JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2023

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)Marks are indicated against each question in square brackets.

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

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Q1. Consider a hypothetical compound. How will you calculate the hydrophobicity of the whole compound? [3] (CO-4)

Q2. Discuss the effect of electron donating group on σ of a ring attached to carboxylic acid? [3] (CO-4)

Q3. Calculate the hydrophobic substituent constant (π) for 'X' if the 'Log P_H'and 'log P_X' values are given as 2.13 and 2.84, respectively. What will be the effect of 'X' substitution on hydrophobicity of the compound? [3] (CO-5)

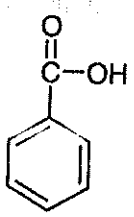
Q4. Draw the structural formulas for the given SMIILES format: [3] (CO-5)

a) **CCN(CC)CC**

b) **CC(C)C(=O)O**

c) **C=CC(CCC)C(C(C)C)CCC**

Q5. Draw the SMILES notations for the given structure: [3] (CO-5)



Q6. Describe the following in context to pharmacokinetic properties of a drug: [2 × 3 = 6] (CO-6)

a) Bioavailability
b) Metabolism
c) Blood brain barrier (BBB)

Q7. Describe the following in context to molecular representations: [2 × 3 = 6] (CO-6)

a) Newman Projections
b) Kekule formulas
c) CAS Registry Number

Q8. Quantitative structure-activity relationship (QSAR) is a computational modeling method for revealing relationships between structural properties of chemical compounds and biological activities. Discuss some properties utilised by Hansch for developing QSAR models. [3] (CO-6)

Q9. 'Rule of 5' helps to predict if a biologically active molecule is likely to have the chemical and physical properties to be orally bioavailable. Describe the rule of 5 and also explain the rotatable bonds and polar surface area criteria for a good drug. [3] (CO-5)

Q10. *In silico* methodologies have become a crucial part of any drug discovery project. Write down an in silico strategy which leads to identification of potential hit compounds. Make your answer presentable by using flowchart scheme. [5] (CO-4)