QP CODE: 213331 **Reg. No:……**

Second Semester M. Pharm Degree Regular/Supplementary Examinations October 2023

M.Pharm (Pharmaceutical Chemistry)

Paper III - Computer Aided Drug Design (MPC203T)

(Common for 2017 and 2019 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 the basics history and development of QSAR.
2. Explain the statistical methods used in QSAR analysis and importance of statistical parameters.
3. Explain the concept of pharmacophore mapping in drug design.

Short Notes **(9x5=45)**

4. Explain the identification of pharmacophore features.
5. Explain the techniques use for the generation of 3D structure of protein with suitable example
6. Explain the 3D-QSAR analysis.
7. Explain Flexible docking with examples.
8. Explain the concept of molecular modeling and docking.
9. Explain methods used for receptor and enzyme cavity size prediction in *de-novo* drug design.
10. What is homology modeling. Give examples.
11. Explain the importance of Taft steric and MR parameters in drug design.
12. Describe the docking of agents acting on acetylcholine esterase (AchE).

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