Pymol Practical Demo

1. **Get the PDB files: 1ALC, 4LYZ and 1TIM**
   i. Go to the Protein Data Bank (PDB) home page (https://www.rcsb.org/).
   ii. Enter the first PDB-ID "1ALC" in search box and click Go
   iii. In the result page, chose the link "Download files" and choose "PDB file (Text)" option to download the file
   iv. Repeat the steps (ii) and (iii) to download the remaining two PDB structures.
2. **Open the file 1TIM and show in cartoon style (hide line style)**
   i. Open the installed Pymol tool. In the file menu, choose the "open" option to load 1TIM pdb file.
   ii. After that, in the Pymol viewer panel, choose the Show option and select the "cartoon" style.
   iii. Choose the Hide option and select the "line" style.
3. **Give different colors for different chains. How many chains are there?**
   Click the color option and choose the " by chain" style.
4. **Remove one chain**
   Right click on the chain and choose Chain->Hide->everything option
5. **Identify the secondary structures with different colors**
   Select the color option and choose "by ss"
6. **Zoom and Rotate to get complete views**
   i. Click and hold the right mouse button and drag the mouse to and fro to zoom in and out.
   ii. Click and hold the left mouse button and drag the mouse to and fro to zoom in and out.
7. **Show the sequence**
   Click the "S" button in the right-side corner (below)
8. **Select the residues 21 to 26: LGELIH**
   Select the given segment in the sequence displayed in the top of the viewer based on the residue numbers
9. **Hide cartoon diagrams**
   i. Choose the hide option and select "cartoon".
   ii. Choose the Show option and select "lines"
10. **Color the selected residues based on different atoms**
    Choose the color option and select "by element"
11. **Identify at least one salt bridge within the protein and list the details of interactions**
    i. Select both the positive and negative charged residues using the command given: "select 1tim///GLU+ARG/"
    ii. Change the appearance to sticks and hide cartoon in the main structure. Now only the selected residues will display
    iii. Select Action->find->polar contacts->Involving side chains
12. **Identify any aromatic stacking interaction and list the details of the interaction**
    i. Select the aromatic residues using the command given below: "select 1tim///PHE+TYR+TRP/"
    ii. Change the appearance to sticks and hide cartoon in the main structure. Now only the selected residues will display
    iii. Double right click on any two residue and enter the "dist" command
13. **Label the residues using atom name and show their van der Waal radii.**
    i. Select the Label option and choose "atom name"
    ii. Select the Label option and choose"vdw radius"

14. **Compute the distance between CG and CD2 in LEU24**
    i. Select the residue LEU 24 and show in sticks format.
    ii. Label based on the atom name
    iii. Select the "measurements" option under the wizard menu
    iv. Select the Distances option in the newly appeared Measurement option
    v. Left mouse click on the mentioned atoms to show the distance
15. **Compute the angle formed by the atoms CD1, CG and CD in LEU24**
    i. Select the option "Angles" in the Measurement option.
    ii. Left mouse click the mentioned atoms to show angle
16. **Compute the dihedral angles of Leu24**
    Phi: C (from GLU 23) – N – CA – C; Psi: N – CA – C – N (from ILE25)
    i. Select the "Dihedrals" in the Measurement option
    ii. Left click the mentioned atoms to show phi angle. Repeat this for Psi angle
17. **Change background white**
    Enter the command "bg_color white"
18. **Make high quality picture (use ray)**
    Click the "ray button" and save in PNG format
19. **Show B-factors to see flexible and rigid regions**
    Select "color->spectrum->b-factor"
20. **Compute the electrostatic potential**
    Select "Action->Generate->Vacuum statistics->protein contact potential"
21. **Save the images in PNG format**
    Choose "File-> save image as ->PNG"
22. **Open the files 1ALC and 4LYZ**
    Open the files one by one using file->open option
23. **Align the structures**
    Command "align 1alc, 4lyz"
24. **Compute RMSD**
    After the alignment, RMS value will be displayed in the command line
25. **Save the aligned protein structures**
    File->save molecule
26. **Download protein structure with ligand(s). Identify the ligand and select residues within 4A. show any one type of interaction between them**
    i. Retrieve the protein structure from PDB "1AQ1"
    ii. Show the sequence and select the ligand. Right click and choose "Actions->around->residues within 4A.
    iii. Select ligand and choose the option "Action->find->polar contacts->within selection
27. **Identify the ligand binidng sites and label them**
    i. Select "Action->preset->ligands"
    ii. Select the interacting residues shown in "dashed lines" and label by residues
28. **Mutate any one of the active site residues and describe the change in the interaction with the ligand before and after mutation**
    i. Select "Mutagenesis" option under wizard.
    ii. Select "No Mutation->any residue"
    iii. Then choose the residue to mutate and give apply in the mutagenesis menu