

Seat No.: _____

Enrolment No. _____

GUJARAT TECHNOLOGICAL UNIVERSITY
B.PHARM – SEMESTER – 8 EXAMINATION – SUMMER-2025

Subject Code: BP807TT

Date: 16-05-2025

Subject Name: Computer Aided Drug Design

Time: 10.30 AM TO 01.30 PM

Total Marks: 80

Instructions:

1. Attempt any five questions.
2. Make suitable assumptions wherever necessary.
3. Figures to the right indicate full marks.

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|-------------|---|-----------|
| Q.1 | (a) What is serendipitous drug discovery? Example with suitable examples. | 06 |
| | (b) Define bioisosterism. Classify various types of bioisosters giving examples. | 05 |
| | (c) Explain in detail about lead discovery based on metabolism. | 05 |
| Q.2 | (a) Differentiate between SAR and QSAR. Give various physicochemical parameters utilized in QSAR. | 06 |
| | (b) How is the Hansch free energy relationship applied in drug design? | 05 |
| | (c) What is 3D-QSAR? Explain in brief about COMFA and COMSIA. | 05 |
| Q.3 | (a) What is Lipinski rule of five? Explain it with suitable example. | 06 |
| | (b) Explain pharmacophore mapping. | 05 |
| | (c) What is pharmacophore based Screening? | 05 |
| Q.4 | (a) What is molecular docking? Enlist various type of molecular docking. | 06 |
| | (b) Explain in detail about De novo drug design. | 05 |
| | (c) Write a note on Chemoinformatics. | 05 |
| Q.5 | (a) Explain in brief about biochemical and pharmaceutical databases | 06 |
| | (b) What is analog Based Drug Design? Explain with suitable examples. | 05 |
| | (c) Discuss Hammett's Substituent constant with examples. | 05 |
| Q. 6 | (a) What is molecular modelling? Explain molecular mechanics in detail. | 06 |
| | (b) Explain various methods for energy minimization. | 05 |
| | (c) Write a note on global conformational minima determination. | 05 |
| Q.7 | (a) Describe rational approaches to lead discovery based on traditional medicine. | 06 |
| | (b) Write a brief note on Free Wilson mathematical model. | 05 |
| | (c) Explain about various stages of drug discovery and development. | 05 |
