Seat No.: _____ Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY

B.PHARM - SEMESTER–VIII • EXAMINATION – SUMMER-2017

Subject Code: 2280006 Date: 09/05/2017

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)**	Write a brief note on importance of drug design approaches in drug discovery.	**06**
	(b)	Explain in brief pharmacophore model based on virtual screening.	**05**
	(c)	Write a short note on multi target inhibitors using pharmacophore model.	**05**
Q.2	**(a)**	Explain in details high resolution protein docking.	**06**
	(b)	Give a brief account of dynamic pharmacophore models.	**05**
	(c)	What is structure based virtual high throughput screening?	**05**
Q.3	**(a)**	Write a short note on genetic algorithms in protein legand docking.	**06**
	(b)	Enumerate scoring functions for evaluation of protein ligand complexes. Explain any one in details.	**05**
	(c)	Explain in details representation of small molecules as “SMILES” in ligand databases for CADD.	**05**
Q.4	**(a)**	Enlist methods to identify protein binding sites and explain any one in detail.	**06**
	(b)	Write a short note on comparative modeling in structure based CADD.	**05**
	(c)	Write a short note on protein-ligand docking in drug design.	**05**
Q.5	**(a)**	Explain in detail 2D description of molecular constitution as molecular descriptor in ligand based CADD.	**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)**	What is pharamacophore? Explain in brief molecular superimposition in pharmacophore mapping.	**06**
	(b)	Explain in brief binary molecular fingerprints as molecular descriptors in ligand based CADD.	**05**
	(c)	Explain in detail pocket matching in structure based CADD.	**05**
Q.7	**(a)**	Explain in brief human ether-a-go-go related gene potassium channel inhibition.	**06**
	(b)	What is toxicity prediction software package? Explain it.	**05**
	(c)	What is compound library filters? Explain it.	**05**

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