Exam. Code: 0043
Sub. Code: 18013

2124

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. I which is compulsory and selecting two questions from each Unit.*

x-x-x

I. Answer the following:-

a) What is the scope of chemoinformatics?

b) Differentiate between flobal and local minima.

c) What is torisional potential?

d) What is the importance of active site in structure based drug design?

e) Give the full form of ADMET.

f) Name any two chemical databases. (6x2)

UNIT - I

II. a) Discuss molecular dynamics simulation and its applications.
b) Explain concept of potential energy surface. (8,4)

III. Write notes on the following:-
a) Chemical structure representations
b) SMILES
c) Molecular graphics (3x4)

IV. a) Discuss the concept of molecular mechanics and give its applications.
b) Briefly explain molecular docking and scoring. (8,4)

UNIT - II

V. a) State Lipinski's rule of five.
b) Differentiate between structure and ligand-based drug design. (2x6)

VI. a) Discuss basic principle of QSAR.
b) What is high throughput screening? (8,4)

VII. Write note on the following:-
a) Virtual screening
b) 2-D and 3-D molecular descriptors (2x6)

x-x-x