JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT
TEST-1, EXAMINATION – 2016
B. TECH. BIOINFORMATICS (VI SEM)

COURSE CODE: 16B11BI611 MAX. MARKS: 15
COURSE NAME: COMPUTER-AIDED DRUG DESIGN
COURSE CREDITS: 4 MAX TIME: 1 HR

Q1. Each question carries 1 mark.

i. Suppose you have a plant extract containing more than 1000 molecules. How do you discover lead molecules using biochemical assay?
ii. What are the important factors that need to be assessed before initiating a drug development project?
iii. What is rational drug design? How is it being used to produce better lead molecules?

Q2. Each question carries 3 marks.

i. Discuss the importance of disease process in drug target identification (explain with example)? How do you decide a drug target against a disease? How do you prioritize a drug target against a disease? (1.5+1+0.5)
ii. Make comparative analyses of clinical trial steps (I, IIa, IIb &III). How do you need to carry out toxicity testing at the lead optimization step? Why many drug molecules were withdrawn after the FDA approval? (2+0.5+0.5)
iii. Suppose receptor flexibility or modification is an important issue for an active site. How do different modules of various softwares (for example IFD, Glide XP, etc.) accommodate receptor flexibility for providing efficient docking? How do you conclude that the consideration of receptor flexibility is important during docking for a particular target? (2.5+0.5)
iv. Discuss the use of molecular mechanics (MM) method for score calculation. How do you use the grid method for calculation of docking score for different conformations of a ligand? Mention the limitations of MM-Based score calculation? (1+1.5+0.5)