**Assignment Submodule 1- Protein Structure**

**Use Pymol software for working on this assignment**

1. Use the pdb file **peptide.pdb** for this problem. Identify the secondary structure of the peptide. What us the secondary structure of the overall peptide? What is the secondary structural element at amino acid residues 87-88-89-90? Identify the hydrogen bonding pattern in the entire molecule. Measure the phi and psi angles at Thr88 and Lys89.

Measure the chi (χ) angle for all side chains in the peptide and report.

Compare the most probable side chain conformation χ angle from the article provided to you. Does the χ angles you have measured fall within the range described in the article?

1. Use **1NWQ.pdb** file for this problem. In the structure of the complex, one end of the two helices interacts with DNA. Describe how is the non-DNA binding part of the helices are stabilized between the two helices. Identify the amino acid residue that is responsible for stabilizing the helices. How are DNA –and protein interact with one another. Identify the amino acids that interact with DNA. What type of non-covalent interaction is observed between DNA-and protein?
2. Use **1o86.pdb** file for this problem. Observe the helices from residues 215-225 and 228 to 261. What is the secondary structure connecting the two helices? Measure the phi and psi values at the secondary structure and report the secondary structure. In the helical structure between 228-261, there is a bend/kink in the structure. Why there is a kink/bend in the helical structure? Is there any end capping at the C-terminal part of the helix. How is the helical structure stabilized?
3. Use **1o86.pd** file for this problem. Display the structure of Lisinopril in the protein showing hydrogen bond and hydrophobic interactions. Describe the hydrophobic interaction that is formed by the protein that stabilizes the structure of the drug. Identify the amino acid residues that form the hydrophobic interactions with Lisinopril.

What is the metal ion present in the protein? How is the metal ion bound to the protein? Identify the amino acid residues that bind to the metal ion.