Printed Pages : 2

EBT-041

(Following Paper ID and Roll No. to be filled in your Answer Book)

PAPER ID : 154753

Roll No.

B. Tech.

(SEM. VII) (ODD SEM.) THEORY EXAMINATION, 2014-15

MOLECULAR MODELING AND DRUG DESIGN

Time : 3 Hours] [Total Marks : 100

Note: Attempt all questions.

1. Attempt any two parts. 10x2=20
   (a) What do you mean by molecular modeling? Explain in detail.
   (b) Discuss the postulates of quantum mechanics.
   (c) Enumerate the drawbacks of mechanical models as compared to graphical models.

2. Attempt any two parts. 10x2=20
   (a) What do you understand by protein folding? Discuss the process of protein folding.
   (b) Discuss the Electrostatic interaction and Van der Waals interactions.
   (c) Write short notes on the following
      (i) Conformational searching
      (ii) Molecular dynamics

3. Attempt any two parts. **10x2=20**

(a) What do you understand by homology modeling? Discuss the homology modeling of proteins.

(b) How Ramachanran plot is used for validation of protein models? Explain.

(c) Discuss the ab initio method for computational modeling of proteins.

4. Attempt any four parts **5x4=20**

(a) What do you mean by linear and non linear QSAR model?

(b) What is drug discovery? Explain the various steps of drug design.

(c) What are artificial neural networks? Explain its application in QSAR.

(d) Write short notes on genetic algorithm.

(e) What are descriptors in QSAR? Explain.

5. Attempt any two parts **10x2=20**

(a) What do you mean by virtual screening? Explain in detail.

(b) What is molecular docking? Discuss the protein-ligand docking with suitable example.

(c) Write short notes on the following

(i) Combinatorial libraries

(ii) ADME properties of lead.