The primary goal of this exercise is to familiarize yourself with the program VMD (Visual Molecular Dynamics). This is a powerful and commonly used tool for analyzing molecular dynamics simulations, as well as performing a variety of structural calculations on macromolecules. It’s much more powerful than PyMOL, but it is also clunkier and more difficult to use. We will use it throughout the course.

**Before class:**

* Download and install VMD: <https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD>
* Bring your laptop to class.

**In class:**

The files you need for this tutorial are here:  
<https://www.ks.uiuc.edu/Training/Tutorials/vmd/vmd-tutorial-files/>

1. We’ll start with loading and visualizing a protein structure. It’s similar to PyMOL, but different enough to be annoying.   
     
   Follow this tutorial up to, but not including, “Sequence Viewer Extension”  
   <https://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node2.html>
2. It is completely non-obvious how to measure the distance between atoms in VMD.   
     
   Go to *Mouse 🡪 Label 🡪 Bonds*, and then click sequentially on any two atoms whose distance you want to measure. If it works, you should see a dashed line with the distance in angstroms between the atoms of interest.
3. The next step is to load a molecular dynamics simulation and visualize it.

Follow this tutorial up to, but not including, “Basics of Movie Making in VMD” <https://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node3.html>

1. During a simulation, molecules are free to drift around in space. We often want to fix the protein in space and watch how parts of the protein move relative to each other. To do this, we need to align each frame to the starting frame.
   1. *File 🡪 New Molecule…* : Browse to and select “ala-ala-ala.gro”. This file holds the starting coordinates of the simulation.
   2. Select the row corresponding to “ala-ala-ala.gro” in the main VMD window.
   3. *File 🡪 Load Data Into Molecule…* : Browse to and select “ala-ala-ala.xtc.” This file holds the steps for the trajectory.
   4. *Graphics 🡪 Representations…* : Draw the protein as lines.
   5. Run the simulation using the player controls on the main VMD window. Notice that the peptide drifts throughout the box.
   6. Go to *Extensions 🡪 Analysis 🡪 RMSD Trajectory Tool*  
        
      Select “Backbone” under “Selection modifiers” and then click “Align.” This will align the backbone residues over the course of the simulation.   
        
      Play the simulation again. Notice that the protein no longer moves relative to the camera.
2. There are many different things you may want to calculate from a simulation. One useful calculation we will do later is a Ramachandran plot.   
   1. Go to *Extensions 🡪 Analysis 🡪 Ramachandran Plot*
   2. Under the “Molecule” dropdown to the right, make sure that “ala-ala-ala.gro” is selected.
   3. Click “Create 3-d histogram.”