Seat No.: _____ Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY

B.Pharm. – SEMESTER VIII • EXAMINATION – WINTER -2022

Subject Code:2280006 Date:31/12/2022

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)**	Enlist protein binding sites identification methods and explain any one in detail.	**06**
	(b)	Explain in details representation of small molecules as "SMILES" in ligand databases for CADD.	**05**
	(c)	Write a short note on comparative modeling in structure based CADD.	**05**
Q.2	**(a)**	Explain multi target inhibitors using pharmacophore model.	**06**
	(b)	Describe in detail applications of Molecular Dynamics simulations in drug design.	**05**
	(c)	Explain in detail pocket matching in structure based CADD.	**05**
Q.3	**(a)**	Explain about genetic algorithms in SBDD.	**06**
	(b)	What do you mean by force field? Describe various methods for energy minimization.	**05**
	(c)	Discuss importance of drug design approaches in drug discovery.	**05**
Q.4	**(a)**	Discuss about Monte Carlo simulation with metropolis criterion.	**06**
	(b)	Define ligand based CADD. Discuss preparation of ligand libraries.	**05**
	(c)	Explain InChIkey.	**05**
Q.5	**(a)**	Explain in detail 3D description of molecular constitution as molecular descriptor in ligand based CADD.	**06**
	(b)	What is pharmacophore? Explain in brief about pharmacophore mapping.	**05**
	(c)	Write about Binary molecular fingerprints.	**05**
Q. 6	**(a)**	Discuss about COMFA and COMSIA methods of QSAR.	**06**
	(b)	What is toxicity prediction software package? Explain it.	**05**
	(c)	Explain in brief human ether-a-go-go related gene potassium channel inhibition.	**05**
Q.7	**(a)**	Write down SAR application in ligand based CADD.	**06**
	(b)	Discuss about Knowledge based Scoring method.	**05**
	(c)	Write down prediction of ADME in detail.	**05**

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