

QP CODE: 213331

Reg. No:.....

**Second Semester M. Pharm Degree Regular/Supplementary Examinations
February 2021**

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. Describe the relationship between physicochemical properties and biological activity in QSAR.
2. Write the protocols to be followed in *In silico* virtual screening
3. Discuss the energy minimization methods in molecular modelling

Short Notes

(9x5=45)

4. Explain the concepts of rigid docking
5. Describe the docking of agents acting on HMG-CoA Reductase.
6. What is log P. How it is determined. Give its significance
7. Give the advantages and disadvantages of Hansch analysis and Free Wilson analysis of QSAR
8. Explain the role of quantum mechanics in drug design.
9. Counter map analysis
10. Explain pharmacophore mapping
11. Give the prediction and analysis of ADMET properties of new molecules in drug design
12. Homology modeling
