Post Graduate Diploma in Chemoinformatics
Annual Examination 2006

Paper PGDC – 102
Medicinal Chemistry

Time Allowed: Three Hours | Maximum Marks: 80

SECTION – I | Marks

Attempt all the question, every question is of equal marks. 1X20=20

1. The nature of the site will determine the interaction energy between _____ and _____.
2. _____ is also known as CPZ.
3. The physical basis of scoring functions is based on _____.
4. Denovo design is a _____ process.
5. clog P stands for _____.
6. Define rule 5.
7. _____ method has been successfully used to construct a model for the G- Protein coupled histamine H-3 receptor.
8. Name four docking tools for virtual screening.
9. Activity in animals does not always translate into efficacy in _____.
10. _____ is a methodology aimed at the rapid analysis of large number of compounds.
11. Name various steps involved in virtual screening.
12. Only about 10% of USAN compounds have a _____ and _____.
13. Marine organisms are rich source of _____ and _____.
14. Define virtual screening.
15. Generic libraries consist of highly _____ covering larger areas in diversity species.
16. Technology that is gaining increasing use in drug discovery is _____.
17. Define Single Cell Analysis.
18. Name two Chemo metric models developed for pharmaceutical analysis in Drug Research and Development.
19. Natural plants are the most consistently successful source of_____.
20. Emperical based methods rely on the availability of _____ with known binding affinity.

SECTION – II

Attempt any six, each questions carries equal marks. 5X6=30

1. Discuss in brief opportunities and challenges for small molecule drug discovery in the post-genomic era.
2. How is target and ligand prepared for docking?

3. Natural products are well recognized source of lead compound, discuss.
4. What do you understand by 2-fold strategy for innovation? Give various phases involved in drug discovery.
5. Give various applications of substructure analysis.
6. Explain microbiological diversity and how it is being exploited in Drug Discovery.
7. Discuss various steps involved in structure based ligand design.
8. Various physio-chemical factors affect the development of lead profile. Enumerate and discuss any two.
9. Define a library. What all information is stored in a library and how is a library used for lead development.

SECTION – III

Attempt any three questions, each question carries equal marks. $10 \times 3 = 30$

1. Structure based virtual screening emerged as a reliable, inexpensive method for identifying lead. Support the statement with examples.
2. Discuss in detail ADME considerations prior to lead optimization.
3. Discuss various natural sources of lead compounds with particular emphasis on natural product, anticancer therapy.
4. What do you understand by terms drug solution and partition-coefficient. How are they related with drug discovery? How will you calculate absolute parameters?