Seat No.: _____ Enrolment No. _____

PARUL UNIVERSITY
FACULY OF PHARMACY
M.Pharm. Summer 2018- 19 Examination

Semester: 2 **Date: 19/04/2019**
Subject Code: MPC 203T **Time: 10:00am to 1:00pm**
Subject Name: Computer Aided Drug Design **Total Marks: 75**

Instructions:
1. Figures to the right indicate maximum marks.
2. Make suitable assumptions wherever necessary.

Q.1 Essay Type Questions. (any 2 out of 3) (15 Marks Each) **(30)**

1. Enumerate the various physicochemical properties of a drug molecule that influence the biological activity and describe lipophilicity parameters in detail.
2. Define QSAR. Mention the advantages and disadvantages of QSAR. Explain Hansch Analysis and Free Wilson analysis.
3. Write a note on 3D-QSAR approaches and contour map analysis.

Q.2 Short Essay Type Questions. (any 5 out of 6) (5 Marks Each) **(25)**

1. Explain the methods to predict ADMET properties of a new drug.
2. Elaborate the various stages in *de novo* drug design.
3. Define energy minimization. Explain various methods of energy minimization.
4. What is molecular docking? Discuss the forces involved in drug-receptor interactions.
5. Define homology modeling and explain how this technique assists in the generation of 3D-structure of protein.
6. Write briefly about pharmacophore mapping.

Q.3 Short Answers. (2 Marks Each) **(20)**

1. Write a note on molecular mechanics.
2. Explain rigid and flexible docking.
3. Briefly explain Lipinski's Rule of Five.
4. Enumerate various virtual screening techniques.
5. Explain extra-precision docking.
6. Discuss molecular docking of agents inhibiting HIV protease.
7. Write briefly about conformational search used in pharmacophore mapping.
8. Explain similarity based methods used in *in-silico* drug design.
9. Define fragment based drug design and ligand based drug design.
10. Explain briefly about quantum mechanics.