JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST-3 EXAMINATION – May 2019

B.Tech 6th Semester

COURSE CODE: 16B11BI611

MAX. MARKS: 35

COURSE NAME: Computer Aided Drug Design

COURSE CREDITS: 4

MAX. TIME: 2HRS

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

1. Write the overview of a typical Structure based Drug Design. What are the advantages and disadvantages of SBDD. **(5 Marks)** **COI**

2. What is a drug target? How does one validate or evaluate drug targets? **(5 Marks)** **COI**

3. What is fragment based drug discovery? How does one find fragment occurrence and what is its significance? **(5 Marks)** **COIII**

4. Describe in detail the various types of QSAR methods and their applications. What are the various statistical methods used in QSAR? Describe in detail **(5 Marks)** **COII**

5. What is oral bioavailability? How is it calculated? How does one determine toxicity of a drug? Explain in detail. **(5 Marks)** **COIII**

6. What are the various molecular mechanisms of antimicrobial resistance? Write about how antibiotic misuse is causing issues in public health. **(5 Marks)** **COIII**

7. What are the two major steps in molecular docking? Compare and contrast the two steps of molecular docking with respect to DOCK and AutoDock. What are the advantages and disadvantages of molecular docking? **(5 Marks)** **COIII**