Enrollment No./Seat No.:

GUJARAT TECHNOLOGICAL UNIVERSITY

Bachelor of Engineering - SEMESTER - VI EXAMINATION - SUMMER 2025

Subject Code: 3160415 **Date: 28-05-2025**

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.

			Marks
Q.1	**(a)**	Write a short note on the methodology of QSAR studies	**03**
	(b)	What are the key features of molecular mechanics force fields?	**04**
	(c)	Write in detail about discovery of Perampanel starting from competitive inhibitor designing upto clinical phase trials. (Each step in brief)	**07**
Q.2	**(a)**	Give Applications of Molecular Dynamics	**03**
	(b)	Differentiate between the perspectives: Statistical mechanics and Molecular dynamics (In the difference table format only)	**04**
	(c)	Explain about Solvent effects in Molecular Dynamics and give detailed note on Implicit Solvent Models.	**07**
		OR	
	(c)	Write in detail about Molecular Dynamics at Constant Pressure and temperature, and approaches to understand molecular dynamics in the given condition.	**07**
Q.3	**(a)**	What is meant by drug-likeness?	**03**
	(b)	Briefly describe the use of genetic algorithms in developing QSAR equations.	**04**
	(c)	What is the workflow of virtual screening? Highlight the applications of 3D database searching in this process.	**07**
		OR	
	(a)	What is the significance of lead optimization in drug discovery?	**03**
	(b)	How are neural networks applied in QSAR studies?	**04**
	(c)	Explain the importance of drug-likeness, compound filtering, and ADMET prediction in successful drug development.	**07**
Q.4	**(a)**	What is the role of bioinformatics in drug design?	**03**
	(b)	Briefly describe the main steps involved in the drug discovery process (Draw only flowchart)	**04**
	(c)	Give a detailed note about rational drug design and high throughput screening as methods of drug designing approaches. Highlight key applications of both approaches along with example.	**07**

OR

	(a)	Explain: protein modelling.	**03**
	(b)	How does bioinformatics assist in modelling target-small molecule interactions?	**04**
	(c)	Compare and contrast Structure-Based Drug Design (SBDD) and Ligand-Based Drug Design (LBDD) with suitable examples.	**07**
Q.5	**(a)**	Give a short-note on the pharmacokinetic properties of Perampanel- an anti-epileptic drug	**03**
	(b)	Differentiate between electrostatic interactions and van der Waals interactions in molecular mechanics.	**04**
	(c)	Explain the strategy for target identification and validation in drug discovery. State how you identify and validate a particular target using different methods.	**07**

OR

	(a)	Give a short-note on the clinical trials of Perampanel- an anti-epileptic drug	**03**
	(b)	Explain the concept of energy minimization and its application in molecular modelling.	**04**
	(c)	Explain the strategy for Modeling of Target-Small Molecule Interactions along with the methods and applications in detail.	**07**

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