Printed pages: 02 Sub Code: NBT 013

Paper Id: 154623 Roll No: [redacted]

B TECH

(SEM VI) THEORY EXAMINATION 2017-18

MOLECULAR MODELLING AND DRUG DESIGNING

Time: 3 Hours *Total Marks: 100*

Note: Attempt all Sections. If require any missing data; then choose suitably.

SECTION A

1. Attempt *all* questions in brief. **2 x10 = 20**

(a) Note down the numerous applications of protein folding.

(b) What do you mean by molecular modeling?

(c) How Ramachandran plot is used for validation of protein models?

(d) What is conformational searching?

(e) Explain the ADME properties of lead.

(f) Give some molecular orbital theories with examples.

(g) Define combination libraries.

(h) What is free energy & salvation?

(i) Discuss the postulates of quantum mechanics.

(j) What are electrostatic interactions?

SECTION B

2. Attempt any *three* of the following: **10 x 3 = 30**

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

(b) What is drug designing? Explain the various steps involved in this process?

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

(d) What are artificial neural network? Explain its applications.

(e) What do you mean by virtual screening? Why it is important?

SECTION C

3. Attempt any *one* part of the following: **10 x 1=10**

(a) What is molecular docking? Discuss the protein – ligand docking with example.

(b) Draw a setup of MD simulation system. Also explain molecular similarity and similarity searching.

4. Attempt any *one* part of the following: **10 x 1=10**

(a) Give an overview of different strategies used for the search of new potential drug.

(b) What are pharmacophores? Explain antihistamine 3D pharmacophore with a suitable diagram.

5. Attempt any *one* part of the following: 10 x 1=10

(a) Keeping in mind the mechanics of molecular modeling, show the number of force field involved in the process of modeling with the use of its various parameters for force field calculation.

(b) Database searching is attractive way to discover new compound. Prove this statement with the structure based de-novo Ligand design**.**

6. Attempt any *one* part of the following: 10 x 1=10

(a) What is the minimal input for molecular modeling process?

(b) Show the structure based design of templates for zeolite synthesis.

7. Attempt any *one* part of the following: 10 x 1=10

(a) How QSAR relates numerical properties of molecular structure to its activity?

(b) What are molecular descriptors? Explain the Jack knifing process in detail.