

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2025

B.Tech-VI Semester (BI)

COURSE CODE (CREDITS): 18B11BI612 (3)

MAX. MARKS: 35

COURSE NAME: Computer Aided Drug Design

COURSE INSTRUCTORS: Dr. Raj Kumar

MAX. TIME: 2 Hours

Note: (a) All questions are compulsory.

(b) The candidate is allowed to make Suitable numeric assumptions wherever required for solving problems

Q.No	Question	CO	Marks
Q1	A search algorithm refers to the computational method used to explore the possible orientations and conformations of a ligand when it binds to a receptor. What are different types of scoring functions. Explain working of a genetic algorithm.	2-5	7
Q2.	Explain how drugs are metabolized in context to ADME? What are different phases of drug metabolism?	5,6	4
Q3.	The Rule of Five, is a set of empirical guidelines developed in the late 1990s to evaluate the "drug-likeness" of compounds, especially their oral bioavailability. Describe various rules, and other possible measures for drug-likeness of unknown compounds?	5,6	5
Q4.	Discuss how linear and parabolic equations are applied to model the relationship between hydrophobicity and biological activity.	5,6	5
Q5.	What is virtual screening, and how does it differ from high-throughput screening in drug discovery?	4,5	5
Q6.	Create molecular structure for given SMILES strings: a) <chem>CC1=CC(CCC1)Br</chem> b) <chem>c1cccc1C(=O)O</chem> c) <chem>c1(Cl)c(O)cc(Cl)c(Cl)c1</chem>	5	3
Q7.	Short notes: a) Bioavailability b) Blood Brain Barrier c) Pharmacophore	2-5	3×2 =6