Course: BT 305

Lab Session 8 and 9: Analysis of simulated structures after MD.

Designed peptides Vs Natural Proteins (Protein G and Trp Cage)

Date: 22 March and 29 March 2023

Aim: MD of the designed peptides as well as Protein G and Trp Cage

Note: Designed peptides means alpha helix, beta sheet you have designed in previous lab sessions

The objectives of current session are as follows:

1. Calculate the net deviation in Ramachandran basin of the 4^{th} and 8^{th} residue of your designed peptides with respect to the starting structure, after:
A) Energy minimization
B) MD simulation for **1ns** in water.
C) Repeat the simulation at 363 K
(Use program rama)

2. Plot the change in the following energetic parameters with time, during MD Simulation. (use *gmx energy*)

A) Total energy (P.E) of the System; B) Coul-SR; C) LJ-SR;

3. Calculate the radius of gyration of the designed structures (helix and sheet) across 1ns trajectory, and compare it with natural proteins. What inference would you get from this analysis with regards to stability of designed peptides. (Use gmx *gyrate*).

4. Cluster the structures of your entire trajectory, output the cluster numbers by varying cut-off as 0.15 nm (or default cut-off) (gmx *cluster*).

5. Repeat the simulation of 1PGB for 1 ns at 363 K. Construct a free energy landscape at 363 K.

Classify and extract the average structure in each cluster, convert it into an image using any protein visualization program. What inference would you get from this analysis?

Materials and methods
Operating System: linux; Computational tools: GROMACS, xmgrace or Any Plotting software.