(i) Printed Pages : 2 Roll No. .....

(ii) Questions : 7 Sub. Code : 1014

Exam. Code : 0043

B.Sc. (Hons.) Bioinformatics 5th Semester

(2122)

MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGN

Paper : BIN-5005

Time Allowed : Three Hours] [Maximum Marks : 60

Note :— Attempt **five** questions in all by selecting **two** questions from each Unit & the first compulsory question.

1. Compulsory Question

   (i) Define Chemo-informatics and give its scope.

   (ii) Briefly explain the concept of potential energy surface.

   (iii) State Lipinski Rule of Five.

   (iv) Differentiate between structure based and ligand based drug design. 4×3=12

UNIT—I

2. (a) What is energy minimization and its importance ? Give any 1 energy minimization method. 6

(b) Write a note on molecular docking & scoring. 6

3. (a) Explain the concept of force fields. 8

(b) Differentiate between quantum mechanics & molecular mechanics. 4

4. (a) What is molecular dynamics simulations and its applications. 8

(b) Briefly explain coordinate system in molecular modeling. 4

UNIT—II

5. (a) Discuss basic concept of ADME and its importance. 6

(b) Discuss protein-ligand interactions in terms of computer aided drug design. 6

6. (a) Discuss virtual drug screening process and its importance. 8

(b) Write a note on the time-lines of drug discovery process from bench to bedside. 4

7. (a) Explain concept of 1D, 2D & 3D molecular descriptors. 8

(b) Give the basic principle and applications of QSAR. 4