

Seat No.: \_\_\_\_\_

Enrolment No. \_\_\_\_\_

**GUJARAT TECHNOLOGICAL UNIVERSITY**  
**B. Pharm. – SEMESTER – VIII • EXAMINATION – WINTER • 2016**

**Subject Code: 2280006**

**Date: 02-12-2016**

**Subject Name: Computer Applications in Drug Discovery**

**Time: 02:30 pm - 05:30 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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|-------------|-----|---|-----------|
| <b>Q.1</b>  | (a) | Write a note on drug discovery process. Give importance of drug design.                               | <b>06</b> |
|             | (b) | Write down Predication of ADME in details.  | <b>05</b> |
|             | (c) | Explain about genetic algorithms in SBDD.   | <b>05</b> |
| <b>Q.2</b>  | (a) | What are the different approaches for new drug discovery? Discuss in brief about each.                | <b>06</b> |
|             | (b) | What is docking? Describe various docking methods.  | <b>05</b> |
|             | (c) | Write in detail about COMFA and COMSIA methods of QSAR.   | <b>05</b> |
| <b>Q.3</b>  | (a) | Explain about QSAR. Discuss various QSAR parameters.  | <b>06</b> |
|             | (b) | Write down steps in Comparative Modeling.   | <b>05</b> |
|             | (c) | Write down applications of Molecular Dynamics simulations in drug design.                             | <b>05</b> |
| <b>Q.4</b>  | (a) | Write a note on Structure-Based Virtual High-Throughput Screening.                                    | <b>06</b> |
|             | (b) | Write about Binary molecular fingerprints.  | <b>05</b> |
|             | (c) | Discuss about Knowledge based Scoring method.   | <b>05</b> |
| <b>Q.5</b>  | (a) | Define Pharmacophore modeling. Write advances, limitations and current application in drug discovery. | <b>06</b> |
|             | (b) | Describe about the target data bases for computer-aided drug design in details.                       | <b>05</b> |
|             | (c) | Explain about 3D Description of molecular configuration and conformation.                             | <b>05</b> |
| <b>Q. 6</b> | (a) | Write a note on Pharmacophore mapping.  | <b>06</b> |
|             | (b) | How to select optimum features in ligand based computer aided drug design?                            | <b>05</b> |
|             | (c) | What do you mean by force field? Describe various methods for energy minimization.                    | <b>05</b> |
| <b>Q.7</b>  | (a) | Discuss on Toxicity Prediction Software Packages and Algorithms.                                      | <b>06</b> |
|             | (b) | Write a note on Ligand databases for Computer-Aided drug design.                                      | <b>05</b> |
|             | (c) | How target structure is derived? How can we determine binding site in the target?                     | <b>05</b> |

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