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

CLASS: MSC (BIOINFORMATICS & COMPUTATIONAL BIOLOGY) **SEMESTER : III**
BRANCH: BIO-ENGINEERING AND BIOTECHNOLOGY **SESSION : MO/2025**

SUBJECT: BI302 CHEMINFORMATICS AND DRUG DESIGN

TIME: 3 Hours **FULL MARKS: 50**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 10 marks and total 50 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
***4*. Before attempting the question paper, be sure that you have got the correct question paper.**
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

			CO	BL
Q.1(a)	Explain various representations of protein 3D structure in chimera software.	[5]	1	2
Q.1(b)	Describe SMILES and their conversion into 2D and 3D formats	[5]	1	2
Q.2(a)	What is Pharmacokinetics? Explain the ADME/T for a drug.	[5]	3	2
Q.2(b)	Describe Physicochemical properties of drug. Briefly explain Lipinski rule of five.	[5]	2	2
Q.3(a)	Describe PubChem and Drug Bank. Explain substructure searching.	[5]	3	2
Q.3(b)	Describe Drug Repurposing. How it is helpful in drug discovery process.	[5]	5	2
Q.4(a)	What is Pharmacophore? Explain the steps involved in pharmacophore-based drug designing using Bioinformatics approach.	[5]	4	3
Q.4(b)	Differentiate between Structure based and Ligand based drug designing	[5]	4	4
Q.5(a)	Describe combinatorial library design and its application in drug design.	[5]	2	2
Q.5(b)	What is virtual screening? Illustrate with example the structure based virtual screening of compound.	[5]	2	3

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