Seat No.: _____ Enrolment No._____

GUJARAT TECHNOLOGICAL UNIVERSITY

B.PHARM – SEMESTER – 8- EXAMINATION –WINTER - 2018

Subject Code: 2280006 **Date: 28/11/2018**

Subject Name: Computer Applications in drug discovery

Time: 02:30 PM TO 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)**	Define ligand based CADD. Enumerate its features and explain binary molecular fingerprints in detail.	**06**
	(b)	Write a note on dynamic pharmacophore model.	**05**
	(c)	What are docking? Describe various docking methods.	**05**
Q.2	**(a)**	Explain how comparative modeling method used for preparation of a target structure for SBDD.	**06**
	(b)	Write a note on knowledge based scoring function and consensus scoring function.	**05**
	(c)	Explain genetic algorithms in SBDD	**05**
Q.3	**(a)**	Write a note on multidimensional QSAR.	**06**
	(b)	Discuss on Toxicity Prediction software packages.	**05**
	(c)	Define force field and describe various methods for energy minimization.	**05**
Q.4	**(a)**	Describe application of QSAR in lingand based CADD.	**06**
	(b)	Write in detail about COMFA and COMSIA methods of QSAR.	**05**
	(c)	Explain about linear regression methods.	**05**
Q.5	**(a)**	Write a note on pharmacophore algorithms and software packages.	**06**
	(b)	Explain how ligand libraries were prepared for CADD?	**05**
	(c)	Describe about the target data bases for computer aided drug design in detail.	**05**
Q. 6	**(a)**	Enumerate different approaches for binding site detection and characterization in SBDD and explain any one in detail.	**06**
	(b)	Write down prediction of ADME in detail.	**05**
	(c)	Explain about 3D description of molecular configuration and conformation.	**05**
Q.7	**(a)**	Explain in detail about SBVS.	**06**
	(b)	Write a note on high resolution docking.	**05**
	(c)	Write a note on importance of various drug design approaches in drug discovery.	**05**

****