

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST 3 EXAMINATIONS – MAY 2018

B.Tech VI Semester

COURSE CODE: 16B11BI611

MAX. MARKS: 35

COURSE NAME: Computer Aided Drug Design

COURSE CREDITS: 04

MAX. TIME: 2 HRS

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

Q1. Describe as to why there is a high rate of failure in designing new drugs that come to market in the last 10 years, compared to the beginning of the century. **5 Marks**

Q2. Compare and contrast 1D, 2D, 3D, and 4D QSAR. Explain the importance of molecular descriptors. **5 Marks**

Q3. Describe the advantages and disadvantages of the following **8 marks**

- a. Structure based drug design
- b. De novo drug design
- c. Receptor based pharmacophore design
- d. Ligand based pharmacophore design

Q4. Explain the role of physicochemical properties in relation to biological activity and drug design. **5 Marks**

Q5. Describe the methods of lead optimization. **5 Marks**

Q6. How are clinical trials performed in the discovery of new drugs? **5 Marks**

Q7. What is ADMET properties and how are they implemented in drug design? **2 Marks**