BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI
BIO F417, BIOMOLECULAR MODELING
FIRST SEMESTER 2017 – 2018
MID-SEMESTER EXAM (CLOSED BOOK)
Full marks: 50 DATE: 12.10.17 DURATION: 90 Mins.

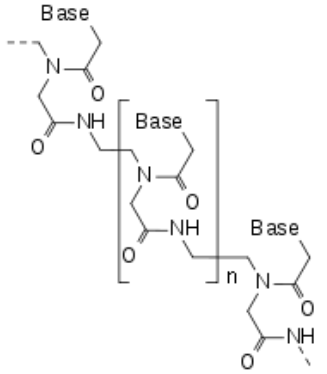
- **Answer to the point**
- **Irrelevant and verbose answer may attract penalty**
- **Steps in each calculation carry marks**

1. Write notes on: **i)** Z-DNA **ii)** γ-turn **iii)** RNA secondary structure **iv)** Levintal's paradox and possible solution **v)** Template selection in Comparative (homology) modeling. **[2X5=10]**

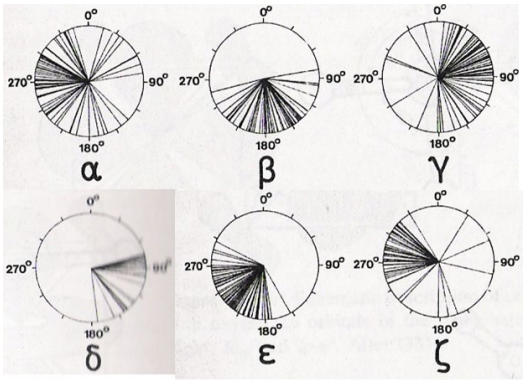
2. a) Show with proper diagram structure of Ala-Ala-Ala-Ala with following combination of phi(ϕ), psi (ψ) and omega (ω) with LLDL configuration of successive alanines. **[5]**
(-,180°, 180°), (0°,180°,180°), (180°,0°,0°), (180°,-,-)

b) Explain the fact that helical structure of collagen is much more stable than α-helix though it contains prolines and glucines. **[2.5]**

c) Peptide nucleic acid (PNA) is artificially synthesized polymer invented by scientists in 1991.The basic structure of PNA is shown in following diagram. Compare all possible stability aspect of PNA/DNA duplex and DNA/DNA duplex (both in vitro and in vivo condition). **[2.5]**



3. a) Justify the following observed torsion angles of standard B-DNA backbone with appropriate Newman projection diagram. [**5**]



b) Justify the fact that among different dinucleotide steps, pyrimidine-purine step is more flexible. **[2.5]**

c) Account all structural changes those lead to transformation of a B-DNA structure to A-DNA. [**2.5**]

4. a) Explain hydrophobic collapse and folding funnel theory of protein folding. What are the major differences of these two theories? **[3]**

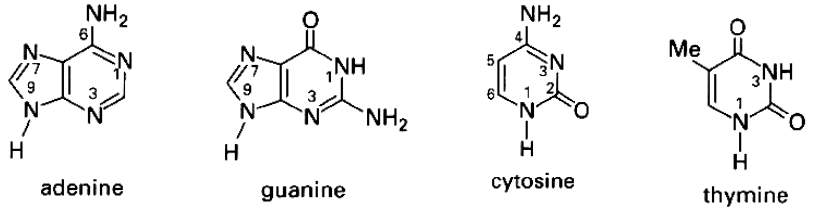
b) What are the major conclusions of Anfinsens's experiments? What is the basis of such conclusions? **[2]**

c) What are the two major steps of comparative modeling? Explain why. **[3]**

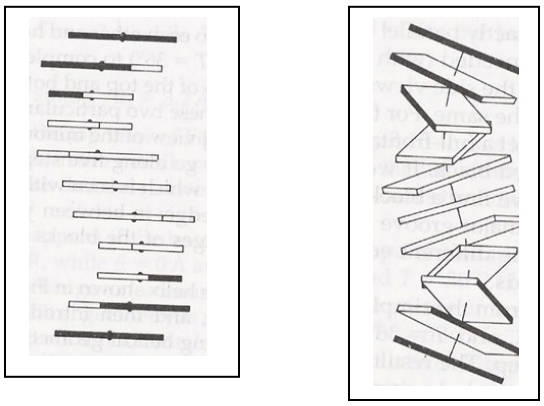
d) Why *ab-initio* technique is less successful in protein structure modeling? **[2]**

5. a) Explain why typical probe radius of 1.4 Å is used to estimate solvent accessible surface area of biomolecules. **[1]**

b) Draw Watson-Crick base pair scheme of GC and AT pair and indicate minor and major groove site. **[3]**



c) The following two diagrams (A and B) represent base pair orientation of DNA double helix. Mention all non-zero basepair, step and helical parameters of each of these arrangements. The base pairs are represented by standard convention. **[2]**



A B

d) What information can be retrieved by the following graphical model of protein? **[2]**

(i) Stick diagram **(ii)** Space-fill diagram **(iii)** Ribbon diagram **(iv)** Wire-frame diagram

e) What would be the common features of proteins that interact with DNA? **[1]**

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