1. Open “fa10\_1usec\_conv.gro” with VMD (opens a static structure)
2. In the “**VMD Main**” window, right click on molecule object ID 0 and select option “*load Data into Molecule*”. This opens “**Molecule File Browser**” window.
   1. Browse and find “fa10\_1usec\_conv\_ns.xtc”. This is a Gromacs XTC Compressed Trajectory file. Load this file. VMD will load the frames (1000)—will take a few seconds.
3. Go to “**Extensions**” in “VMD Main” window.
   1. Select “*Tk Console*”. This opens a command prompt.
   2. Load vmdrc.txt. This file contains functions for VMD. For example, on my windows laptop I typed this on the Tk Console command prompt:

% source /Users/Inspiron/Dropbox/Temp/visualization\_for\_Tredinnick/vmdrc.txt

* 1. Now run a function to align all the dynamics frames to the first frame (keeps protein from jumping around).

% align\_frames\_alpha 0

1. Go to “**Graphics**” in “**VMD Main**” window.
   1. Go to “*Representations…*”
      1. In “*Selected Atoms*” line type “resname lig” (this will create object for the drug molecule).
         1. Note: you are in the “Draw style” subtab
         2. In “*Drawing Method*”, select VDW (rendering style for drug)
         3. In “Coloring Method”, select “ColorID”, and “1 Red” for now.
      2. Click “Create Rep” button new top of “Graphical Representations” window
         1. In “Selected Atoms” line replace “resname lig” with “protein”
         2. In “Drawing Method”, select “NewCartoon”
         3. In Coloring method”, select “Secondary Structure”
      3. Note, so far you have been working in the “Draw style” subtab.
         1. Click on the “Trajectory” subtab,
         2. Change “Trajectory Smoothing Window Size” to something like 5
         3. Do this for both the drug and protein objects.

NOTE: go ahead a play with the rendering choices and stuff to find what looks best.