

GUJARAT TECHNOLOGICAL UNIVERSITY
B.PHARM – SEMESTER – 8- EXAMINATION – WINTER - 2018

Subject Code: 2280006**Date: 28/11/2018****Subject Name: Computer Applications in drug discovery****Time: 02:30 PM TO 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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|-------------|-----|---|-----------|
| Q.1 | (a) | Define ligand based CADD. Enumerate its features and explain binary molecular fingerprints in detail. | 06 |
| | (b) | Write a note on dynamic pharmacophore model. | 05 |
| | (c) | What are docking? Describe various docking methods. | 05 |
| Q.2 | (a) | Explain how comparative modeling method used for preparation of a target structure for SBDD. | 06 |
| | (b) | Write a note on knowledge based scoring function and consensus scoring function. | 05 |
| | (c) | Explain genetic algorithms in SBDD | 05 |
| Q.3 | (a) | Write a note on multidimensional QSAR. | 06 |
| | (b) | Discuss on Toxicity Prediction software packages. | 05 |
| | (c) | Define force field and describe various methods for energy minimization. | 05 |
| Q.4 | (a) | Describe application of QSAR in ligand based CADD. | 06 |
| | (b) | Write in detail about COMFA and COMSIA methods of QSAR. | 05 |
| | (c) | Explain about linear regression methods. | 05 |
| Q.5 | (a) | Write a note on pharmacophore algorithms and software packages. | 06 |
| | (b) | Explain how ligand libraries were prepared for CADD? | 05 |
| | (c) | Describe about the target data bases for computer aided drug design in detail. | 05 |
| Q. 6 | (a) | Enumerate different approaches for binding site detection and characterization in SBDD and explain any one in detail. | 06 |
| | (b) | Write down prediction of ADME in detail. | 05 |
| | (c) | Explain about 3D description of molecular configuration and conformation. | 05 |
| Q.7 | (a) | Explain in detail about SBVS. | 06 |
| | (b) | Write a note on high resolution docking. | 05 |
| | (c) | Write a note on importance of various drug design approaches in drug discovery. | 05 |
