2012
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 Z-factor in HTS?

   b) Write any one common drug in SMILES format?

   c) Explain non-bonded interactions giving suitable examples.

   d) What is the importance of PubChem?

   e) Briefly explain 2D molecular descriptors?

   f) What are the applications of Cheminformatics?   (6x2)

UNIT - I

II.   a) Explain molecular mechanics force field and various bonded and non-bonded terms associated with it.

      b) How are chemical structures represented?   (10,2)

III. Write notes on the following

      a) Potential Energy surface

      b) Concept of Co-ordinate system

      c) Molecular graphics   (3x4)

IV.   a) Discuss Steepest and Conjugate gradient methods of energy minimization.

      b) Briefly explain molecular docking scores and their importance.   (8,4)

UNIT - II

V.   Write notes on the following:-

      a) Virtual Screening

      b) Concept of ADME   (2x6)

P.T.O.

VI.   a) Give the overview of drug development process?

        b) Explain the approaches used in Active Site Prediction?   (8,4)

VII.   a) Discuss protein-ligand interactions and various molecular forces stabilizing ligand binding.

        b) Compare and contrast COMFA and COMSIA   (8,4)

x-x-x