Exam. Code : 206603
Subject Code : 5018

M.Sc. Bio-Informatics 3rd Semester

MOLECULAR MODELING & COMPUTER AIDED DRUG DESIGN

Paper : BI–634

Time Allowed—3 Hours] [Maximum Marks—75

Note :— Attempt any **five** questions, selecting at least **one** question from each Section. The **fifth** question may be attempted from any Section. Each question carries equal marks.

SECTION—A

1. (a) What are the basic principles of molecular mechanics ? Define the term 'force field' by citing suitable examples.

   (b) What is the importance of energy minimization in molecular modeling ? Discuss the Conjugate gradient method of energy minimization and its limitations.

2. (a) Compare Molecular Dynamics and Monte Carlo simulations.

   (b) Define global minima and local energy minima. Discuss the random method of conformational searching.

SECTION—B

3. (a) Classify QSAR descriptors with at least one example.
   (b) Describe Hansch QSAR model and its applications.
4. (a) What is pharmacophore ? Describe various steps involved in pharmacophore mapping.
   (b) What is partial least square analysis ? Describe its advantage over other multi-variate regression method.

SECTION—C

5. Discuss structure, function and pharmacology of GPCR.
6. (a) Write short note on mitotic apparatus as target of drugs.
   (b) Discuss the designing of new anti-viral drugs.

SECTION—D

7. (a) Describe general steps of structure based drug designing.
   (b) Describe various types of docking analysis.
8. (a) How to explore database searching for identifying and optimizing lead molecule.
   (b) Explain role of ADMET prediction and its significance in drug discovery and development.