M

Exam. Code : 206603
Subject Code : 4665

M.Sc. Bio-Informatics 3rd Semester

MOLECULAR MODELING & COMPUTER AIDED DRUG DESIGN

Paper—BI–634

Time Allowed—3 Hours] [Maximum Marks—75

Note :— Candidates are to attempt **FIVE** questions, **ONE** from each section. **Fifth** question may be attempted from any section. All questions carry equal marks.

SECTION—A

I. (a) What are the different kinds of internal energies associated with the molecular structure ? 7.5

(b) Name various energy minimization methods. Explain the energy minimization method by conjugate gradient. 7.5

II. (a) What is the principle of molecular dynamics ? Describe its applications. 7.5

(b) Name various method used for conformational analysis. Explain the systematic search method of conformational analysis. 7.5

SECTION—B

III. (a) Describe the various steps involved in the development of Hansch QSAR model. 7.5

(b) Describe various steric descriptors used in 2D QSAR. 7.5

IV. (a) Discuss the conformational analysis in pharmacophore mapping. 7.5

(b) Name various regression methods used in QSAR analysis. Discuss any one in detail. 7.5

SECTION—C

V. Discuss structure, function and pharmacology of an ion channel. 15

VI. (a) Describe reversible and non-reversible enzyme inhibitors. 7.5

(b) Discuss the designing of classical anti-viral drugs. 7.5

SECTION—D

VII. (a) Explain the role of molecular recognition in drug design. 7.5

(b) Compare structure based drug designing and ligand based drug designing. 7.5

VIII. (a) Explain the principles of docking analysis. 7.5

(b) Describe Lipinski's rule of five and its application. 7.5