Seat No.: _____ Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY

B. Ph. – SEMESTER 8 – EXAMINATION – WINTER -2024

Subject Code: 2280006 Date: 02/12/2024

Subject Name: Computer Applications in drug discovery

Time: 02:30PM to 05:30PM 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)**	Explain drug discovery process. Write the importance of drug design.	**06**
	(b)	Write a note on binary molecular fingerprints.	**05**
	(c)	Explain in brief representation of small molecules as “SMILES” and “InChIKey” in ligand databases for CADD.	**05**
Q.2	**(a)**	Write the stepwise procedure of Comparative Modeling.	**06**
	(b)	Write a note on Energy-based approaches used for Binding Site Detection and Characterization.	**05**
	(c)	Explain Monte Carlo Search with Metropolis Criterion.	**05**
Q.3	**(a)**	What is docking? Enumerate various docking methods and explain one in detail.	**06**
	(b)	Discuss the applications of Molecular Dynamics simulations in drug design.	**05**
	(c)	Explain dynamic pharmacophore model with its importance.	**05**
Q.4	**(a)**	Write a note on Structure-Based Virtual High-Throughput Screening.	**06**
	(b)	Discuss linear regression method in QSAR models.	**05**
	(c)	Explain pocket matching in structure based CADD.	**05**
Q.5	**(a)**	Write a note on 2D description of molecular constitution as molecular descriptor in ligand based CADD.	**06**
	(b)	Explain about 3D description of molecular configuration and conformation.	**05**
	(c)	Explain molecular superimposition in pharmacophore mapping.	**05**
Q. 6	**(a)**	Explain Predication of ADME.	**06**
	(b)	Write a note on human ether-a-go-go related gene potassium channel inhibition.	**05**
	(c)	What is toxicity prediction software package? Write its applicability.	**05**
Q.7	**(a)**	Write a note on genetic algorithms in SBDD.	**06**
	(b)	Write a note on multidimensional QSAR.	**05**
	(c)	Discuss about Knowledge based Scoring method.	**05**

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