Practical 12
11 April 2022
Questions

1. Get the PDB files, 1ALC, 4 LYZ and 1TIM
2. Open the file 1TIM and show in cartoon style (hide line style)
3. Give different colors for different chains. How many chains are there?
4. Remove one chain (right click on the chain and hide)
5. Identify the secondary structures with different colors
6. Zoom and rotate to get complete views
7. Show the sequence
8. Select the residues 21 to 26: LGELIH
9. Hide cartoon diagrams
10. Color the selected residues based on different atoms
11. Identify at least one salt bridge within the protein and list the details of interaction.
12. Identify any hydrophobic interaction / aromatic stacking interaction protein and list the details of interaction.
13. Label the residues using atom name and show their van der Waal radii.
14. Compute the distance between CG and CD2 in Leu24
15. Compute the angle formed by the atoms CD1, CG and CD2 in Leu24.
16. Compute the dihedral angles of Leu24
17. Change background white
18. Make high quality picture (use ray)
19. Show B-factors to see flexible and rigid regions (color by spectrum, b-factor)
20. Compute the electrostatic potential (A -> generate -> vacuum statistics -> protein contact potential)
21. Save the image in PNG format
22. Open the files 1ALC and 4LYZ
23. Align the structures
24. Compute rmsd
25. Save the aligned protein structures
26. Download a protein structure with ligand(s). Identify the ligand and select residues within 3.5Å. Show any one type of interaction between them.
27. Mutate any one of the active site residue and describe the change in the interaction with the ligand before and after mutation.

Deadline: 17th April 2022