Printed Pages: 4 **NBT-013**

(Following Paper ID and Roll No. to be filled in your Answer Books)	
Paper ID :154663	**Roll No.**

B.TECH.

Theory Examination (Semester-VI) 2015-16

MOLECULAR MODELING & DRUG DESIGN

Time : 3 Hours ***Max. Marks : 100***

Section-A

Q1. Attempt all sections. All sections carry equal marks. Write answer of each section in short. (10×2=20)

(a) Compare the drawbacks of mechanical models with graphical models.

(b) Using examples of simple models introduce the term Molecular dynamics.

(c) Note down the numerous applications to protein folding.

(d) What are linear and non-linear modeled equations?

(e) Give some molecular orbital theories with suitable examples.

(f) Describe Ramchandran plot with diagram.

(g) What is Molecular Modeling and molecular modeling by homology? What is it good for?

(h) Incorporate additional features into 3-D pharmacophore.

(i) Define the following

(i) Free energy and salvation.

(ii) Combinational libraries.

(j) Draw a simple setup of a MD Simulation model.

Section-B

Q2. Attempt any five questions from this section. **(5×10=50)**

(a) (i) What are the Minimal Input for Molecular Modeling process.

(ii) Methodology opted for accurate mass measurement of small molecules (*ab-initio* method).

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

(c) Give an overview of the different strategies used for the search of new potential drugs.

(d) (i) What are pharmacophores. Show' with the help of diagram the antihistamine 3D pharmacophore.

(ii) Elucidate the steps involved in the optimization and validation of protein models.

(e) How Quantitative-structure Activity Relationships (QSAR) relates numerical properties of the molecular structure to its activity.

(f) Database "searching is an attractive way to discover new compounds." Prove this statement with the structure-based D*e-novo* ligand design.

(g) Derive some postulates of quantum mechanics.

(h) Define the following terms:-

(i) Molecular similarity and Similarity searching.

(ii) Molecular descriptors.

Section-C

Attempt any two questions from this section. (2×15=30)

Q3. (a) What does Molecular docking mean and also score functions for molecular docking.

(b) Applications of 3-d based searching and docking.

Q4. Questions in this segment are related to QSAR, therefore answer as per following:-

(a) How selecting of compounds for QSAR Analysis is done?

(b) Derive the QSAR equation.

(c) Interpreting a QSAR equation.

(d) Jack knifing process involved

Q5. Keeping in mind the mechanisms of molecular modeling show the number of force field involved in the process of modeling with use of its various parameters for force field calculations.