

QP Code: 827006

Reg. No.....

Eighth Semester B. Pharm Degree Supplementary Examinations
October 2025
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 analog based drug design. Explain the concept of bioisoterism and classify it with examples.
2. Explain the molecular docking procedures involved in rigid docking and flexible docking.

Short Notes

(7x5=35)

3. What is meant by the terms local and global energy minima, and what is their relevance to conformational analysis.
4. Explain the different stages involved in rational drug discovery process.
5. Explain 3D QSAR approaches.
6. Explain the different methods of lead optimization.
7. Explain the case study on the design of HIV protease inhibitors using docking.
8. Explain Free-Wilsons method for QSAR with its merits and demerits.
9. Explain ADME databases and its applications.

Answer Briefly

(10x2=20)

10. Role of bioinformatics in drug design.
11. Hansch equation
12. Write about history of drug discovery and development
13. What is pharmacophore mapping.
14. Binding site identification in docking.
15. Define force field used in molecular modeling.
16. What is semi empirical method in quantum mechanics.
17. Define molecular dynamic simulation technique.
18. Define bioisoterism with an example.
19. Define the term chemoinformatics.

CORRECTION / NO-CORRECTION FILE
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QPCODE: 827006

Dated: 24-10-2025

Question No.18

Replaced with "Electronic effect with an example."

Corrections/Modifications/Replacement of Questions if any shall be made available to all students. Take the print out of the Correction File in such cases and distribute to all students.

(Sd/-)

CONTROLLER OF EXAMINATIONS