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

CLASS: PHARM SCI TECH **SEMESTER: II**
BRANCH: PHARMACY **SESSION: SP2024**

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.	Elaborate the Hancsh equation with its application along with the physicochemical parameters commonly used for QSAR equation	[7]
1b.	Define Topliss Scheme for aromatics and aliphatics with relevant explanation	[8]
2a.	Demonstrate the preparation of ligands in a 3D SAR study	[7]
2b.	Explain conformational analyses and the various methods	[8]
3a.	Detail out the role of Molecular Modelling in the process of drug discovery	[7]
3b.	Define the terms: (i) Molecular Mechanics (ii) Molecular dynamics (iii) Ab initio methods (iv) Semiempirical methods	[8]
4a.	Define molecular docking. Classify them with a brief description.	[7]
4b.	Why protein require preparation before molecular docking simulation? Discuss briefly.	[8]
5a.	Explain why we need FBDD? Discuss the aspects in which it differs from SBDD.	[7]
5b.	What is the need for ADME-TOX predictive models? Discuss on the challenges in developing ADME-TOX models.	[8]
6a.	Discuss upon internal and external validation(s) in any QSAR studies.	[7]
6b.	What are decoys? Where they will be used? How will you prepare a decoy set?	[8]
7a.	Discuss in detail about the enrichment studies used in any HTVS. Discuss about the various parameters used for the purpose of validating the HTVS protocol.	[7]
7b.	Write a note on ROC. Discuss about its significance in HTVS.	[8]

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