VMD Tutorial
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This is an example for visualizing the trajectories from the M2TM Molecular Dynamics simulations, performed in the Biomedical Research Foundation of the Academy of Athens as part of the project "Study of the interaction of aminoadamantane derivatives with the influenza A virus M2 channel through docking and FEP/MD calculations" with lead investigators Prof. Kolocouris and Dr. Cournia.

The following example corresponds to the trajectory of amantadine (ligand4) from the last window of the 6 -> 4 mutations in the system with the DPPC lipid bilayer, but can be easily used for the other ligands.

A. To load the trajectory

1. Open vmd

2. Go to **File > New Molecule** and in the Filename put the name of the first frame **analysis1.gro** and then press "ok" and "load" (Figure 1). The first frame has been loaded.
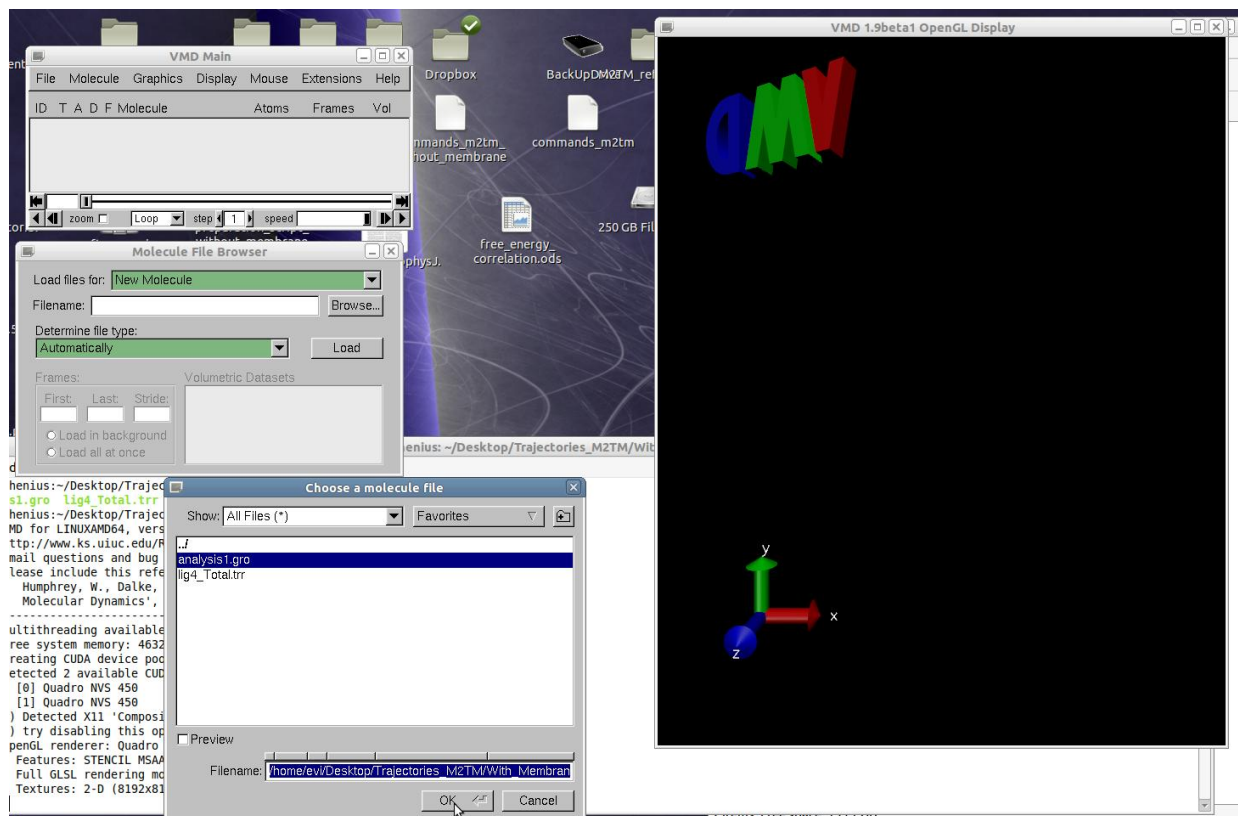

Figure 1

3. Right-click on the entry analysis1.gro and press "Load Data Into Molecule". In the Filename put lig4_Total.trr and press "ok" and "load". The total 2-ns trajectory has been loaded (85 frames). You can see any of the frames as shown in Figure 2.
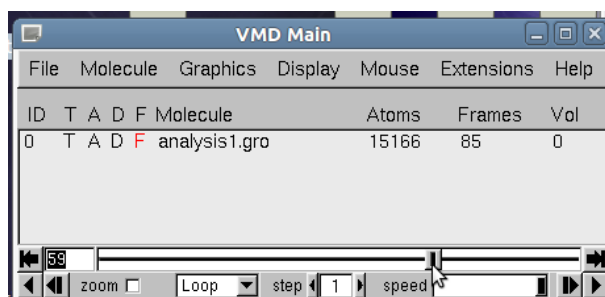

Figure 2

B. Visualization

1. Go to Display and choose **Orthographic** instead of **Perspective** viewing options.

2. Protein representation: Go to **Graphics > Representations**, select protein in the selected atoms section and in the Drawing Method choose **NewCartoon** (Figure 3).
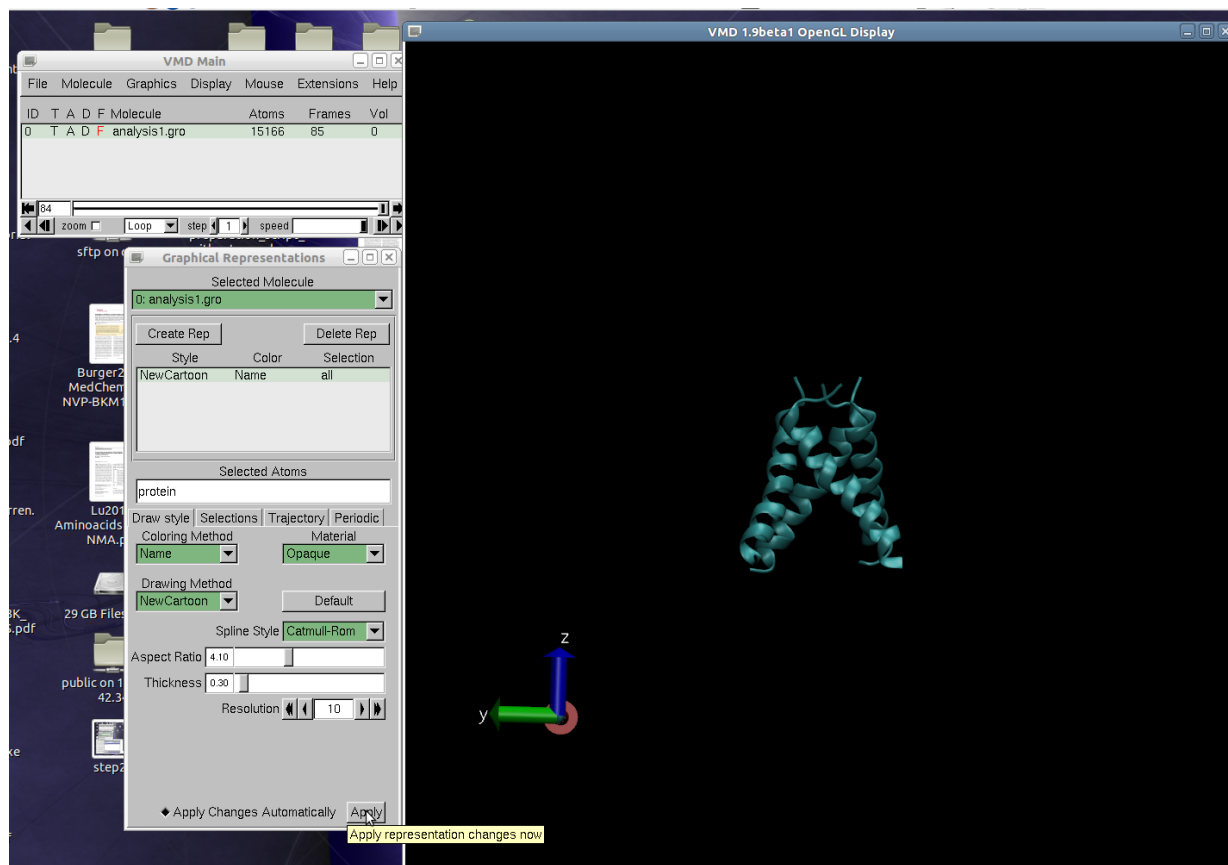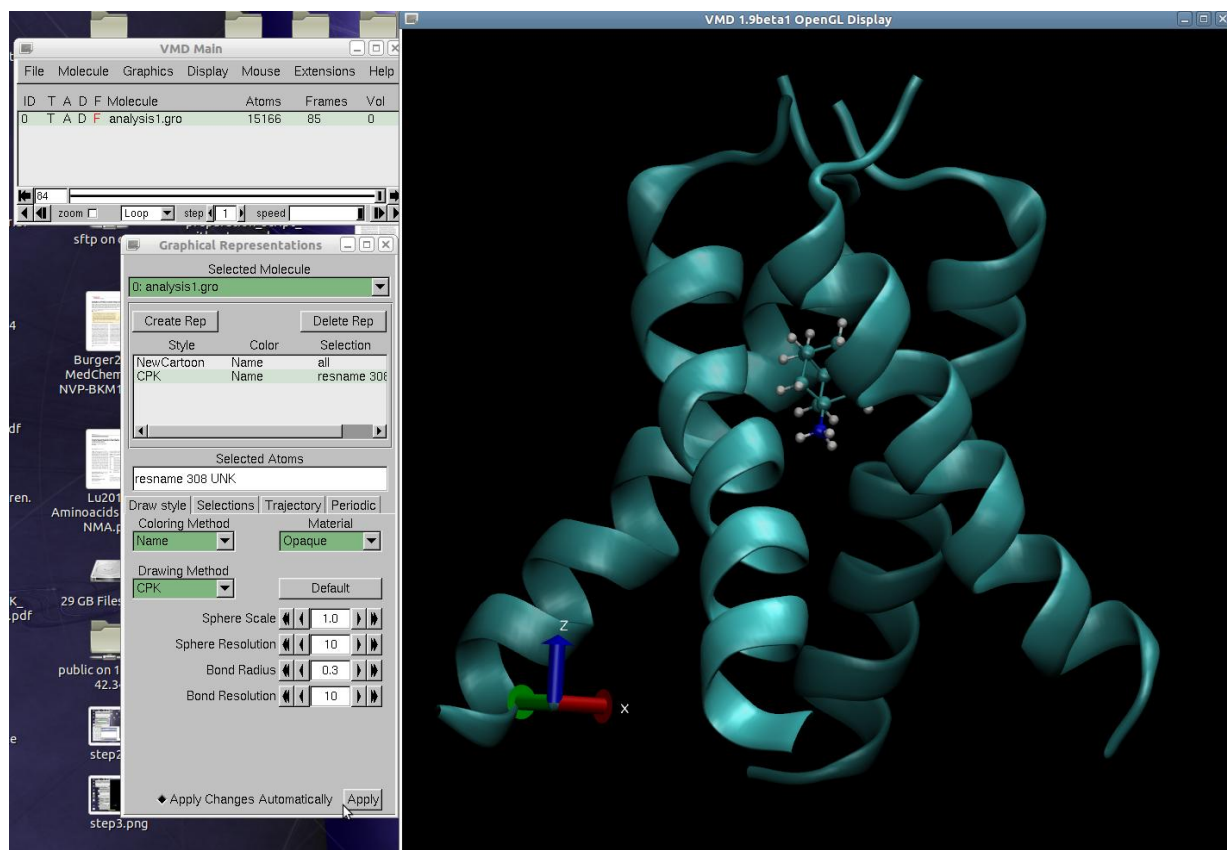

Figure 3

3. <u>Ligand representation</u>: Press **Create representation**, in the selected atoms space put "**resname 308 UNK**" and in the Drawing Method choose **CPK**.

Figure 4

4. <u>Water representation</u>: Press Create representation; in the selected atoms space put "**resname T3P**" (the Drawing Method can be whatever is better for the eye - you can choose among different choices - just press the arrow at the drawing method section). To keep only the water at a certain distance from the ligand4 instead of "resname T3P" in the selected atoms you should put "**resname T3P and within 9 of resname 308 UNK**", where 9 is the distance in Angstroms from the ligand and can be changed (Figure 5). Don't forget to go to the Trajectory tab (third) and chose Update Selection Every Frame!

5. <u>Ion representation</u>: Press Create representation, in the selected atoms space put "**resname CL NA**". You can again keep only the ions at a certain distance from the ligand as described above.

6. To visualize a specific protein residue or a specific atom, go to Selections (the second tab in the Graphical Representations), and chose a keyword and the value you want. For example, to visualize the histidines, you will chose **resname HIS** (Figure 6).

7. To hide any of the representations, just double-click on the selection (Figure 6 – the hidden entries are shown in red).
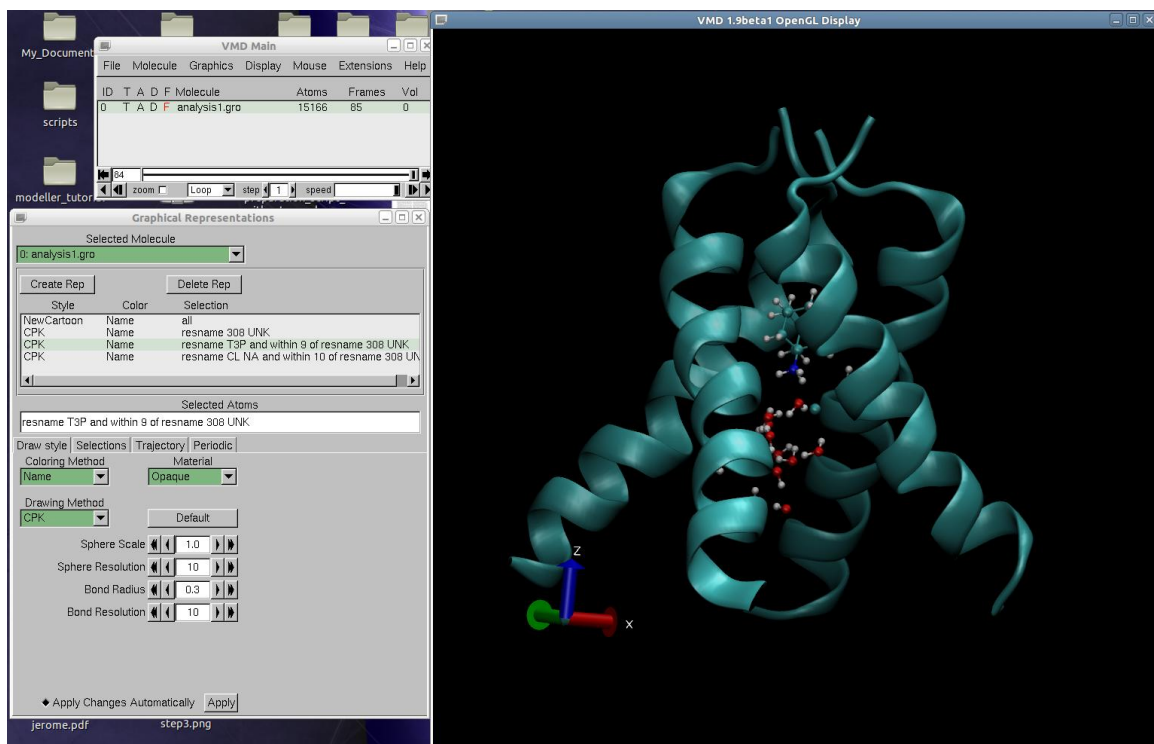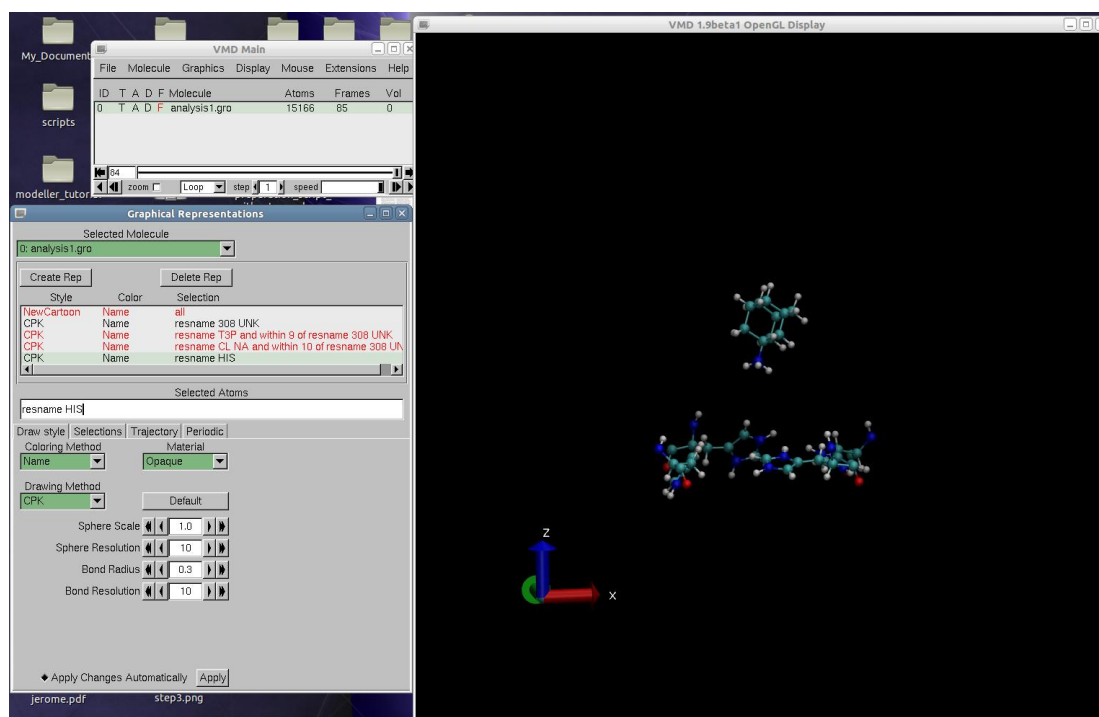
Figure 5

Figure 6

6. To visualize the hydrogen bonds: create a new representation and chose **(resname T3P and within 9 of resname 308 UNK) or resname 308 UNK** and in the drawing method choose **HBonds**. You can change the distance and the angle cutoff (Figure 7). Again you need to choose Update Selection Every Frame in the Trajectory tab.
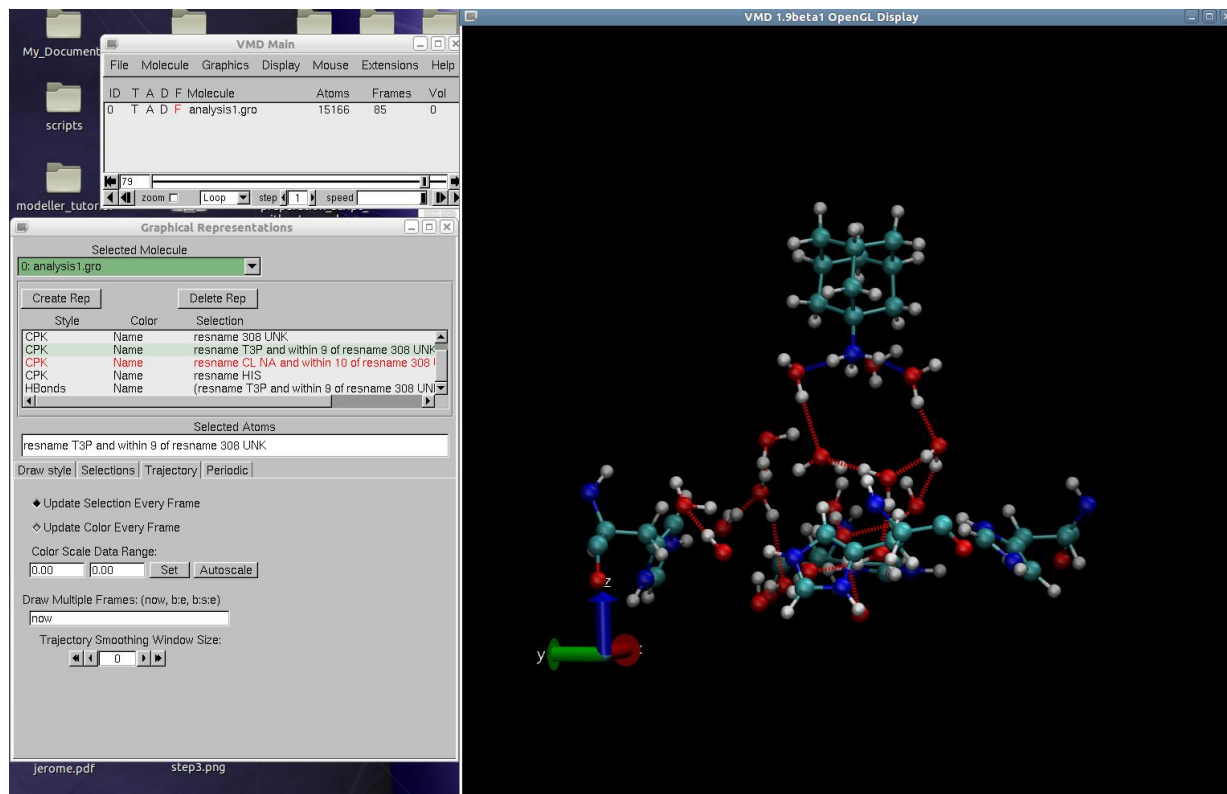

Figure 7

VMD is a very powerful visualization tool, relatively easy to use. For more advanced options, I am attaching two more documents.