Exam. Code: 0442
Sub. Code: 25971

2056

M.Sc. (Bio-Informatics) Fourth Semester

MBIN-8018: Molecular Modeling and Pharmacoinformatics

Time allowed: 3 Hours | Max. Marks: 60

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

x-x-x

1. Answer briefly:
   a) QSAR
   b) Lead optimization
   c) PubChem
   d) Similarity
   e) Individualized therapy
   f) Fingerprints (6x2)

UNIT - I

2. a) Explain empirical potential energy functions used in molecular mechanics.
   b) Describe molecular surfaces and types such as van der Waals and solvent-accessible surfaces. (2x6)
3. a) Discuss different force field methods used in molecular mechanics.
   b) Explain energy minimization methods and their role in conformational analysis. (2x6)

UNIT - II

4. a) Explain the principles of rational drug design with suitable examples.
   b) Discuss high-throughput screening and its advantages and limitations. (2x6)
5. a) Explain the concepts of similarity and complementarity in drug design.
   b) Elaborate on the development of HANSCH QSAR equation. (2x6)

UNIT - III

6. a) Discuss molecular descriptors and fingerprints in cheminformatics.
   b) Describe ADME in drug development. (2x6)
7. a) Discuss gene-drug interactions and their importance in personalized medicine.
   b) Explain the role of genomics in drug target identification and disease diagnosis. (2x6)

x-x-x