

**PARUL UNIVERSITY**  
**FACULTY OF PHARMACY**  
**M.Pharm., Summer 2017-18 Examination**

**Semester: 2****Subject Code: MPC203T****Subject Name: Computer Aided Drug Design****Date: 18-05-2018****Time: 10:00AM to 01:00PM****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. Write a short note on Hansch analysis and Free Willson analysis. Describes the relationship between them with advantages and disadvantages.
2. Explain in details about the De novo drug design with explanation of Fragment based drug design.
3. Write a short note on Molecular docking and drug receptor interactions with examples of types of docking.

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

1. Write a note on Homology modeling and generation of 3D-structure of protein.
2. Describes the Pharmacophore mapping in brief.
3. Explain in brief about prediction and analysis of ADMET properties of new molecules.
4. Describes: Energy Minimization Methods in brief.
5. Write brief note on Hammett equation and electronic parameters.
6. Give a brief overview of virtual screening techniques.

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

1. Define: Pharmacophore
2. Which agents are acting on HMG-CoA reductase?
3. What do you mean by Quantum Mechanics?
4. Write importance of statistical parameters in QSAR.
5. Explain effects of lipophilicity in QSAR.
6. Write notes on agents acting on choline esters.
7. What do you mean by template recognition in homology modeling?
8. Explain in brief about bioactive conformation.
9. Enlist application of QSAR.
10. Write Lipinski's rule of five.