Exercise 03

GROMACS simulation setup

Deadline: Please hand in Exercise 03 by **Friday, 29 May, 10.15 a.m.**

1.1 Download PDB file and visualize with VMD (10)

In this exercise you can practice how to download a pdb structure and visualize it wih VMD. Download from the Protein Data Bank (PDB) website a structure of Langerin:
(http://www.rcsb.org/pdb/explore/explore.do?structureId=3P5H).
Open downloaded pdb file in a text editor and extract the Langerin monomer A, by deleting other monomers, crystal water, and Ca^{2+} ions. (5)

Using VMD visualize Langerin structure (New Cartoon as view style) and highlight the α-helicies in red, β-sheets in blue, and loops and coils in silver. Set background color to white. Include a snapshot of VMD representation in your report. (5)

1.2 Gromacs Set Up - Structure minimization (20)

Using GROMACS minimize the structure in vacuum and solvate it. Are ions needed? Why? (*use AMBERff99SB-ILDN as a force field and TIP3P water model. Use a dodahedron box and place Langerin in the center of it, at least 1 nm from the box walls*). (8)

Check the size of the simulation box. How many water molecules are needed to solvate such a protein? How many atoms atoms are in the solvated system? (2)

Check if the system is truly minimized by using the g_energy command of GROMACS and plotting the potential energy, the kinetic energy and the total energy. Can you plot the kinetic energy at this stage the structure preparation? (4)

Change the number of minimization steps (try 5000, 10000, and 15000 steps) in minim.mdp file and check again the potential energy. Is anything changed ? (2)

Change the energy cutoff (try 50, 100, and 150). What happens at different values of emtol? (2)

What can you conclude from this plots? Include plots made in xmgrace in the report and comment. (2)

1.3 Gromacs Set Up - Equilibration in NVT ensemble (20)

Modify given nvt.mdp file so that, integration step is 2 fs, NVT equlibration lasts for 100 ps, trajectory is updated every 1 ps, equilibration temperature is 300K, and Berendsen thermostat is used. Include **modified nvt.mdp** file into your report. (10)

Run NVT equilibration, detect the time needed for NVT equilibration, and check total, potential, and kinetic energy of the system by using g_energy command. (10)

2 Files

Necessary files are provided.