In-class Assignment on computer simulation of Protein

Copy the content from accompanying "trpcage" folder.

In this exercise, you will use Gromacs for Molecular Dynamics (MD) simulations of Trpcage, a tiny mini-protein. Please feel free to use previous instructions of gromacs for this project.

Process 1: preprocessing using in-built programmes of Gromacs

A. The folder contains an initial configuration of a mini-protein called Trpcage. Visualize the protein in VMD. Save a snapshot. Write What do you see? Please generate topology files (topol.top) of this conformation using Gromacs for CHARMM27 forcefield.

B. Solvate the system in 3.5 nm cubic box and add necessary number of Chloride (CL) anion to neutralize the system (using gmx solvate and gmx genion tool). *Please note that for gmx grompp you need to use -maxwarn 2*

C. Now energy-minimize the system using min.mdp file. What is the maximum force on minimized system? Finally update the simulation protocol files (npt.mdp) to run 500 picosecond MD simulation. Note and write the performance in ns/day.

D. Before going ahead, please post-process the trajectory by centering protein at the box and removing periodic image related artifact (using gmx trjconv). Now visualize the post-processed trajectory in VMD. Write what are the observations you make? Take a screen-shot of starting and final screen-shots and save them.

E. Then let's do some analysis:

i) Calculate and plot RMSD of protein relative to reference structure (conf.gro) (using gmx rms tool).

ii) Calculate and plot Root mean squared fluctuation of each residue (RMSF) of the protein structure (using gmx rmsf)

iii) Calculate and plot the size of protein by calculating Radius of gyration (gmx gyrate)

iv) Calculate the number of hydrogen bonds present within protein as a function of time (gmx hbond).

v) Calculate the C_α-C_α radial distribution function.

Process 2: Using CHARMM-GUI

Carry out the same process as in Process 1, but now using Charmm-Gui. In this case use "Solution Builder" input generator Module of "Charmm-Gui". Use RCSB PDB code 1L2Y to obtain the coordinate directly in Charmm-gui. Use Charmm36 forcefield there.

Write a report on your observations. Specify your working directory in the computer in the report so that the instructor can find them. Upload your report in a "google classroom"