6. (a) What is protein structure validation and refinement? Name and state the principle of any one computational tool used for performing each of these activities.

(b) What do you mean by molecular mechanics? How is it useful in drug design and discovery? How is the ab-initio method different from Monte Carlo methods? (9,9)

[This question paper contains 4 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 1177 **I**

Unique Paper Code : 3183010009

Name of the Paper : Drug Design and Discovery

Name of the Course : **B.Sc. (H) Biomedical Science (NEP-UGCF) : DSE**

Semester : V

Duration : 3 Hours Maximum Marks : 90

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Each question is of **18** Marks.
3. Attempt any **Five** questions in total.
4. Attempt subparts of a question together.

1. (a) Explain the significant features of a peptide bond. What are dihedral angles in a peptide chain?

(b) How is free energy calculated in computational biology for a given biomolecule? How does a local minimum differ from a global minimum?

(c) What desirable properties must a molecule have to be considered a drug? Explain how pharmacological parameters differ from pharmacokinetic parameters? (6,6,6)

2. (a) What is pharmacovigilance, and what role does it play in regulatory approvals during clinical trials?

(b) Describe the key steps in structure based drug design.

(c) What are the main stages in the drug discovery pipeline? List and briefly describe each. (6,6,6)

3. (a) Explain homology modeling method for protein structure prediction. How is it different from the fold recognition method?

(b) Using suitable examples, explain what are molecular descriptors? Describe in detail any one application of molecular descriptor.

(c) What are molecular fingerprints, and how are they used in substructure searching? (6,6,6)

4. (a) What is a conformational search? Describe all the key steps involved in this approach.

(b) What are the main phases of clinical trials, and what is the primary goal of each phase?

(c) Compare and contrast the SCOP and CATH databases in terms of their classification systems for protein structures. What are the advantages of each system? (6,6,6)

5. (a) Write short notes on the following **(Any three)** :

(i) Virtual Screening

(ii) "Proof of Concept" in drug development

(iii) Lipinski's rule of five

(iv) Protein BLAST

(b) Discuss different levels of protein structure with illustration. (9,9)

P.T.O.