Chemistry 438/550: Computational Chemistry, Spring 2020

Homework #7, due 8 April

The goal of this homework project is to have you work through the key parts of tutorials B0 and B1, which can be found at ambermd.org/tutorials/Introductory.php. I do not expect you to follow every step, but do enough so that you feel comfortable in carrying out such simulations. Make a mistake somewhere (on purpose, if necessary), and see what happens. Look through the human-readable log files from *sander* to familiarize yourself with what sort of information is there. As noted in Remote Lecture 4, you should use *tleap* in place of *xleap*.

1. Once you have done this, go to tutorial B3, at ambermd.org/tutorials/basic/tutorial3/index.htm. This tutorial walks you through a protein folding simulation on a fairly short peptide called the *Trp cage*. But I just want you to follow the tutorial up through the minimization step, to the end of section 3. Please modify the tutorial by changing the second amino acid in the peptide from leucine to isoleucine. Build the system as in Section 2, and minimize as in section 3.

2. "Hand this in" by doing the following:

   ```
   cp min1.pdb lastname.txt
   cp lastname.txt /home/dacase/ccb550/homework7
   ```

   (Again this is a pretty trivial thing to "hand in". The point is to make sure you are actually learning how to prepare systems in *tleap*, and to use those files in e.)