

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT  
Test 2 EXAMINATION- Apr 2018  
B.Tech. (Bioinformatics) VI Semester

COURSE CODE : 16B11BI611  
COURSE NAME: Computer Aided Drug Design

MAX MARKS : 25  
MAX. TIME: 1.5 Hrs.

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*Note: All questions are compulsory. Attempt all questions of a particular section at one place.  
Answer each question to the point.*

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1. What is cheminformatics? Discuss with examples the uses of various file formats of small molecule representation. (3 marks)
2. What are molecular fingerprints? Write a short note on the fingerprint based library searches for drug discovery. (3 marks)
3. Explain the uses of molecular similarity and diversity in lead discovery process. (3 marks)
4. Discuss Tanimoto Coefficient. What is the difference between similarity and distance based matrices in high throughput screening of small molecules? (3 marks)
5. Explain the general drug discovery process. Discuss each stage in the process from target identification to market launch. (3 marks)
6. Write a short note on Zinc library for virtual screening. (3 marks)
7. Discuss the principles of receptor – ligand interactions. How can receptor fitting be employed in drug discovery? Discuss. (4 marks)
8. Write a short note on induced fit docking. (3 marks)