Seat No./Enrollment No.: _____

GUJARAT TECHNOLOGICAL UNIVERSITY
BACHELOR OF ENGINEERING – SEMESTER 6 – EXAMINATION – SUMMER 2026

Subject Code: 3160415 **Date: 29/05/2026**

Subject Name: Rational Drug Design

Time: 10:30 AM TO 01:00 PM **Total Marks: 70**

Instructions:

1. **Attempt all questions.**
2. **Make suitable assumptions wherever necessary.**
3. **Figures to the right indicate full marks.**
4. **Simple and non-programmable scientific calculators are allowed.**

Q.1	**(a)**	Define drug discovery process.	**03**
	(b)	Explain the role of bioinformatics in drug design.	**04**
	(c)	Discuss structure-based and ligand-based drug design approaches with examples.	**07**
Q.2	**(a)**	Define molecular mechanics.	**03**
	(b)	Explain components of molecular mechanics energy function.	**04**
	(c)	Explain hydrogen bonding and van der Waals interactions in drug–receptor binding.	**07**
		OR	
Q.2	**(c)**	Describe application of energy minimization in drug discovery.	**07**
Q.3	**(a)**	Define molecular dynamics.	**03**
	(b)	Explain importance of solvent effects in MD simulations.	**04**
	(c)	Describe conformational changes studied using MD simulation.	**07**
		OR	
Q.3	**(a)**	Explain constant temperature and pressure simulations.	**03**
	(b)	What are time-dependent properties measured in MD?	**04**
	(c)	Discuss application of MD in drug discovery.	**07**
Q.4	**(a)**	Define molecular docking.	**03**
	(b)	Explain types of molecular docking.	**04**
	(c)	Describe virtual screening workflow.	**07**
		OR	
Q.4	**(a)**	Define combinatorial chemistry.	**03**
	(b)	What is drug likeness?	**04**
	(c)	Explain ADMET property prediction.	**07**
Q.5	**(a)**	Define pharmacophore.	**03**
	(b)	List descriptors used in QSAR.	**04**
	(c)	Explain QSAR methodology.	**07**
		OR	
Q.5	**(a)**	Define QSPR.	**03**

(b) Explain role of neural networks in QSAR. **04**

(c) Describe pharmacophore-based virtual screening. **07**

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