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JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATIONS-2022

B.Tech-VI Semester (BT)

COURSE CODE: 18B11BI612

MAX. MARKS: 25

COURSE NAME: Computer Aided Drug Design

COURSE CREDITS: 3

MAX. TIME: 1 Hour 30 Min

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

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Q1. How will you introduce receptor flexibility in a docking experiment?[2 Marks] (CO-2)

Q2. How will you validate a docking program for your customized docking experiment?[2 Marks](CO-2)

Q3. Discuss the basis of conformational search analysis by a search algorithm. [2 Marks](CO-3)

Q4. Suppose a computational receptor geometry having 10 right-angle of same dimensions having base length of 5nm and height of 10nm. Only 3 such triangles form the void in the receptor. What is the area of void? [3 Marks](CO-2)

Q5. How does a stochastic search algorithm differ in finding conformations for a ligand than an exhaustive search algorithm? [3 Marks](CO-4)

Q6. A variety of scoring schemes are available for ranking the docking poses. Discuss the basis of binding energy calculations by a force-field based scoring function.[3 Marks](CO-3)

Q7.CASTp is an important program to predict the binding sites on the receptor. Describe the discrete flow method for identifying and measuring pockets on a receptor surface. [5 Marks](CO-4)

Q8. Virtual screening is an important approach in rational drug discovery. Discuss the various stages involved in identification of a lead molecule. [5 Marks](CO-3)