

GUJARAT TECHNOLOGICAL UNIVERSITY
B.Pharm. -SEMESTER-VIII • EXAMINATION – SUMMER -2022

Subject Code: BP807TT**Date:06/06/2022****Subject Name: Computer Aided Drug Design****Time:10:30AM TO 01:30PM****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 molecular mechanics? Discuss its applications in details. | 06 |
| | (b) Write a note on lead discovery based on drug metabolism. | 05 |
| | (c) Discuss about Hansch analysis in QSAR. | 05 |
| Q.2 | (a) Write down various stages of drug discovery and development. | 06 |
| | (b) Write a note on quantum mechanics in drug discovery. | 05 |
| | (c) Define drug likeness. Discuss about virtual screening of drug likeness. | 05 |
| Q.3 | (a) Define Bioisosterism. Discuss classification & bioisosteric replacement in details. | 06 |
| | (b) Write a note on de novo drug design. | 05 |
| | (c) Discuss in details about concept of pharmacophore mapping. | 05 |
| Q.4 | (a) Write about COMFA and COMSIA methods of 3D-QSAR. | 06 |
| | (b) Write about serendipitous drug discovery in details. | 05 |
| | (c) Discuss in details about ADME databases. | 05 |
| Q.5 | (a) Write about energy minimization methods in molecular modeling. | 06 |
| | (b) Differentiate between SAR and QSAR in details. | 05 |
| | (c) Write a note on pharmacophore based screening. | 05 |
| Q.6 | (a) Define docking. Discuss various docking methods. | 06 |
| | (b) Write about free wilson analysis in QSAR. | 05 |
| | (c) Discuss in details about bioinformatics in drug design. | 05 |
| Q.7 | (a) Discuss various physicochemical parameters in QSAR. | 06 |
| | (b) Write about global conformational minima determination. | 05 |
| | (c) Write a note on lead discovery based on clinical observation. | 05 |
