

## Modeling and Simulations of Molecules

Assignment 6, due beginning of last meeting on **Thursday, December 19**, or **Friday, December 20**, 2013

**1. Analysis of dihedral angle dynamics**

In class we learned how to monitor the distance between the oxygen atoms of the two spin labels as a function of time. (Read the relevant section of the VMD tutorial if you need to remember how this was done.)

In this question you will examine how the values of the  $\phi_1$  and  $\phi_2$  dihedral angles of the two spin labels change in time. (Remember, the dihedral angles were defined as follows:  $\phi_1$  : CR1 – CR3 – N4 – C4 and  $\phi_2$  : CR3 – N4 – C4 – C5.)

- a.** Upload the relevant `.dcd` trajectories and select the two dihedral angles of the first spin label (attached to base number 6 on RNA1).

Produce a plot showing the values of these dihedral angles as a function of time.

Examine the plot to determine which conformations (of the six possibilities introduced in Assignment 3) are visited by the first spin label.

- b.** Now select the two dihedral angles of the second spin label (attached to base number 16 on RNA1).

Produce a plot showing the values of these dihedral angles as a function of time.

Examine the plot to determine which conformations (of the six possibilities introduced in Assignment 3) are visited by the second spin label.

Bring the two plots of parts **a** and **b** to our meeting. Also, write a few sentences explaining whether the spin labels remained in their starting conformations during the entire duration of the trajectories that you examined or whether they changed their conformations. At what points have such changes occurred?