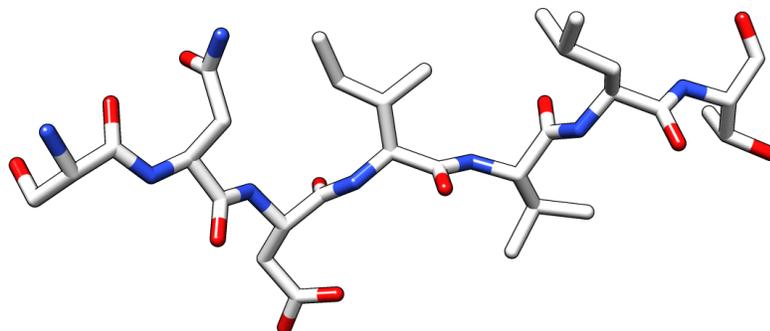


Hands-On Thirteen

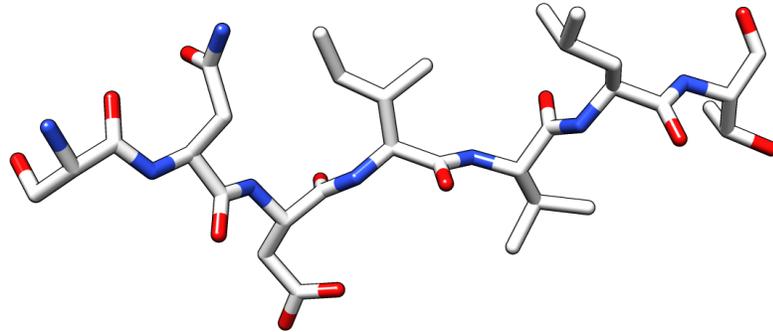
Protein Secondary Structure and Visualization

In this Hands-on Exercise, you will learn how to:

1. Identify the repeating structure of the peptide backbone
 2. Identify the different N and C termini of a peptide chain
 3. Identify the side chains associated with a polypeptide from the 3D structure
1. Examine the image below, and decide which of the following sequences accurately describes the primary structure of this peptide:
 - a. SDNVLIT
 - b. SNDIVLT
 - c. TLVIDNS
 - d. TVLIENS



2. Download the peptide sequence in the PDB format (ho13ex1.pdb) from <http://salilab.org/~nkhuri/Rabat2013/>
 3. Start the UCSF Chimera viewer and open the file you downloaded by selecting “File”, then “Open”. Try to rotate the peptide and identify the amino acids by pointing atoms with the computer mouse.
 4. You can display the entire peptide sequence by selecting “Tools”, then “Sequence” and “Sequence”. Did you identify the amino acids correctly?
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5. Using the image shown below, label on it the different amino acid side chains with their single- and three-letter codes.



6. To complete the next exercise, close current session in Chimera by selecting “File”, then “Close Session”.
7. Download ho13ex3.pdb from <http://salilab.org/~nkhuri/Rabat2013/> and open the file in Chimera. You should see a 3D structure of an alpha helix. Display the peptide’s backbone and side chain atoms by selecting “Actions”, then “Atoms/bonds”, “backbone only” and “full”. Hide the ribbon representation by selecting “Actions”, then “Ribbon” and “hide”.
8. As mentioned in the lecture, different kinds of secondary structure can be distinguished on the basis of their patterns of inter-backbone hydrogen-bonding. Display all potential hydrogen bonds for the peptide by selecting “Tools”, then “Structure analysis” and “FindHBond”. Accept all default parameters and click on “OK” to view the potential hydrogen bonds. Does the hydrogen-bonding follow the alpha helix pattern?
9. Close current session in Chimera. You will now examine the hydrogen-bonding pattern of a small beta sheet. Download ho13ex4.pdb from <http://salilab.org/~nkhuri/Rabat2013/> and open the file in Chimera. Display peptide’s backbone and side chain atoms and hide the ribbon representation. Identify all potential hydrogen bonds. Is this beta sheet parallel or anti-parallel?