

**QP CODE: 213331**

**Reg. No:.....**

**Second Semester M.Pharm Degree Supplementary Examinations  
January 2019**

**M.Pharm (Pharmaceutical Chemistry)**

**Paper III - Computer Aided Drug Design (MPC203T)**

**(2017 Scheme)**

**Time: 3 Hours**

**Total Marks: 75**

- Answer all Questions.
- Draw Diagrams wherever necessary.

**Essays**

**(3x10=30)**

1. Discuss in detail the different energy minimization methods and its applications in molecular modeling
2. Give a detailed account on de novo drug design.
3. Statistical methods used in QSAR analysis and importance of statistical parameters

**Short Notes**

**(9x5=45)**

4. Role of ADMET parameters in designing new molecules.
5. Homology modeling.
6. Pharmacophore mapping.
7. Taft steric parameter.
8. Applications of quantum mechanics in drug design.
9. Structure based in-silico virtual screening protocol
10. Free Wilson analysis.
11. Rigid docking and flexible docking.
12. Advantages and disadvantages of 2D -QSAR

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