JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATIONS- 2026

B.Tech-VI Semester (BI)

COURSE CODE(CREDITS): 18B11BI612 (3) MAX. MARKS: 35

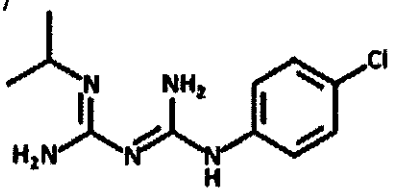
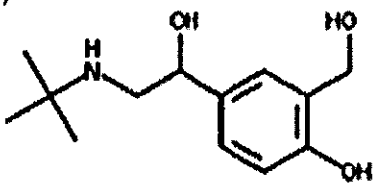
COURSE NAME: Computer Aided Drug Design

COURSE INSTRUCTOR: 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

(c) Use of calculator is allowed

Q.No	Question	CO	Marks
Q1	Explain role of hydrophobic substituent constant in drug discovery. The LogP value of benzene is 2.13 and the LogP value of toluene (-CH_3 substituent) is 2.73. Calculate the hydrophobic substituent constant value for the methyl substituent.	6	5
Q2	Differentiate between the straight-line and parabolic LogP equations used in QSAR studies.	5	5
Q3	Create SMILES strings for the given compounds: a)  b) 	4	5
Q4	Explain the roles of Phase I and Phase II metabolism in the detoxification processes of the liver that facilitate the excretion of drug molecules.	6	4
Q5	Explain the role of Lipinski's Rule of Five and Veber's Rule in drug discovery in predicting drug-likeness.	6	4
Q6	A patient receives a 150 mg oral dose of a drug. If the bioavailability is 60%, calculate the amount of drug that reaches systemic circulation.	6	3
Q7	A drug is distributed between n-octanol and water. At equilibrium, the concentration of the drug in n-octanol is 80 mg/mL and in water is 20 mg/mL.Calculate the partition coefficient (P).	5	3

Q8	Describe the training set selection criteria for 3DQSAR pharmacophore modelling using Hypogen algorithm.	5	3
Q9	Explain various assumptions taken for Hanch's analysis for QSARs?	5	3