Dr C. Rout

JAYPEE UNIVERSITY OF INFORMATRION TECHNOLOGY, WAKNAGHAT

MID SEMESTER EXAMINATION-2015

B.Tech 6th Semester

COURSE CODE: 10B11BI613 MAX. MARKS: 30

COURSE NAME: Drug Designing Techniques

COURSE CREDITS: 4 MAX. TIME: 2 HRS

Note: *All questions are compulsory.*

Section A **(Marks: 1x 6= 6)**

1. What are the limitations of traditional drug design technique in pharma industry? How computer aided drug design technique helps in overcome these limitations?
2. What are the different approaches of computer aided drug design (CADD) technique? Give two examples of successful drug developed by CADD and are in the clinic.
3. What is a drug target? How we validate that it is a good drug target?
4. What are the challenges in finding a new drug to solve a complex disease?
5. What are the reasons for developing resistance to antimicrobials by microorganisms such as bacteria?
6. Why the computational results predicted using different docking softwares are most likely not consistent?

Section B **(Marks: 3x3= 9)**

1. How do we score a binding site? Give the mathematical expression in scoring a binding site using any site prediction program. Briefly explain the characteristic features of different parameters being used.
2. Why it is hard to correlate the docking score of a ligand with its *in vitro* activity? How we can improve the docking score? Briefly explain the alternative strategies along with the mathematical expression if anything.
3. How do we discover a lead molecule to begin with drug development process? Mention the various strategies being followed in pharma industry in refinement and optimization of lead molecule to become a drug.

Section C **(Marks:5x3= 15)**

1. Enumerate the various task of drug discovery process for developing a novel drug for a disease such as cancer.

2. Assuming a protein structure has various binding sites. How we would select a good binding site (or active site) pertaining to inhibitor design? Briefly explain the various properties being consider by any one binding site prediction program.
3. "The secrete of life is molecular recognition; the ability of one molecule to recognize another through weak binding interaction." How these non bonding interactions are being implemented in modeling the protein-ligand interaction? What are the limitations of empirical docking score calculations? How these limitations could be overcome?