Exercise 03

GROMACS simulation Setup

Deadline:

1.1 Download PDB file and visualize with VMD (6)

In this exercise you can practice how to Download a pdb structure and visualize it wih VMD. Download from the Protein Data Bank website a structure for AIPP:
(http://www.rcsb.org/pdb/files/3G7V.pdb),
also called amylin or more formally Pancreatic islet amyloid. It is a characteristic feature of type 2 diabetes and is released in response to the stimuli that lead to insulin secretion.

Using VMD superimpose the full amylin structure (use Ribbons as view Style) and a replica that only includes the fragment FGAIL. Highlight the fragment by choosing Licorice as a view style. Include a snapshot of VMD in your report. (3)

From the pdb file extract the FGAIL fragment and make it capped. (3)

1.2 Gromacs Set Up (11)

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 cubic box and place your peptide in the center of it at at least 1 nm from the box walls*). (4)

Check the size of the simulation box. How many water molecules are needed to solvate such a fragment?(1)

Check that the system is truly minimized using the g_energy command of GROMACS and plotting the potential energy, the kinetic energy and the total energy. (1)

Change the number of simulation steps of the minimization and check again the potential energy. Is anything changed ? (2)

Change the energy cutoff. What happens at higher/smaller values of emtol? (2)

What can you conclude from this plots? (1)

Include plots in the report and comment.

2 Files

An example of mdp file for minimization is included.