PROJ 102 Fall 2013

Modeling and Simulations of Molecules

Assignment 4, due beginning of meeting on **Thursday**, **November 28**, or **Friday**, **November 29**, 2013

0. Complete your work on Assignment 3

For question **2**(a), make sure you observe that spin-label configurations 4, 5 and 6 interfere with the hydrogen bonding between the spin-labeled Cytosine and its Guanine partner on the other chain of the RNA.

Fill out the table in question **2**(b).

In this Assignment you will perform molecular dynamics (MD) simulations using the program NAMD. Before starting to work on the questions make sure you have downloaded the NAMD executable file and have figured out how to run NAMD.

1. Vacuum simulation of spin-labeled, double-helical RNA

Using the "protein structure file" `rna_6-16.xpsf` and one of the coordinate files `a-rna.pdb`, `ap-rna.pdb` or `a-dna-rna.pdb` perform molecular dynamics simulations of the spin-labeled RNA at a temperature of 310 K and for a total duration of 100 ps. Save the simulation trajectory (i.e., `.dcd` file) once every 500 steps. (You need to modify the NAMD input script `vacuum.conf` that we used in class such that it reflects these choices.)

How long did the simulation take?

At the beginning of our meeting you should be able to show the resulting trajectory using VMD.

2. Simulation of spin-labeled, double-helical RNA in water

Use VMD to immerse the spin-labeled RNA contained in the files `a-rna.pdb`, `ap-rna.pdb` or `a-dna-rna.pdb` in a box of water with dimensions of $80\,\text{Å} \times 80\,\text{Å} \times 80\,\text{Å}$. Subsequently, put Na and Cl ions at a concentration of 150 mM (milli Molar) into the simulation box. (If you have already performed these two steps in class and have generated the files `ionized.psf` and `ionized.pdb` you do not need to repeat them.)

Perform molecular dynamics simulations of the resulting system at a temperature of 310 K and for a total duration of 2 ps. Save the coordinates to a `.dcd` file once every 50 simulation steps. As before, you will need to modify the NAMD input script `water.conf` that we used in class.

To perform the desired MD simulations you will need to use the new parameter file `par_all36_na_lipid_sl.prm` that came in the email containing this assignment. (The previous parameter file that I gave you did not have parameters for chloride ions.)

How long did the simulation take?

At the beginning of our meeting you should be able to show the resulting trajectory using VMD.