

QP CODE: 213331

Reg. No:.....

**Second Semester M. Pharm Degree Supplementary Examinations  
September 2022**

**M.Pharm (Pharmaceutical Chemistry)**

**Paper III - Computer Aided Drug Design (MPC203T)**

**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 the theoretical approaches for the determination of various physicochemical parameters.
2. Explain the factors involved in energy minimization methods.
3. Explain the concept of *in silico* virtual screening in drug design.

**Short Notes**

**(9x5=45)**

4. Explain the pharmacophore-based screening methods.
5. Describe the methodology involved in de novo drug design.
6. Differentiate between 2D-QSAR and 3D-QSAR.
7. Describe rigid docking with suitable example.
8. Explain the concept of fragment-based drug design.
9. Explain the concept of drug-receptor and drug-enzyme interaction with examples.
10. What is contour map analysis. Give examples.
11. Explain the parameter Log P and its application in drug research.
12. Explain how the determination of steric effects help in drug design.

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