Seat No.: _____ Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY

B. Pharm. - SEMESTER–8 • EXAMINATION – SUMMER -2018

Subject Code: 2280006 Date: 09/05/2018

Subject Name: Computer Applications in drug discovery

Time: 10:30 AM TO 01:30 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)**	What do you mean by force field? Describe various methods for energy minimization.	**06**
	(b)	What is compound library filters? Explain it.	**05**
	(c)	Discuss potentials of in silico toxicology.	**05**
Q.2	**(a)**	Write a note on Pharmacophore mapping	**06**
	(b)	Discuss about Consensus – scoring function.	**05**
	(c)	Explain in detail molecular dynamics – based detection in SBDD.	**05**
Q.3	**(a)**	Describe multi target inhibitors using common pharmacophore models.	**06**
	(b)	Write a note on high resolution docking.	**05**
	(c)	Discuss about Monte Carlo Search with metropolis criterion.	**05**
Q.4	**(a)**	Write a note on drug discovery process. Give importance of drug design.	**06**
	(b)	Write in detail about COMFA and COMSIA Methods of QSAR.	**05**
	(c)	Write a note on ligand databases for CADD.	**05**
Q.5	**(a)**	Enlist methods to identify protein binding sites and explain any one in detail.	**06**
	(b)	Write a short note on multidimensional QSAR in drug discovery.	**05**
	(c)	Explain in brief linear regression method in QSAR models.	**05**
Q. 6	**(a)**	Explain in detail 3D description of molecular configuration and conformation in ligand based CADD.	**06**
	(b)	Write a note on InChIKey- the IUPAC International Chemical Identifier.	**05**
	(c)	Explain role of octanol / water partition coefficient and polarizability as a molecular descriptors in ligand based CADD	**05**
Q.7	**(a)**	What is pharmacophore? Explain in brief molecular superimposition in pharmacophore mapping.	**06**
	(b)	Write a note on Receptor – dependent 3D/4D QSAR.	**05**
	(c)	Discuss about Knowledge based scoring function.	**05**

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