Exam.Code:0043
Sub. Code: 1014

1127

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 atleast two questions from each Unit.*

x-x-x

I. Answer briefly:

a) SMILES

b) Pharmacoinformatics

c) 2D chemical structure representation

d) Energy minimization

e) Molecular Mechanics

f) Hits and Leads

g) Molecular descriptors

h) Active site of protein (8x1½)

UNIT – I

II. Elaborate on the Aim, Scope and Role of Chemoinformatics in pharmaceutical and chemical research. (12)

III. a) Explain the Coordinate systems and concept of potential energy surface.
b) Write a note on Molecular docking and Scoring. (2x6)

IV. Write notes on:
a) Angle bending
b) Bond Stretching
c) Non-bonded interactions (12)

UNIT – II

V. a) Explain the drug development process.
b) Describe the process of High Throughput Screening. (2x6)

VI. a) Explain the Lipinski's Rule of Five in the context of drug screening.
b) What are the basic principles and applications of QSAR? (2x6)

VII. Differentiate between Structure based and ligand based drug designing. (12)

x-x-x