JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATION- APRIL-2023

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

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Q. Drug target identification is an essential part of modern rational drug design projects. Discuss important considerations for identification of a suitable drug target. (CO-3) [5]

Q. Suppose you have an unknown protein 3D structure. How will you: (CO-4)

a) find out the sequence of the protein? [1]
b) probable function for the protein? [2]
c) ligand-binding site? [2]

Q. LBDD and SBDD are two important approaches in computational drug design. Enlist some important LBDD strategies to identify potential hit compounds. (CO-2) [3]

Q. There are thousands of potential drug targets under investigation. What are the major classes of current drug targets? (CO-3) [3]

Q. CASTp is based on theoretical and algorithmic results of computational geometry. If three angles of same dimensions having base length of 10nm and height of 20nm form the void in the receptor. The calculate the area of void? (CO-4) [3]

Q. Give a brief account on: (CO-3) [2 × 3 = 6]

a) Hit vs. Lead
b) Microarray for target validation
c) Receptor flexibility in docking