JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATION- 2024

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 Minutes

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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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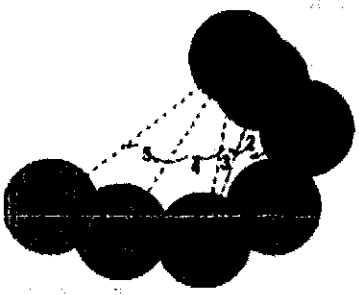
Q1. List some important methods of ligand-based drug design. (CO-1,2) [2]

Q2. Target identification is the first step in drug discovery. How do researchers prioritize potential drug targets for further investigation and validation? (CO-2,3) [3]

Q3. New target validation is the basis of completely new drug exploration and the initial step of drug discovery. Discuss important steps to target validation process. (CO-2,3) [2]

Q4. Demonstrate how can a biological pathway can be targeted for cancer therapeutics? (CO-2,3) [5]

Q5. Consider a binding pocket consisting of triangles of equal arm lengths L = 10 cm. Calculate the total area of binding site pocket given below: (CO-2,3) [3]



Q6. Short notes: (CO-3,4,5) [2 × 5 =10]

a) Pocket Vs. cavity
b) Exhaustive systematics search
c) Genetic algorithm
d) Forcefield scoring function
e) Docking limitations