Seat No.: _____ Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY

M.PHARM - SEMESTER–2 EXAMINATION – SUMMER-2019

Subject Code: MPC203T Date: 31/05/2019

Subject Name: Computer Aided Drug Design

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)**	Describe history and applications of CADD.	**06**
	(b)	Give brief introduction to QSAR. Enumerate various physicochemical parameters used in QSAR.	**05**
	(c)	Write about determination of lipophilicity parameters.	**05**
Q.2	**(a)**	Write applications, advantages and disadvantages of Free Wilson analysis.	**06**
	(b)	Explain how QSAR equations are derived? What are the importance of this equations?	**05**
	(c)	What is 3D-QSAR? Write in brief about contour map analysis.	**05**
Q.3	**(a)**	Make a note on various statistical methods used in QSAR analysis.	**06**
	(b)	Discuss electronic parameters used in QSAR.	**05**
	(c)	Describe different energy minimization methods for conformations.	**05**
Q.4	**(a)**	Explain the role of quantum mechanics in drug design.	**06**
	(b)	Define molecular docking. Describe in brief various types of docking.	**05**
	(c)	Explain molecular docking by taking DHFR and cholinesterase enzymes.	**05**
Q.5	**(a)**	Which parameters of drug-receptor interaction are to be analysed in de novo drug design?	**06**
	(b)	Describe the importance of ADMET properties of new molecules in drug design.	**05**
	(c)	Explain how new drugs are discovered based on receptors / enzymes.	**05**
Q. 6	**(a)**	Write a short note on fragment based drug discovery.	**06**
	(b)	What is homology modelling? What are the uses of this technique?	**05**
	(c)	Explain about pharmacophore mapping.	**05**
Q.7	**(a)**	Write a note on pharmacophore modelling.	**06**
	(b)	What is in silico drug design? How drugs are designed based on pharmacophore.	**05**
	(c)	Write about various virtual screening techniques.	**05**

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