PROJ 102 Fall 2013

Modeling and Simulations of Molecules

Assignment 3, due beginning of meeting on **Thursday**, **November 21**, or **Friday**, **November 22**, 2013

1. Tcl scripting

The script `chi1.tcl` that we considered in class rotates the second spin label on the RNA double helix around the bond between carbon 4 and nitrogen 4 on the cytosine base (see Figure 1).

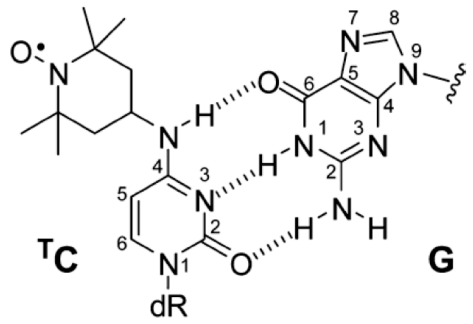

Figure 1: A representation of our spin label, which is covalently bonded to cytosine. Here it is shown forming three hydrogen bonds with guanine. The numbers next to the atoms show the universally accepted numbering for the cytosine and guanine bases.

(a) Write another script, `chi2.tcl`, which will rotate the second spin label around the bond between nitrogen 4 and the carbon on the six-membered ring of the spin label containing the unpaired electron.

(b) Write a script `phi2.tcl` that rotates the first spin label around the bond between carbon 4 and nitrogen 4 on the cytosine base at position 6 on the strand `RNA1`.

(c) Write a script `phi1.tcl` that rotates the first spin label around the bond between nitrogen 4 on the cytosine base at position 6 on the strand `RNA1` and the carbon on the six-membered ring of the spin label containing the unpaired electron.

Print the three scripts that you wrote and bring the print-out to the meeting.

2. Distances between the spin labels

The energy surface associated with the rotations of a spin label around the two bonds that you studied in the previous question is shown in Figure 2. The molecular models, numbered from 1 to 6, show the conformations of the spin label at the local minima of the energy surface. The energies of these conformations are given in Table 1.

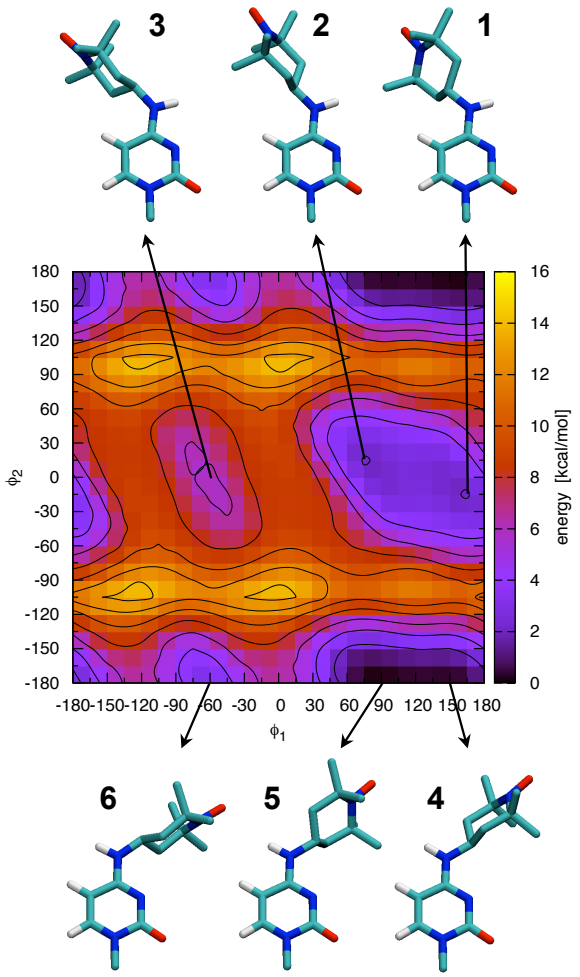

Figure 2: Possible conformations of the spin label shown on the energy surface associated with rotations about the two bonds that you examined in the first question.

Note that the dihedral angles ϕ_1 and ϕ_2 constituting the axes of Figure 2 correspond to the rotations performed by the scripts `phi1.tcl` and `phi2.tcl` in parts (c) and (b) of Question 1. Unfortunately, in the case of the second spin label, ϕ_1 corresponds to `chi2.tcl` and ϕ_2 corresponds to `chi1.tcl`.

(a) Use the scripts `phi1.tcl` and `phi2.tcl` that you wrote in Question 1 to rotate the first spin

Table 1: Energies (in kcal/mol) and corresponding dihedral angles of the spin label conformations shown in Figure 2.

conf.	1	2	3	4	5	6
energy	2.0	2.0	5.5	0.0	0.0	2.6
ϕ_1	160°	80°	−60°	160°	80°	−60°
ϕ_2	−10°	10°	0°	180°	180°	180°

label into conformations 4, 5, and 6. Argue why these conformations are not expected to be seen in a double-helical RNA.

[Argue means that you should write a few sentences which explain your evidence. If you wish, you can also present the evidence as a figure.]

(b) Use the scripts `phi1.tcl`, `phi2.tcl` as well as `chi1.tcl`, `chi2.tcl` to rotate the first and second spin labels in the conformations listed in Table 2. Measure the distances between the **oxygen** atoms of the two spin labels for the four possibilities and write the value in the last column of the table.

Table 2: Distances between spin labels 1 and 2 when the two spin labels are in the specified conformations.

label 1	label 2	distance (Å)
1	1	
1	2	
2	2	
2	1	

Bring your answer to part (a) and the filled-out table 2 in written form to our meeting.