PROJ 102 Fall 2013

Modeling and Simulations of Molecules

Assignment 5, due beginning of meeting on **Thursday**, **December 5**, or **Friday**, **December 6**, 2013

In this assignment you will use NAMD to position the two spin labels in the conformations introduced in question 2 of Assignment 3. To do so, you need to download the *NAMD User's Guide* and find the subsection titled *Constraints and Restraints*. In this section, you will find instructions on how to restrict a dihedral angle to remain around a desired value.

1. Indices of atoms in dihedral angles

First you need to identify the index of the atoms comprising the ϕ_1 and ϕ_2 dihedral angles (defined in Assignment 3) of the two spin labels. To remind you, the names of the atoms involved in the two dihedral angles were

$$\phi_1: \quad \text{CR1} - \text{CR3} - \text{N4} - \text{C4}$$
$$\phi_2: \quad \text{CR3} - \text{N4} - \text{C4} - \text{C5}.$$

Fill out the following table with the indices of the relevant atoms:

	spin label 1				spin label 2			
	atom 1	atom 2	atom 3	atom 4	atom 1	atom 2	atom 3	atom 4
ϕ_1:								
ϕ_2:								

Bring the filled out table to our next meeting.

2. Simulation with restrained dihedral angles

Following the instructions in the *NAMD User's Guide*, prepare a file that contains information about the dihedral angles you want to restrain. (You may call this file `dih-restr.dat`.)

In this file, select the reference values of ϕ_1 and ϕ_2 such that spin label 1 is in conformation 2, and spin label 2 is in conformation 1. Set the value of the spring constant to 200 (in whatever units NAMD uses).

Modify the NAMD configuration file `vacuum.conf` such that the non-hydrogen atoms of your RNA are *harmonically restrained* around their starting positions (contained in one of the files `a-rna_lbl.pdb`, `a-rna_lbl.pdb` or `a-dna-rna_lbl.pdb`) with spring constants as specified in one of the files

`a-rna_lbl.cons.pdb`, `a-rna_lbl.cons.pdb` or `a-dna-rna_lbl.cons.pdb`.

(Remember, this part we already did in class.)

At the end of this modified file, add additional instructions for constraining the desired dihedrals using the information contained in the file (`dih-restr.dat`) that you already prepared.

Once everything is ready, run the modified `vacuum.conf` file for 5000 steps.

Use VMD to measure the ϕ_1 and ϕ_2 dihedral angles for both of the spin labels at the *beginning* and at the *end* of the simulation.

Write down the values of these angles (both at the beginning and at the end) and observe whether they change as desired.

Bring a table containing your measured values and a written statement of your observation to our next meeting.