonds". Change to wireframe 1.25 and color them blue.

(type: select sulfur ➔ press enter➔ type: wireframe 1.25➔press enter➔type: color blue).

11. How many disulphide bonds are founds in insulin protein.
12. Show for each disulphide bridge the position of each Cys and the chain involved.
13. Move the structure 0 360 0 0 0 0 0 0 10. (type: move 0 360 0 0 0 0 0 0 10 ➔press enter)
14. Save the protein structure.