Course: BT 305

Lab Session 8

Section 1: Analysis of simulated structures after MD at higher temperatures.

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

Section 1

1. Repeat the simulation of 1PGB (with same parameters of lab session 7) 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 at higher temperature?

2. VMD is installed in all your designated lab computers. Try to make a video of the MD trajectory at 300 K and 363 K. Compare the results and explain your observations.

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

Section 2

Download the tool open babel and install it in your system.

https://openbabel.org/docs/dev/Installation/install.html

http://www.cheminfo.org/Chemistry/Cheminformatics/FormatConverter/index.html

Exercise 1

1. Convert at least two structures that you have designed and downloaded small protein molecule 1PGB from PDB to internal coordinate format.
   Convert it back, means internal coordinate to PDB file. Calculate the RMSD between the original pdb and newly generated pdb from internal coordinate.

2. Attempt to convert the PDB file of ALA, PHE, GLU and LYS to smiles

Exercise 2

Browse through the open babel tool. Design a unique question yourself and find answer with open babel, and present it in your record book as a regular exercise.