Exam. Code : 206603
Subject Code : 4622

M.Sc. Bio-Informatics Semester—III
BI–634 : MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGN

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)   Non-bonding drug receptor interactions

    (ii)   Applications of CHARMM force field

    (iii) Internal coordinates of molecules

    (iv) Bioactive conformation

    (v)   Indicator variables used in free Wilson approach

    (vi) Constraint Docking

    (vii) Principal Component Analysis

    (viii) Competitive Enzyme Inhibitors

    (ix) Ligand based virtual screening

    (x)   Eigen value. $10 \times 1.5 = 15$

SECTION—B

UNIT—I

2. (a) Describe various strains of structure of molecules that are considered to calculate potential energy in Force Field. 6

   (b) Briefly describe two graphics visualization systems of modeling graphics workstation. 6

3. Name various algorithms available for energy minimization. Describe any two method in detail. 12

UNIT—II

4. (a) How does solvent effect incorporate into molecular dynamics ? 6

   (b) Discuss Monte Carlo Simulation of flexible molecules. 6

5. (a) Enlist various methods used to explore conformational space. Describe any one in detail. 7

   (b) Briefly describe protein engineering by homology modeling. 5

UNIT—III

6. (a) Explain the role of molecule recognition in Drug Design. 6

   (b) Describe the rules for deriving Hansch QSAR model. 6

7. (a) Give brief account of Multiple Linear Regression analyses recommended for 3D QSAR analysis. 6

 (b) Describe evaluation of pharmacophore models. 6

UNIT—IV

8. (a) Comment on the signal transduction mechanism through GPCR. 6

 (b) Give critical account of active site-directed irreversible inhibitors. 6

9. (a) Give an overview on design of new Antiviral Agents. 6

 (b) Explain role of DNA strand breakers in cancer therapy. 6

UNIT—V

10. Describe general steps of direct drug designing using docking methods. 12

11. (a) Process of drug discovery and development is costly and time consuming. Justify. 6

 (b) How does CADD technique accelerate the process of Drug Discovery ? Justify by citing one successful story. 6