JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATIONS-2022

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: *All questions are compulsory. Marks are indicated against each question in square brackets.*

Q1.SMILES isa specification in the form of a line notation for describing the structure of chemical species using short ASCII strings.How can you define different types of bonds in SMILES? [3](CO-4)

Q2. Write down various valid SMILES strings for the given structure. [3](CO-5)

CH_2=CH-CH_2-CH=CH-CH_2-OH

Q3. According to QSAR, activity is the function of molecular property. Discuss some properties utilised by Hanschfor developing QSAR models.[3](CO-5)

Q4. How can you calculate LogP? What is its importance in QSAR? [3](CO-4)

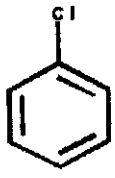
Q5. What will be the effect of electron withdrawing group on σ of a ring atcched to carboxylic acid? [3](CO-4)

Q6. Claculate the Tanimoto coefficient of subset (A, B, C, D, E) and subset (I, H, G, F, E, D)?[3](CO-6)

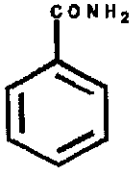
Q7. How can you calculate the bioavailability of an oral drug? [2](CO-6)

Q8. Calculate the hydrophobic substituent constant for the given benzene substituents.What will be the effect of benzene substituents on the hydrophobicity? [5](CO-5)

Benzene
(Log *P* = 2.13)



Chlorobenzene
(Log *P* = 2.84)



Benzamide
(Log *P* = 0.64)

Q9. Different schemes can be utilised for molecular structure representation in 2D and 3D. Discuss some 2D schemes which can represent 3D structures. [5] (CO-4)

Q10. What are the rules for multiple ring structure representations in SMILES? Write down valid SMILES string for the given structure.[5](CO-5)