



[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. Explain Hansch and Free Wilson method of analysis with a suitable example and relationship between them.
2. Discuss the approaches for 3D-QSAR analysis.
3. Write the protocols to be followed in In silico virtual screening.
4. Discuss the energy minimization methods in molecular modeling.

SHORT ESSAY (Answer any Nine)

9 X 5 = 45 Marks

5. Describe the docking of agents on AchE.
6. Explain the method of generation of 3D-structure of a protein.
7. What is log P? How it is determined? Give its significance.
8. Explain the docking of agents on DHFR enzyme.
9. Explain pharmacophore mapping.
10. Discuss homology modeling of a protein.
11. Describe extra precision docking.
12. Explain the electronic parameters to be considered in QSAR.
13. Write a note on counter map analysis.
14. Discuss the role of computer aided drug design in drug discovery.

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