BT 305 End Semester Examination (Lab)

Date: April 16, 2024. **Maximum Marks: 25. Time 90 minutes**

Your answer book has 6 entries, of which you should present 5 correct ones for maximum marks. 5 marks for each correct entry

Aim: Design a signature peptide with your name

(Sequence should be a combination of your name and surname with sequence length of maximum 10 amino acids. For example, VIBIN RAMAKRISHNAN, sequence will be VIINRAMAKR)

1. Use Ribosome and PROSS already installed

2. Design peptides with the above sequence (with your name). Generate PDB file (**first entry**)

3. You may use dihedral angles (Phi, Psi, omega) as -57, -47, 180

4. box type: cubic, size: 1 nm from the edge of the peptide.
Note the energy difference. Report box dimensions as the **second entry** in your answer sheet.

5. Solvate the peptide. Note down the number of water molecules as the **third** entry in your answer sheet.

6. Energy minimize in water. Energy difference between the starting structure and final structure as **fourth** entry

7. Perform 200 ps MD run at 300 K.

8. Plot RMSD (**5th entry**) and number of hydrogen bonds with time (**6th entry**)

Material and methods

Operating System: linux
Computational tools: Ribosome, PROSS, Any other software of your choice.