BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: M.PHARM. **SEMESTER: II**
BRANCH: PHARMACY **SESSION: SP2025**

SUBJECT: MPC203T COMPUTER AIDED DRUG DESIGN

TIME: 3.00 Hours **FULL MARK: 75**

INSTRUCTIONS:

1. The missing data, if any, may be assumed suitably.
2. Before attempting the question paper, be sure that you have got the correct question paper.
3. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.
5. Answer any five questions.

1a.	Define QSAR with the various physicochemical descriptors associated with 2D QSAR.	[7]
1b.	Elaborate (i) Hammett Substituent Constant (ii) Hydrophobicity constant (iii) F and R	[8]
2a.	Explain the following: (i) Advantages of 3D QSAR over 2D QSAR (ii) Craig Plot	[7]
2b.	Elaborate Topliss Scheme for aromatics and aliphatics with relevant explanation.	[8]
3a.	Demonstrate the preparation of ligands in a ComFA study.	[7]
3b.	Elaborate conformational analyses and the various methods	[8]
4a.	Analyze the role of Molecular Modelling in the process of drug discovery.	[7]
4b.	Define the terms: (i) Molecular Mechanics (ii) Quantum Mechanics (iii) Molecular Dynamics (iv) Semiempirical methods	[8]
5a.	Discuss the importance of prediction and analysis of ADMET properties in drug design.	[7]
5b.	Writes notes on (i) Fragment based drug design (ii) Receptor cavity size prediction.	[8]
6a.	Explain Homology modelling with suitable examples.	[7]
6b.	Explain Pharmacophore mapping.	[8]
7a.	Explain Docking studies with suitable examples and flowchart.	[7]
7b.	Write notes on (i) Similarity based methods (ii) Pharmacophore based screening	[8]

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