2053
M.Sc. (Bio-Informatics) Fourth Semester
MBIN-8018: Molecular Modeling and Pharmacoinformatics

Time allowed: 3 Hours

Max. Marks: 60

NOTE: *Attempt* <u>*five*</u> *questions in all, including Question No. I which is compulsory and selecting atleast one question from each Unit.*

x-x-x

I. Attempt the following:-

   a) Define model.

   b) Define empirical force fields.

   c) Explain active site of protein.

   d) Define 3D conformations.

   e) Define clogP.

   f) Discuss Fingerprints.

   g) What is similarity coefficient?

   h) Discuss small molecules   (8x1½)

UNIT - I

II.   a) What are coordinate systems and its applications?

     b) Write a note on molecular surfaces.   (6,6)

III. a) Discuss role of molecular minimization & its application.

     b) What are molecular surface and its significances?   (6,6)

UNIT - II

IV. a) What are the different methods for target identification?

     b) Differentiate between scoring and docking.   (6,6)

V.   a) What is the importance of molecular descriptor in QSAR?

     b) Discuss process scoring and lead optimization.   (6,6)

UNIT - III

VI. a) Discuss Pharmacogenomics & its applications.   (6,6)

     b) Write a note on future of drug therapy.

VII. a) What are molecular descriptor & name three descriptors?

     b) Discuss Pubchem *vs* eMolecules.   (6,6)

x-x-x