Seat No.: _____ Enrolment No._____

GUJARAT TECHNOLOGICAL UNIVERSITY

B. Pharm. – SEMESTER – VIII • EXAMINATION – WINTER • 2016

Subject Code: 2280006 Date: 02-12-2016

Subject Name: Computer Applications in Drug Discovery

Time: 02:30 pm - 05:30 pm Total Marks: 80

Instructions:

1. **Attempt any five questions.**
2. **Make suitable assumptions wherever necessary.**
3. **Figures to the right indicate full marks.**

Q.1	**(a)**	Write a note on drug discovery process. Give importance of drug design.	**06**
	(b)	Write down Predication of ADME in details.	**05**
	(c)	Explain about genetic algorithms in SBDD.	**05**
Q.2	**(a)**	What are the different approaches for new drug discovery? Discuss in brief about each.	**06**
	(b)	What is docking? Describe various docking methods.	**05**
	(c)	Write in detail about COMFA and COMSIA methods of QSAR.	**05**
Q.3	**(a)**	Explain about QSAR. Discuss various QSAR parameters.	**06**
	(b)	Write down steps in Comparative Modeling.	**05**
	(c)	Write down applications of Molecular Dynamics simulations in drug design.	**05**
Q.4	**(a)**	Write a note on Structure-Based Virtual High-Throughput Screening.	**06**
	(b)	Write about Binary molecular fingerprints.	**05**
	(c)	Discuss about Knowledge based Scoring method.	**05**
Q.5	**(a)**	Define Pharmacophore modeling. Write advances, limitations and current application in drug discovery.	**06**
	(b)	Describe about the target data bases for computer-aided drug design in details.	**05**
	(c)	Explain about 3D Description of molecular configuration and conformation.	**05**
Q. 6	**(a)**	Write a note on Pharmacophore mapping.	**06**
	(b)	How to select optimum features in ligand based computer aided drug design?	**05**
	(c)	What do you mean by force field? Describe various methods for energy minimization.	**05**
Q.7	**(a)**	Discuss on Toxicity Prediction Software Packages and Algorithms.	**06**
	(b)	Write a note on Ligand databases for Computer-Aided drug design.	**05**
	(c)	How target structure is derived? How can we determine binding site in the target?	**05**

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