QP CODE: 213331	Reg. No:
<b></b>	

## Second Semester M. Pharm Degree Regular/Supplementary Examinations November 2024

## 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 in detail about various 3D-QSAR approaches and its advantages over 2D-QSAR
- 2. Explain fundamentals of QSAR in drug design. Add a note on QSAR Parameters related to chemical structure and biological Activity
- 3. Explain theory and applications of Molecular and Quantum mechanics in drug design

Short Notes (9x5=45)

- 4. Elaborate the Hansch equation
- 5. Explain the concept of de-novo drug design
- 6. Write the principles of computer aided drug design
- 7. Explain free Wilson analysis and its importance
- 8. Briefly explain Lipinsky's Rule of five
- 9. Explain molecular docking of agents acting on enzymes. Dihydrofolate reductase and choline esterase
- 10. Write a short note on Virtual screening techniques
- 11. Write a note on the importance of prediction and analysis of ADMET properties in drug design
- 12. Explain fragment based Drug Design

\*\*\*\*\*\*