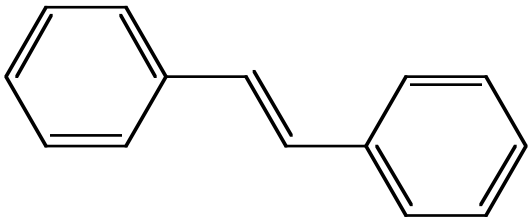
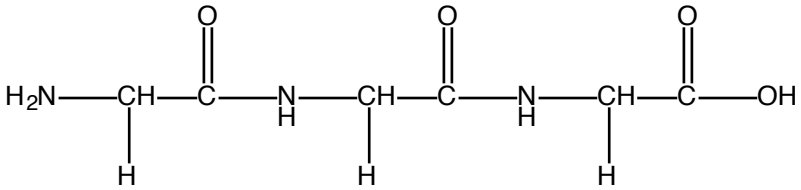
Computers in Chemistry—CHEM 3111 Problem Set 5
Use ChemDraw to draw molecules and perform simple calculations.

In this exercise, you will use ChemDraw and Chem3D to draw some simple and not so simple molecules, then determine their 3D structure, and setup and pertorm some simple molecular dynamics calculations. You should submit either a ChemDraw or MSWord document with the pictures, structures, and descriptions. These can be emailed to me or simply uploaded to your account on k2.chem.uh.edu

1. Practice using ChemDraw to make the following molecules:
   a.) trans-stilbene

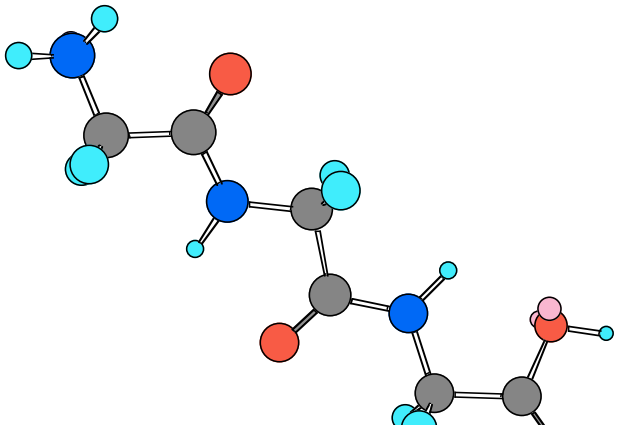


   b.) water
   c.) an amino acid sequence of 4 amino acids: (e.g)

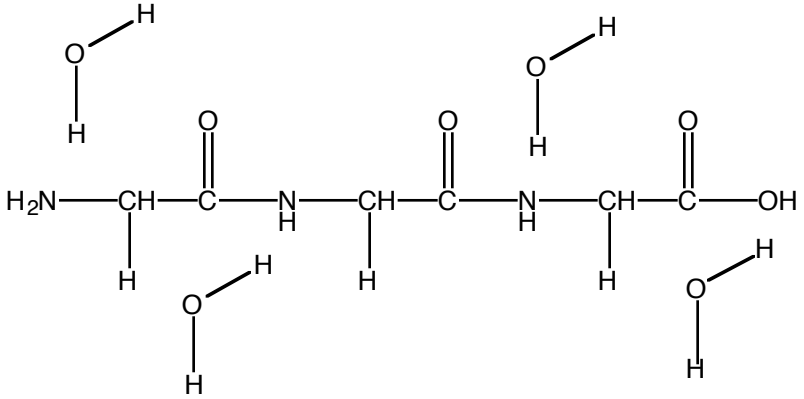


   d.) caffine

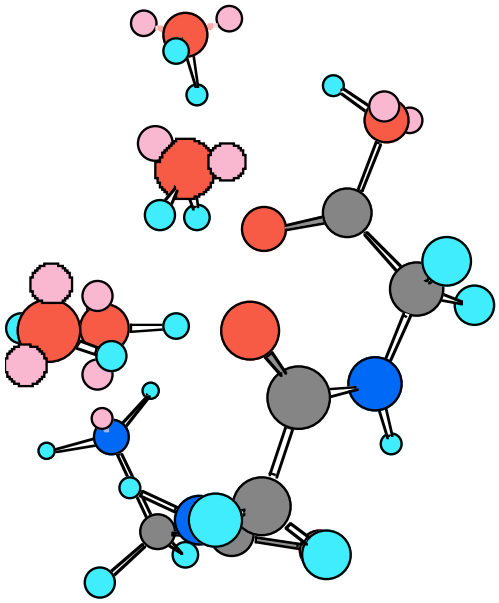
2. Using the "Scripts" menu, determine the 3D structure of each of the molecules or clusters you just drew. For eacn case, use Chem3D to use MM2 to minimize the energy of the molecule. (e.g. for the amino acid sequence above, the minimal energy structure looks like:



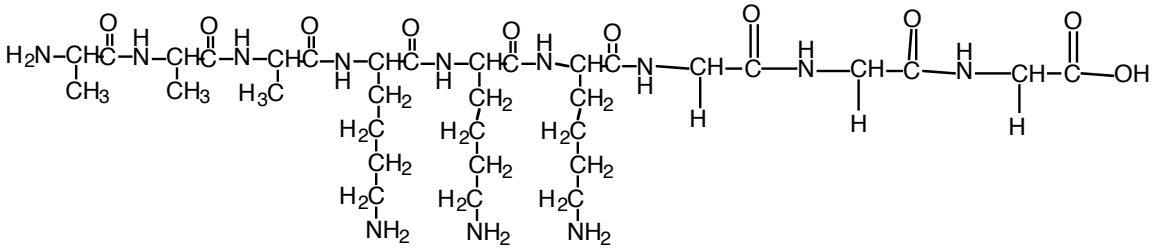
3. For the amino acid sequence, add some water molecules about it (using ChemDraw), then setup and perform a molecular dynamics calculation at 300K. Let the system run for about 10000 steps (I'd suggest using a 1fs time step.) and discuss the location of the water molecules about the amino acid chain. (eg. For the chain above, adding 4 waters:



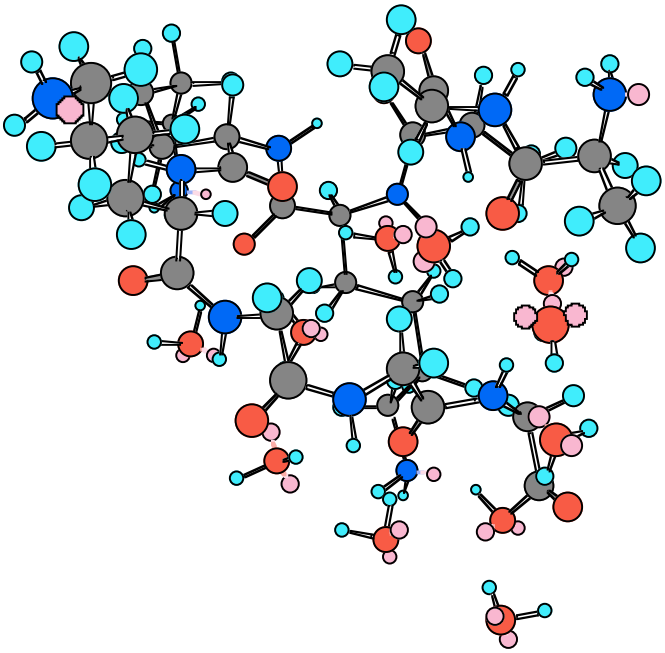
then running the calculation produces the following configuration.



4. Finally make a block polymer of 3 blocks of different amino acids. Choose the middle segment to have hydrophobic side chains. For example:



Place some waters around it and minimize the energy. Run a MD simulation for about 5000 steps and discuss the structures you observe. For example, here's a snap shot of a simulation based on the molecule above with 10 waters. Notice the waters tend to avoid the alkane side chain segments.



Looking at the output data, plot the total energy, potential energy, and temperature as a function of time. Has the system approached thermodynamic equilibrium at 300K at the end of your calculation?