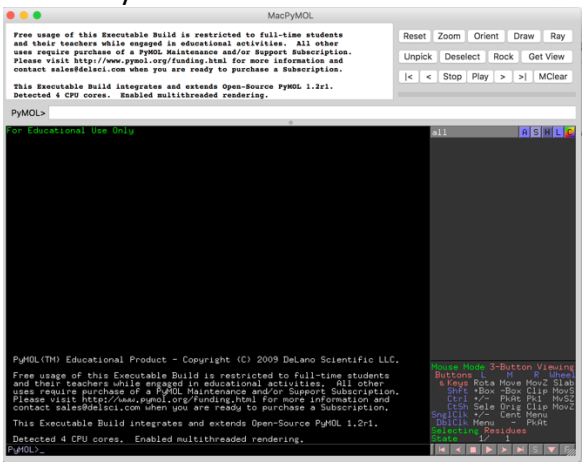
PyMol Assignment 1: Making a tripeptide

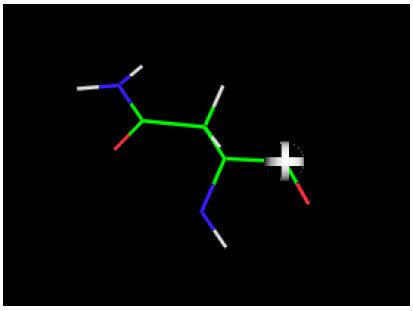
Install PyMol on your computer from either the Mac or PC versions of this program that are provided on the Canvas site for the class.

Launch PyMol. It should look like this:



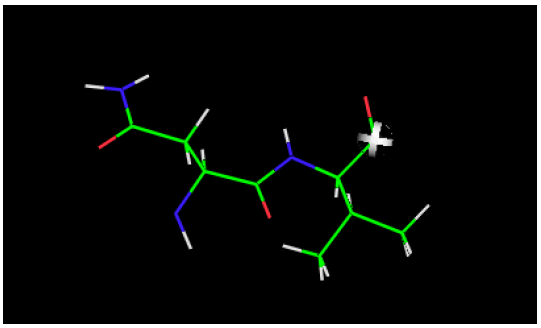
Make a tripeptide with amino acids corresponding to your initials. I will use my initials, NVH, as an example. Use yours for the assignment. If you only have two initials, add your favorite amino acid as your middle initial. If you have an initial for which an amino acid is not assigned, then use the letter that is closest to your initial in the English alphabet.

To select your first amino acid go to the pulldown menu Build->Residue->(your first amino acid). I selected Asparagine for N. This is what appeared on my screen.

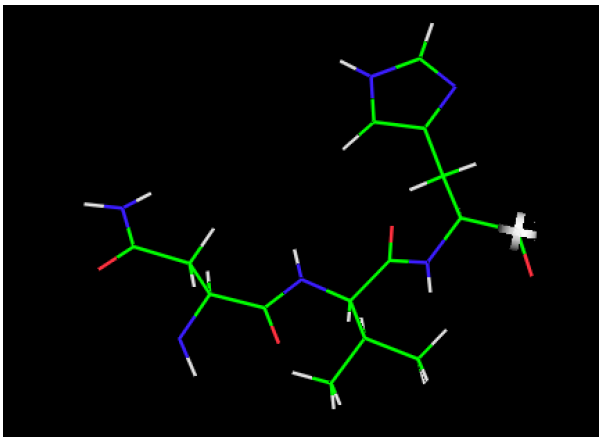


Notice that the last carbon atom of is surrounded by a while banded sphere. That is a special type of atom selection that is designated a pk1. This selection is where the next residue will be attached.

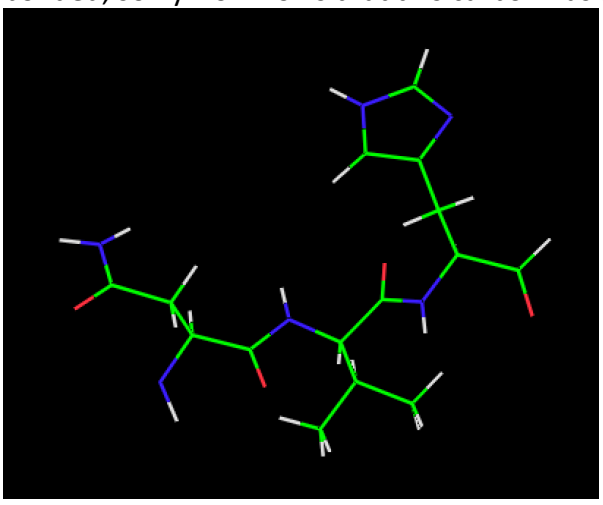
Go to Build->Residue->(your second amino acid) to add the next residue in your tripeptide. I added valine so my growing peptide changed to:



Do the same for your third initial. Mine is H, so I added a histidine. Now my peptide looks like this:

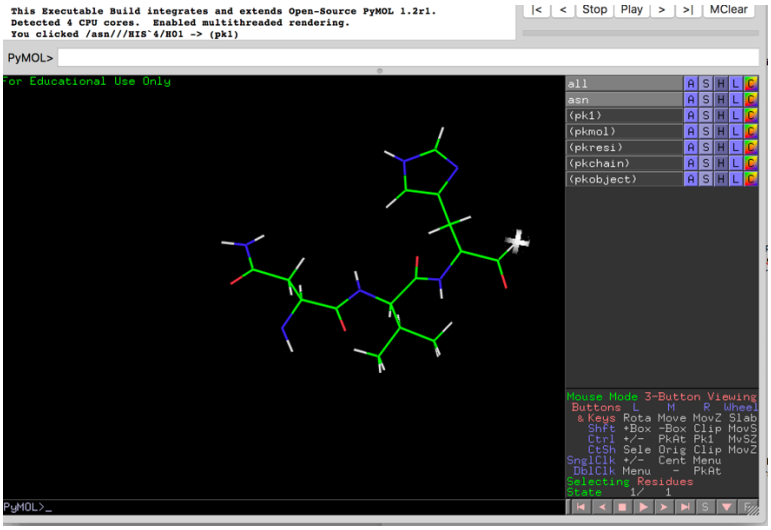


Now it is necessary to terminate the peptide properly. We can do this in two steps. Go to Build->Fragment->Carbon to confirm that this atom is to be a carbon. Notice that PyMol has added just one hydrogen to this carbon. That is because the oxygen attached to this carbon is double bonded, so PyMol knows that this carbon has sp2 hybridization.



Now you need to change that hydrogen that PyMol added to an oxygen. Do this by a “special” selection of the hydrogen. On a Mac you can hold down the control key and use two fingers on

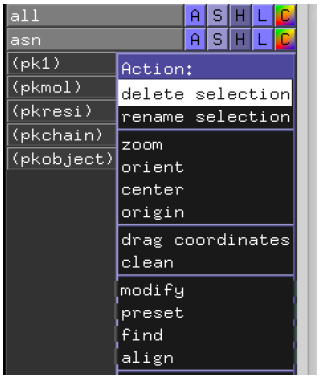
your mouse pad to select this atom while your cursor is over this atom. On a PC your can use CTRL-right click. When selected properly the peptide now looks like this:



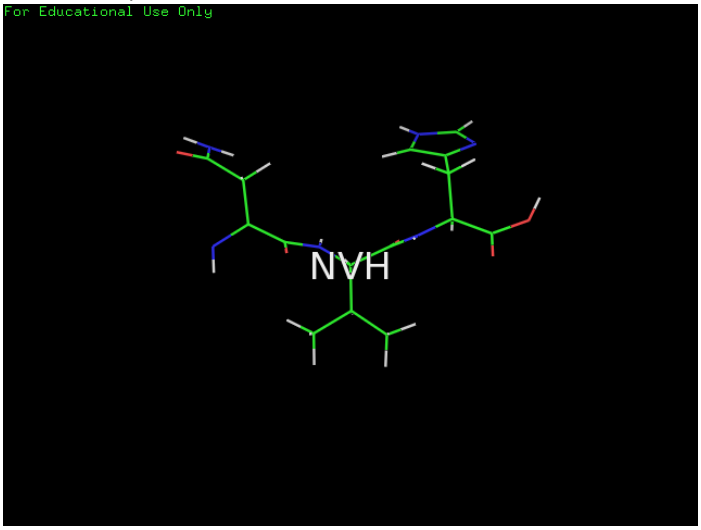
Now go to Buld->Fragment->Oxygen to change the hydrogen to an oxygen. Your peptide is finished. The peptide ends are not charged, in the -NH2 and -COOH states, but that is OK for this exercise.

Now center your peptide in the screen by doing the pk1 selection on an atom near the center of the peptide and then by typing >**center pk1** in the command line of PyMol (without the >). Your peptide will move to the center. You can now use your mouse or track pad to rotate your peptide into a nice view. There are online tables that tell you which mouse commands can be used to move, rotate, or resize your structure.

Add your initials at the pk1 selected atom by typing >**label pk1, "NVH"**, bu twith your initial. Then go to Labels->Setting->Size and increase the font size so that your initials are easy to see. Go to the pk1 selection, click on the A and go down to delete selection to remove the banded sphere.



After that, mine looked like this:

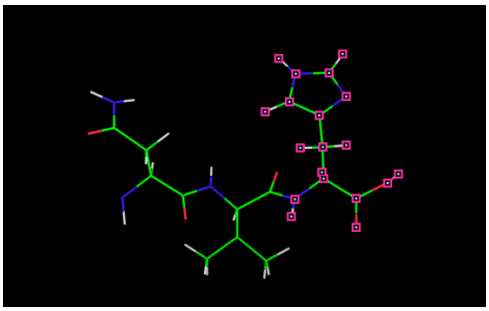


Make an image of your peptide with initials using File->Save Image As -> PNG.
Save this image to some place on your computer where you can easily find it later.

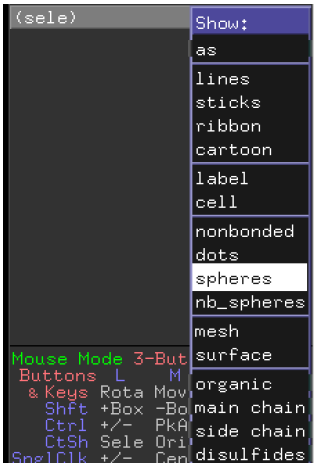
Clear initials from your peptide by selecting the atom to which they are attached as pk1. Then enter into the command line >**label pk1, “”**

Now, make sure that your Selecting level is set to Residues. You will see this in the bottom right section of the PyMol screen. If it is set so something else, like Atoms, Molecules, Objects, just click on the word after Selecting until it shows Resdidues.

Select one of the residues on your peptide. When it is selected it should have red squares around each atom. Like this:

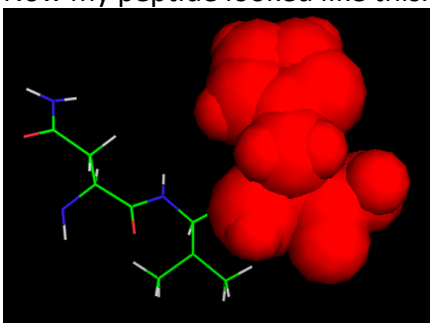


Now move your cursor to the “S” (for Show) that is at the right of the (sele) tab that appeared when you selected the residue. Tap on the “S” to reveal the different ways that you can render the amino acid. I selected “spheres”.



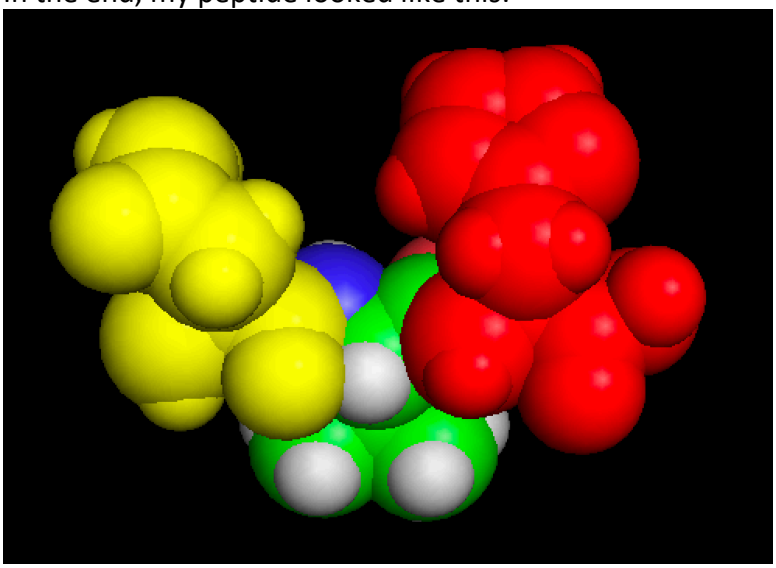
Next, move your cursor to the “C” at the far right of (sele) to select a color scheme for your residue. I selected red under the reds tab to make all atoms in my residue red.

Now my peptide looked like this.



To de-select the residue, as I did before taking this picture, just click your mouse someone in the PyMol window where there is blank space (no atom).

Change the appearance of the other two residues until you have something you like. If you change to something that you do not like, you can remove it by using the “H” (for hide) button, just like you use the “S” button.
Increase the quality of your image by using the tab Display->Quality->Maximum Quality.
In the end, my peptide looked like this:



Save a PNG format image of your final peptide.

To complete your assignment, import the two PNG images you saved into a word processing document (such as Word). That is, the stick rendering of your peptide with your initials on it and the one what you changed to have different rendering styles and colors. Have these fit onto a single page. Put your full name on the page. If you found any useful options in PyMol by yourself or with the help of an online tutorial that were not mentioned above, write about these below your images.

Convert your document to a PDF file and submit as your completed assignment.