



[Time: 3 Hours]

[Max. Marks: 75]

Computer Aided Drug Design -II

Q.P. CODE: 5159

Your answers should be specific to the questions asked.

Draw neat, labeled diagrams wherever necessary.

LONG ESSAY (Answer any Three)

3 X 10 = 30 Marks

1. Discuss the techniques used in virtual screening.
2. Explain Hammett equation and electronic parameters and how they are determined?
3. Explain fragment based drug design.
4. Write about receptor ligand interaction and how is it analysed?

SHORT ESSAY (Answer any Nine)

9 X 5 = 45 Marks

5. Describe the docking of agents on HMG-CoA reductase.
6. Explain in detail In silico drug design.
7. How the contour map is generated and analysed?
8. Write a note on effect of substituents on log P.
9. Discuss rigid docking.
10. Explain how the pharmacophore features can be identified?
11. Discuss how the ADMET properties of an experimental molecule can be predicted?
12. Describe drug-receptor interaction.
13. Explain the role of molecular modeling in drug design.
14. Explain the statistical methods used in QSAR analysis.

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