Exam.Code:0043
Sub. Code: 1014

1128

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 briefly:-

a) MOL

b) Molecular Graphics

c) Molecular Docking

d) Ligand

e) Non-bonded interactions

f) Active-site

g) Molecular descriptors

h) Angle bending (8x1½)

UNIT – I

II. a) Define Molecular Mechanics. Explain the factors contributing to the same.

b) Describe the different types of structure representations using ChemSketch. (8,4)

III. Explain Molecular Dynamics Simulation and its applications. (12)

IV. a) Write short notes on:

i) SMILES ii) SDF

b) Define Energy Minimization. Explain Local and Global Energy Minima. (6,6)

UNIT – II

V. Give an overview of the Drug development process with special emphasis on Structure Based Drug Design. (12)

VI. a) Explain ADME with reference to drug handling by the body.

b) Discuss the Lipinski's rule of five. (6,6)

P.T.O.