

QP Code: 827006

Reg. No.....

**Eighth Semester B. Pharm Degree Regular/Supplementary
Examinations March 2026
Computer Aided Drug Design
(2017 Scheme)**

Time: 3 Hours

Max. 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 diagrams wherever necessary

Essays

(2x10=20)

1. What is molecular docking. Explain the different types and components of molecular docking (2+8)
2. Explain the term 'Pharmacophore'. What is bioisosterism. Classify with examples and write a note on importance of pharmacophore and bioisosterism in drug design. (2+8)

Short Notes

(7x5=35)

3. Explain homology modeling of proteins.
4. Explain Hansch equation and Hammett equation.
5. Explain the significance of Lipophilicity and Steric effects in QSAR.
6. Explain the ligand and structure based drug design.
7. What is meant by the terms local and global energy minima, and what is their relevance to conformational analysis.
8. Explain the different approaches of 3D-QSAR.
9. Mention the applications of cheminformatics and bioinformatics in the field of drug discovery.

Answer Briefly

(10x2=20)

10. Biochemical database.
11. Difference between SAR and QSAR
12. Write briefly on History of drug discovery and development.
13. Define the term Rational drug discovery.
14. Explain the role of computer applications in lead drug discovery.
15. Taft's steric constant.
16. What is pharmacophore mapping. What is its role.
17. Application of quantum mechanics in drug design.
18. What is de novo drug design.
19. What is force field.
