JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT
MAKEUP EXAMINATION-May-2016
B.Tech. VI Semester (BI)

COURSE CODE: 16B11BI611   MAX. MARKS: 25

COURSE NAME: COMPUTER AIDED DRUG DESIGN

COURSE CREDITS: 04   MAX. TIME: 1.5 HRS

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

Q1. Each question carries 3 marks.   **(3x5=15)**

i. How do you calculate molecular descriptors (explain with example)? Discuss the significance and applications of 3D descriptors? When do you expect that 2D descriptors can be used for lead molecule identification and why?

ii. Explain the principle used to discover lead molecule using *de novo* method? How was lead molecules optimized using this principle? Why is this principle not so popular today? (1.5+1+0.5)

iii. Suppose you have 500 descriptors for a set of active/inactive molecules against a receptor target. How do you use feature reduction and selection technique to develop optimal QSAR model? How do you validate this model? How do you use this model to design more potential lead molecules?

iv. Why does most software use grid principle for calculating score of docking and how grid values are calculated? How do you refine potential molecules (determined in docking step) using database search as well as analog (derivative) design method? How do you validate docking score? (1.5+1+0.5)

v. How do you develop a database which can be used for virtual screening (what are the components that need to be included and how those data are to be acquired)? How do you convert it into a pharmacophoric database? (2+1)

2. Each question carries 5 marks.   **(5x2=10)**

i. One conformation each from two molecules including distance data will provided. Determine graph from these two conformations and how do you determine clique from the graph? If you have set of active molecules, how do you use clique detection technique to determine pharmacophore? (3.5+1.5)

ii. Refer the case study entitled "Pharmacophore determination of Dopamine D3 receptor antagonist". Suppose you have a set of active molecules against a particular enzyme, how do you determine the pharmacophore? Two pharmacophores will be provided. How do you perform ZINCPharmar database search using those pharmacophore? How do you evaluate the performance of database searching? (3+1+1)