Exam. Code : 206603
Subject Code : 5148

M.Sc. Bio-Informatics 3rd Semester

MOLECULAR MODELING & COMPUTER AIDED DRUG DESIGN

Paper—BI-634

Time Allowed—3 Hours] [Maximum Marks—75

Note :— Attempt ***six*** questions in all. Section A is compulsory. Attempt any ***five*** questions from Section B i.e. ***one*** question from each unit.

SECTION—A

1. Explain briefly :
   (i) Give specific application of DREIDING force field.
   (ii) What are Sterimol parameters ?
   (iii) What is systematic conformational searching ?
   (iv) Define two statistical measures used to evaluate stepwise multiple regression equation.
   (v) What are allosteric modulators ?
   (vi) Differentiate global energy minima from local energy minima.
   (vii) What is the important structural feature of nitrogen mustard class of anticancer agent ?
   (viii) What is flexible docking ?
   (ix) What is uncompetitive enzyme inhibition ?
   (x) Why the antiviral chemotherapy has evolved very slowly at the start ? Give at least two reasons. 1.5×10

  (Contd.)

SECTION—B

UNIT—I

2. Write notes on :
   (a) Potential Energy Surfaces
   (b) Limitations of Force Field Models. 2×6

3. (a) Name various energy minimization methods. Describe any one method in detail. 6
   (b) Describe applications of energy minimization. 6

UNIT—II

4. Write short notes on :
   (a) Conformational Changes from Molecular Dynamics Simulations. 6
   (b) Monte Carlo Simulations of Rigid Molecules. 6

5. Name various conformational search methods. Discuss systematic methods for exploring conformational space. 12

UNIT—III

6. (a) Describe generation and representation of pharmacophore feature in pharmacophore mapping. 6
   (b) Discuss Enthalpic contributors of drug receptor interactions. 6

7. (a) Describe rules recommended by Unger and Hanch for the selection of QSAR regression model. 5

(b) What are advantages of PLS analysis over conventional multivariate regression analysis ? 4

(c) Describe two critical statistical measures used to select best PLS model. 3

UNIT—IV

8. (a) Discuss the fundamental architecture of ion channels. 6

(b) Write a short note on nuclear receptors. 6

9. (a) What are the various strategies used by enzyme to stabilize transition-state structure ? Give critical account of any one. 6

(b) Give critical account on compounds which inhibit the replication of the Human Immunodeficiency Virus (HIV). 6

UNIT—V

10. Describe common steps involved in drug designing by molecular docking. 12

11. Describe optimization of lead obtained from natural sources using bioinformatics tools. 12