

**GUJARAT TECHNOLOGICAL UNIVERSITY**  
**B.PHARM - SEMESTER-VIII • EXAMINATION – SUMMER-2017**

**Subject Code: 2280006**

**Date: 09/05/2017**

**Subject Name: Computer Applications in drug discovery**

**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.

- |             |   |           |
|-------------|---|-----------|
| <b>Q.1</b>  | (a) Write a brief note on importance of drug design approaches in drug discovery.                               | <b>06</b> |
|             | (b) Explain in brief pharmacophore model based on virtual screening.  | <b>05</b> |
|             | (c) Write a short note on multi target inhibitors using pharmacophore model.                                    | <b>05</b> |
| <b>Q.2</b>  | (a) Explain in details high resolution protein docking.   | <b>06</b> |
|             | (b) Give a brief account of dynamic pharmacophore models.   | <b>05</b> |
|             | (c) What is structure based virtual high throughput screening?  | <b>05</b> |
| <b>Q.3</b>  | (a) Write a short note on genetic algorithms in protein ligand docking.   | <b>06</b> |
|             | (b) Enumerate scoring functions for evaluation of protein ligand complexes.<br>Explain any one in details.      | <b>05</b> |
|             | (c) Explain in details representation of small molecules as “SMILES” in ligand<br>databases for CADD.           | <b>05</b> |
| <b>Q.4</b>  | (a) Enlist methods to identify protein binding sites and explain any one in detail.                             | <b>06</b> |
|             | (b) Write a short note on comparative modeling in structure based CADD.   | <b>05</b> |
|             | (c) Write a short note on protein-ligand docking in drug design.  | <b>05</b> |
| <b>Q.5</b>  | (a) Explain in detail 2D description of molecular constitution as molecular<br>descriptor in ligand based CADD. | <b>06</b> |
|             | (b) Write a short note on multidimensional QSAR in drug discovery.  | <b>05</b> |
|             | (c) Explain in brief linear regression method in QSAR models.   | <b>05</b> |
| <b>Q. 6</b> | (a) What is pharmacophore? Explain in brief molecular superimposition in<br>pharmacophore mapping.              | <b>06</b> |
|             | (b) Explain in brief binary molecular fingerprints as molecular descriptors in ligand<br>based CADD.            | <b>05</b> |
|             | (c) Explain in detail pocket matching in structure based CADD.  | <b>05</b> |
| <b>Q.7</b>  | (a) Explain in brief human ether-a-go-go related gene potassium channel<br>inhibition.                          | <b>06</b> |
|             | (b) What is toxicity prediction software package? Explain it.   | <b>05</b> |
|             | (c) What is compound library filters? Explain it.   | <b>05</b> |

\*\*\*\*\*