

Course: BT 305

Lab Session 7: Practice Energy minimization and MD simulation

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

Date: 15/03/2023

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

1. Run Energy minimization of Protein G and Trp Cage
2. Plot the change in Potential Energy during minimization. What do you understand from this?
3. Perform Molecular Dynamics Simulations of both molecules for 1 ns.
4. Plot the change in potential energy during the production run of MD? How is it different from energy minimization?
5. How much time did it take to complete the MD simulation
6. How are temperature and pressure maintained? Plot your P and T during the production run.

Materials and methods

Operating System: Linux; Computational tools: GROMACS, Any Plotting software.