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JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATION- April-2019

B.Tech Bioinformatics VI Semester

COURSE CODE: 16B11BI611

MAX. MARKS: 25

COURSE NAME: Computer Aided Drug Design

COURSE CREDITS: 4

MAX. TIME: 1.5 Hours

*Note: All questions are compulsory. Carrying of mobile phone during examinations will be treated as case of unfair means.*

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|---|-----------------|-------|
| 1. Explain the methodology of converting a smiles format into a 3D coordinate.  | (2 Marks)       | COII  |
| 2. What is the advantage of using machine learning based methods in QSAR?   | (2 Marks)       | COIII |
| 3. List the various linear and non-linear methods used in QSAR.   | (2 Marks)       | COIII |
| 4. Explain in detail the method of CoMFA, using a suitable example.   | (3 Marks)       | COIII |
| 5. Explain in detail the method of CoMSIA, using a suitable example.  | (3 Marks)       | COIII |
| 6. Define the following:  | (1X5 = 5 Marks) | COIII |
| a. PLS  |                 |       |
| b. MLR  |                 |       |
| c. ANN  |                 |       |
| d. SVM  |                 |       |
| e. PCA  |                 |       |
| 7. What is molecular docking? What are its limitations? Explain the steps involved in DOCK with the help of a suitable diagram. | (5 Marks)       | COIV  |
| 8. What are the various molecular surface generation methods?   | (3 Marks)       | COIV  |