(b) De-abbreviate the following and briefly describe them :

  (i) 3D-QSAR

  (ii) PDB

  (iii) ADMET   (6,9)

[This question paper contains 4 printed pages.]

Your Roll No...............

Sr. No. of Question Paper : 2008

Unique Paper Code   : 2174001209

Name of the Paper   : GE: Molecular Modelling, Artificial Intelligence and Machine Learning

Name of the Course   : **B.Sc. (H)/ B.Sc. (Prog.)**

Semester   : II

Duration : 2 Hours   Maximum Marks : 60

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.

2. Attempt **any two** questions each from **Section A** and **Section B.**

3. **All** questions carry equal marks.

4. Answer four questions in all.

Section A

1. Write short notes on any three of the following.

   (i) Density functional calculations

P.T.O.

(ii) Semiempirical calculations

(iii) Force fields

(iv) Scoring function of Molecular Docking   (5×3)

2. (a) What do the torsional and non-bonded energy terms represent in a molecular mechanics force field?

   (b) Draw and discuss the potential energy diagrams of ethane a; a function of torsion angle.

   (c) Define intrinsic reaction coordinate. How will you differentiate between a minimum and a saddle point?   (5×3)

3. (a) What are the advantages of computational chemistry as compared to the conventional experimental chemistry'?

   (b) Molecular mechanics cannot be used to calculate electronic properties like dipole moment. Explain with reason.

   (c) Using the case of a diatomic molecule I-D potential energy surface, derive and show that the first and second derivatives of the energy with respect to the geometric parameters, can be used for geometric optimization.   (5×3)

Section B

4. (a) Define Data Search. Describe various types of Data Search.

   (b) Explain Hill Climbing Algorithm with a suitable example.

   (c) What do you understand by the term Artificial Intelligence (AI)? Discuss various applications of AI in chemistry.   (5×3)

5. (a) What is a lead molecule? Discuss the various steps involved in identification ofa lead molecule.

   (b) What is genetic algorithm? Explain various types of genetic algorithms.

   (c) Give the basis on which you can predict the potency of molecule as an effective drug?
                                                    (5×3)

6. (a) Differentiate between

      (i) Linear and non-linear search

      (ii) Ligand based and structure based drug design