Analysis of Protein Conformations Using Computer Simulations

We use a program called AMBER, on Western Kentucky University’s computing cluster, to run molecular simulations. AMBER uses a Linux command line and is good at organizing data and files. For each protein that we ran using AMBER we created a new directory to organize the files that go with each individual protein both left and right. We used a basic min, heat, and prod file for each protein that we ran and a submit file to go along with each of the min, heat, and prod files.

To get the information about the individual proteins, we download the pdf of the proteins and then we run tleap to create the prmtop, a list of all the atoms in the protein, and inpcrd, coordinates for the location of the individual atoms in the complex protein, files. We then run the submit files to run the protein. We heat the proteins to a very high temperature and then cool the proteins back down to see if they have changed their confirmation. Once all the files have been submitted and have finished running, the files can be viewed by importing files to VMD (visual molecular dynamics). By importing the inprcd files it shows how the protein changes throughout the running of the simulation, therefore can be used to predict a proteins conformation. Also, RMSD (root-mean-squared deviation) analysis is used to measure the deviation of a reference set of coordinates to a target set of coordinates.

Eventually we hope to be able to compare the bound and unbound proteins, extract interesting structures from our MD runs, and perform tagdock on our proteins.