BT4110 COMPUTATIONAL BIOLOGY LABORATORY
MOLECULAR DYNAMICS MODULE
ASSIGNMENT 2 – MD SIMULATION USING GROMACS

Instructions:

- *This assignment is organized into 5 tasks with 2 questions each (total of 10 questions** 1 mark = 10 marks). Please perform the tasks in the order they are listed, step by step.
- Please use the pdb id assigned to you to perform the tasks and answer the questions. You can use the same mdp files from the lab session.
- Please provide plots in png format and VMD snapshots/file screenshots wherever indicated.
- Your submission should be in pdf format with the name "Roll number_Assignment2"
- Deadline for submission: 10th September 2024, 2 pm

Task 1. Generate topology file from the pdb file using charmm27 forcefield.

Q1a. Compare the gro and pdb files. Comment on the units of distance used in both the formats.

Q1b. What is the net charge on the protein?

Task 2. Create a cubic box around the protein and solvate it in water. Neutralize your system by adding ions to counter the charge.

Q2a. Open the system in VMD. Provide a snapshot of the protein present in the water box with ions (protein: in New Cartoon representation, water: in Points representation, ions: in VDW).

Q2b. What is the volume of the box generated? How many water molecules were added at this step?

Task 3. Edit the mdp file and perform energy minimization for 50023 steps.

Q3a. Provide a screenshot of the edited mdp file.

Q3b. Plot potential vs time for your system in XM Grace. In how many steps did the system converge to its least energy state?

Task 4. Perform NVT equilibration for the system at temperature 310 K.

Q4a. What is the average temperature at the end of the run?

Q4b. Provide a plot of temperature vs time.

Task 5. Perform NPT equilibration at temperature 310 K and 1 bar pressure.

Q5a. What is the average pressure at the end of the run?

Q5b. Provide a plot of pressure vs time.

After submitting this assignment, perform production MD for your system (500000 steps/1 ns) also at 310 K & 1 bar pressure and keep ready for the next assignment.