Seat No.: _____ Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY

B.Pharm - SEMESTER– VIII • EXAMINATION – SUMMER -2026

Subject Code: BP807TT Date: 05/05/2026

Subject Name: Computer Aided Drug Design

Time: 10:30AM TO 01:30PM 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 in detail about different stages of drug discovery.	**06**
	(b)	How lead can be discovered based on drug metabolism? Write about it.	**05**
	(c)	What is QSAR? Write a note on QSAR parameters.	**05**
Q.2	**(a)**	Define the term: Bioisosterism. Classify the bioisosters.	**06**
	(b)	Discuss about Hansch analysis in QSAR.	**05**
	(c)	Explain: SAR vs QSAR.	**05**
Q.3	**(a)**	What do you mean by pharmacophore? Explain in detail about pharmacophore based screening.	**06**
	(b)	Write a note on docking with suitable examples.	**05**
	(c)	Write a note on de novo drug design.	**05**
Q.4	**(a)**	Define and explain in brief about direct and indirect molecular modeling.	**06**
	(b)	Write a note on Random and non-random screening.	**05**
	(c)	Make a detailed note on Free Wilson analysis.	**05**
Q.5	**(a)**	Write about COMFA and COMSIA methods of 3D-QSAR.	**06**
	(b)	Discuss Hammett's Substituent constant and Taft's steric constant and give their importance.	**05**
	(c)	Explain the concept of molecular mechanics in drug design.	**05**
Q. 6	**(a)**	Write a note on Chemoinformatics.	**06**
	(b)	Define Bioinformatics. Mentioned applications of bioinformatics.	**05**
	(c)	Discuss in details about ADME databases.	**05**
Q.7	**(a)**	What do you mean by docking? Explain in detail about rigid docking.	**06**
	(b)	Write about global conformational minima determination.	**05**
	(c)	Define drug likeness. Discuss about virtual screening of drug likeness.	**05**

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