Post Graduate Diploma in Chemoinformatics
Annual Examinations – 2006

Paper: PGDC – 108
Drug Design and Discovery

Time allowed: Three hours | Maximum Marks: 80

SECTION –I

Q1. Fill in the blanks. 1X20

(i) IC_{50} stands for _____.
(ii) _____ is an example of rapid reversible inhibition.
(iii) Most drugs are small molecules of molecular weight less than _____.
(iv) Amprenavir and Nelfinavir developed against HIV protease were designed using mainly _____.
(v) Albert in 1958 was the first to introduce the concept of _____.
(vi) Remifentanil, a short acting m-opoid receptor agonist is a _____.
(vii) The rule of 5 (five) was given by _____.
(viii) The most commonly used method of identifying a lead molecule for a protein target is _____ of compound database.
(ix) A hydrogen bond occurs when a proton is shared between _____.
(x) ACD stands for _____.
(xi) _____ and _____ are used for small molecular proteins.
(xii) Fragment docking can be done by _____ docking software.
(xiii) Molecular modelling is study of _____.
(xiv) Standard C-C bond length is _____.
(xv) Phase I reactions involve metabolic modification of drug; commonly _____, _____ or _____.
(xvi) The substrate for cytochrome $P_{450}IA_2$ is _____.
(xvii) For rational drug design the first necessary step is _____.
(xviii) Information about protein structure can be obtained from _____.
(xix) B- lactamase enzyme has a _____ at the active site that cleaves the B-lactam ring of an antibiotic.
(xx) According to rule of five, a calculated log of partition coefficient (c log P) should be _____.

SECTION-II

Q2. Attempt any six questions 5X6

(i) How can a structure be evaluated for structure based drug design?

(ii) Explain with example, factors to be taken into consideration while protein ligand interaction patterns are analyzed.

(iii) Name various softwares used for docking of ligand in the target protein. Discuss any one in detail.

(iv) What are the various scoring functions used in DOCK and what do they signify?

(v) What is the use of energy calculations to drug design?

(vi) Discuss the role of P_{450} enzyme in drug metabolism.

(vii) Explain the terms Pro drug, Hard drug and Soft drug. Various factors affect the response of a drug after administration into the system. Enumerate

(viii) What are affinity labels? Illustrate with examples.

SECTION-III

Attempt any three questions 10X3

Q3. Discuss in details Phase II metabolism.

Q4. How can the prediction of physiochemical properties of molecules be important?

Q5. FLUDI is used for De NOVO drug design. Explain the procedure and applications of computational De NOVO drug design methods.

Q6. Define selective and non-selective enzyme inhibition. Discuss in detail various factors (forces) involved in formation of enzyme inhibition complex.

Q7. What is the need of computer modelling? What are the advantages of using computer models over physical models?