

QP CODE: 213331

Reg. No:.....

**Second Semester M. Pharm Degree Regular/Supplementary Examinations
November 2025**

M.Pharm (Pharmaceutical Chemistry)

Paper III - Computer Aided Drug Design (MPC203T)

(Common for 2019 and 2024 Scheme)

Time: 3 Hours

Total Marks: 75

- *Answer all questions to the point neatly and legibly • Do not leave any blank pages between answers • Indicate the question number correctly for the answer in the margin space*
- *Answer all parts of a single question together • Leave sufficient space between answers*
- *Draw table/diagrams/flow charts wherever necessary.*

Essays

(3x10=30)

1. Explain advantages, disadvantages and applications of Free Wilson approach. How 2D-QSAR equations are derived. Explain the importance of these equations.
2. Enlist DHFR inhibitors and explain its interaction with DHFR. What do you mean by rigid, flexible and extra-precision docking.
3. Write short note on fragment based drug design. What is homology modelling. What are the uses of this technique.

Short Notes

(9x5=45)

4. Discuss Taft steric and MR parameters used in QSAR study.
5. What is 3D-QSAR. Write in brief about contour map analysis.
6. Explain role of quantum mechanics in drug design.
7. Write a note on pharmacophore modelling.
8. Explain applications of Hammett equation and electronic parameters in drug design.
9. Explain in detail the docking of drugs that act on HMG-CoA reductase enzyme.
10. Write about various virtual screening techniques.
11. Discuss various energy minimization methods used in drug design. Add a note on global minimum conformation.
12. What is the use of topliss scheme and Craig plot.
