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	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

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Section-A

- Q1. Attempt all sections. All sections carry equal marks.Write answer of each section in short. $(10 \times 2=20)$
 - (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?



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- om Give some molecular orbital theories with suitable (e) examples.
- (f) Describe Ramchandran plot with diagram.
- What is Molecular Modeling and molecular model-(g) ing by homology? What is it good for?
- into 3-D Ranker additional features Incorporate (h) pharmacophore.
- (i) Define the following
 - Free energy and salvation. (i)
 - (ii) Combinational libraries.
- (i) Draw a simple setup of a MD Simulation model.

Section-B

Q2. Attempt any five questions from this section.

 $(5 \times 10 = 50)$

- What are the Minimal Input for Molecular Mod-(a) (i) eling process.
 - (ii) Methodology opted for accurate mass measurement of small molecules (ab-initio method).



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- (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.
- 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 De-novo ligand design.
- (g) Derive some postulates of quantum mechanics.
- (h) Define the following terms:-
 - (i) Molecular similarity and Similarity searching.
 - (ii) Molecular descriptors.

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Attempt any two questions from this section. $(2 \times 15 = 30)$

- 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.