

2125

B.Sc. (Hons.) Bio-Informatics

Fifth Semester

BIN-5005: Molecular Modeling and Computer Aided Drug Design

Time allowed: 3 Hours

Max. Marks: 60

NOTE: Attempt five questions in all, including Question No. 1 which is compulsory and selecting two questions from each Unit.

x-x-x

I. Answer the following:-

- a) Distinguish between local and global minima.
- b) What is the importance of 1D, 2D & 3D chemical structure representations?
- c) Briefly explain non-bounded interactions.
- d) What are molecular descriptors?
- e) State Lipinski's rule of five.
- f) Briefly explain high throughput screening. (6x2)

UNIT - I

- II. a) Write a note on SMILES and SDF format.
b) Discuss any one energy minimization methods. (2x6)
- III. a) What are the force fields and their importance?
b) Discuss the concept of potential energy surface. (2x6)
- IV. a) Discuss molecular dynamics simulation and its applications.
b) What is the role of chemoinformatics in pharmaceutical research. (8,4)

UNIT - II

- V. a) Discuss computer aided drug design and its applications.
b) Give an overview of concept of therapeutic drug targets. (8,4)
- VI. a) How do 3D and 2D QSAR differ?
b) Discuss virtual screening and its applications. (2x6)
- VII. a) Give an overview of drug development process.
b) Write a note on chemical databases. (2x6)

x-x-x