Assignment 13

Nucleic Acids

(Submit November 15, 2K18)

(NB. While writing the assignment sheet you submit, please do not consult any available published figure. Try to do the assignment on your own)

1. Clearly draw the Lewis structures of the five bases A, T, U, G, C, showing all the lone pairs and the hydrogen atoms. Label each of the structures, indicating the three edges (Watson Crick, Hoogsteen and Sugar) and the hydrogen bond donors and acceptors.

2. Clearly draw the Lewis structures of A:T and G:C base pairs in their Watson Crick:Watson Crick Cis geometry. Indicate the Sugar attachment with a filled circle. Hence label the minor and the major groove edges and label the hydrogen bond donor and acceptor atoms.

3. Use Rasmol, Pymol, VMD or any other molecular visualization software, and familiarize yourselves with the structures of A and B and Z DNA molecules. The pdb files of the molecules are attached.

4. For the following questions, use the coordinates supplied in the attached pdb files.

   a. From each of the A DNA and B DNA structures, choose one A:T and one G:C base pair respectively. In each case, find out their nucleotide number; identify the backbone torsion angles (α, β, γ, δ, ε and ζ); the glycosidic angle (χ) and the sugar pucker (C2′/C3′ and endo/exo). Prepare a table to report the values.

   b. From the Z DNA molecule, choose any four consecutive base pairs and report parameters for each of the nucleotides in a table similar to what you have done for part a. above.