JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2024

B.Tech-VI Semester (BI)

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

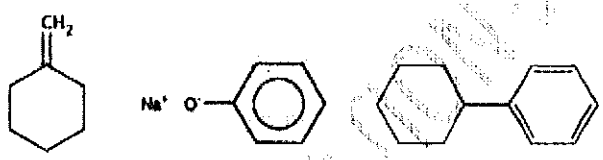
COURSE NAME: Computer Aided Drug Design

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

---

Q1. Write the SMILES string for the given molecules: (CO-3,5) [2×3 = 6]



(a) (b) (c)

Q2. Discuss about the Quantitative Structure-Activity Relationship (QSAR) and how does it differ from qualitative SAR? (CO-3,5) [3]

Q3. Describe practical steps involved in the process of developing a QSAR model? (CO-3) [3]

Q4. Discuss the role of partition coefficient in drug design. What is the effect of a high value of partition coefficient on a potential drug molecule? (CO-4) [3]

Q5. Calculate the hydrophobic substituent constant and discuss the effect of –CH3 group substitution on benzene? Given π value of, benzene = 2.13, toluene = 2.69. (CO-5) [3]

Q6. Professor Corwin Hansch was a prominent chemist known for his significant contributions to the field of medicinal chemistry. Discuss the Hansch equation, which is a foundational concept in QSAR studies. (CO-6) [5]

Q7. Enlist the important rules for predicting the drug-likeness properties of potential drug molecules? (CO-6) [3]

Q8. Discuss the statistics of failure of compounds in drug development phase with respect to the pharmacokinetic properties. (CO-5,6) [3]

Q9. Discuss important parameters in selection of compounds for training set in QSAR modeling. (CO-5,6) [3]

Q10. Short notes: (CO-3-6) [1×3 = 3]

a) CAS Registry Number
b) Wedge-dash diagrams
c) Oral bioavailability