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JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -1 EXAMINATION- February 2018

B.Tech. (BI) VIth Semester

COURSE CODE: **16B11BI611** MAX. MARKS: 15

COURSE NAME: Computer Aided Drug Design

COURSE CREDITS: 4 MAX. TIME: 1 Hr

Note: *All questions are compulsory. Carrying of mobile phone during examinations will be treated as case of unfair means. Provide example and diagram wherever possible.*

Q1. Each question carries 2 marks. Answer any three. **(2 x 3 = 6)**

i. High risk is involved in a drug design project, why? What are the important factors that need to be taken into account before implementing a drug development project and why? (0.5+1.5)

ii. How different stages of clinical trials are being carried out and discuss their basis? Why many drugs are being withdrawn from the market after FDA approval? (1.5+0.5)

iii. Suppose for a target enzyme inhibitor is known. How do you modify the inhibitor molecule through analyzing enzyme-inhibitor complex? (1.5+0.5)

iv. Discuss the role of chemoinformatics in lead design. Why 2D representations like SMILES are preferred in chemoinformatics?

Q2. Each question carries 3 marks. **(3 x 3 = 9)**

i. Discuss the importance of understanding the disease process in a drug development setting to identify protein target of a disease? Suppose you do not know the disease process then how do you identify drug targets? (2+1)

ii. Discuss the mechanism of *de novo* lead molecule design method which was used to design lead against a target whose active ligand is not known. Discuss the major limitations of this approach. (2.5+0.5)

iii. How docking score is calculated? What are poses of a ligand and how are these poses determined? Why grid-based score calculation is preferred in docking?