2123
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 importance of computer aided drug design?

    b) Give application of chemsketch.

    c) Briefly explain coordinate system.

    d) Give full form of ADMET.

    e) Differentiate between structure and ligand based drug design.

    f) Name any two 2-D molecular descriptors.   (6x2)

UNIT - I

II.   a) Differentiate between global and local minima.

    b) Write a note on molecular docking and scoring.   (2x6)

III. a) Discuss concept of potential energy surface.

    b) What are the applications of molecular dynamics simulations?   (8,4)

IV.   a) Discuss molecular mechanism and force fields.

    b) Explain SMILES giving suitable example.   (10,2)

UNIT - II

V.   a) Write a note on virtual screening process and applications.

    b) State Lipinski's Rule of Five.   (8,4)

VI. a) What is high throughput screening?

b) Write a note on chemical databases and their applications.   (2x6)

VII. a) Give basic principle and applications of QSAR.

b) Explain concept of therapeutic drug targets.   (8,4)

x-x-x