

QP CODE: 213331

Reg. No:.....

**Second Semester M. Pharm Degree Supplementary Examinations
February 2026**

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. Describe history and applications of CADD. Discuss about the basic history and development of QSAR. (5+5)
2. Write a note on significance of 3D-QSAR in drug design. Make a note on various statistical methods used in QSAR analysis. (5+5)
3. Write a note on *in-silico* drug design and virtual screening techniques. Explain the significance of ADMET property prediction and its analysis. (5+5)

Short Notes

(9x5=45)

4. Write about determination of lipophilicity parameters.
5. Distinguish Hansch and Free Wilson analysis.
6. Explain role of molecular mechanics in drug design.
7. Enumerate various energy minimization methods and explain any one in detail.
8. Explain *De novo* drug design in detail
9. Explain fragment based drug design.
10. Briefly explain the terms: CoMFA and CoMSIA
11. What is drug likeness. Write a note on utility of Lipinski rule of five.
12. Define pharmacophore and pharmacophore mapping. Explain the importance of conformation search in pharmacophore mapping.
