JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATION- 2025

B.Tech-VI Semester (BI)

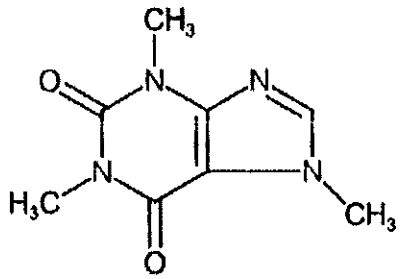
COURSE CODE (CREDITS): 18B11BI612 (3) MAX. MARKS: 25

COURSE NAME: Computer Aided Drug Design

COURSE INSTRUCTORS: Dr. Raj Kumar MAX. TIME: 1 Hour 30 Min

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 drug target is a specific molecule in the body that a drug interacts with to produce a therapeutic effect. Give a brief overview of current molecular targets for drug discovery.	1,2	3
Q2	Identification and evaluation of surface binding-pockets and occluded cavities are initial steps in protein structure-based drug design. Discuss some shapes of possible binding sites?	2,3,4	3
Q3	Describe the working principle of CASTp program.	2,3,4	5
Q4	A scoring function is a mathematical model used in molecular docking to predict the binding affinity or stability of a ligand–protein complex. Discuss in detail the formulation of AutoDock scoring function used to predict binding affinity.	2,3,4	6
Q5	Validating a docking program is a critical step to ensure that the predictions from a molecular docking experiment are reliable. Describe the strategy how will you validate a docking program for your docking experiment?	2,3,4	5
Q6	Design three possible SMILES strings for the given molecule: 	5,6	3