

### Computational Bio lab ASSIGNMENT-1 (10 Marks)

Answer the following questions using the PDB IDs assigned to YOU

1. Read the remarks sections of the PDB file and describe your protein in a maximum of 2-3 lines.
2. Is your PDB structure determined by NMR or X-RAY? Which technique can result in resolving hydrogen atoms and provide hydrogen co-ordinates?
3. Represent the protein in Licorice and color the protein according to its elements.
4. Does your protein have crystal waters? If yes, represent using VDW.
5. Change the background color to white, hide the axes and render the image in orthographic mode. (Use **this layout for answering rest of the questions**)
6. Show all hetero atoms (need not include waters) lying within 2.0 Angstrom of your protein in CPK form. List them.
7. Represent in VDW the first atom of your PDB ID using keyword: index and serial. What do you infer from the observation?
8. Represent the first 5 residues in CPK. Find the angle between any three non-consecutive atoms and display the angle value in red and atom labels in blue.
9. Load the same PDB twice and place them next to each other in different color.
10. Display the contact map of protein. What do you interpret from the graph?