Assignments for the course Computational Chemistry and Classical Molecular Dynamics (CCCMD): Lectures 36 to Lecture 41 Week - 8

The assignments are listed lecture-wise and weekly. For example, Assignment (5.1) will be the first assignment after lecture 5. There are a total of 41 lectures.

36.1) What is the information stored in a topology file?
36.2) Suppose you want to view a file water.pdb. What is the command you will use to view it?
36.3) What is meant by tolerance in the inp file of water?
36.4) What is the command genbox used for?
36.5) Let us consider a cubical box having 1500 water molecules and you are performing a simulation. You have created initial configuration using the software PACKMOLE. Total number of atoms for which the coordinates are created is _____.

37.1) What does nbfunc 1 stands for?
37.2) What are the files required for energy minimization?
37.3) What is the input file for mdrun?
37.4) Which gro file that is used for full molecular dynamics simulations?
37.5) Suppose I am creating an index file for water molecules. I type the following commands,

make_ndx –f em.gro –o index.ndx
a OW

What does **a** stands for here?

38.1) How does one execute an inp file in PACKMOLE?
38.2) Which command is used to generate a tpr file?
38.3) Which files are used for generating a tpr file?
38.4) Which are the files required to calculate the diffusion coefficient of methanol molecules?
38.5) Fill in the blanks:
g_rdf –___ full.xtc –s full.tpr -___index.ndx –o msdmethanol.xvg

39.1) What are the prerequisites for installation of GROMACS?

39.2) Which command is used to know the full path of any folder or any directory?

40.1) A topology file can be created with the help of _____ command.

40.2) In the MD simulations of s-peptide, which command is used to solvate the peptide?

40.3) In the command given below,

editconf –f speptide.gro –o out.gro –d 0.5 –c

a. What does –d specify?
b. What does –c specify?

40.4) What is the unit of potential energy obtained after energy minimization?

41.1) Which method is used to calculate the hydration free energy of methane using gromacs?

41.2) Which command is used to prepare a simulation box around a molecule?

41.3) Consider the following command,

editconf –f methane.pdb –o box.gro –bt dodecahedron –d

What is bt?

41.4) Which integrator is used for calculation of hydration free energy?

41.5) Which command is used to compute the free energy of hydration?