

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

Subject Code: 2280006**Date: 10/06/2022****Subject Name: Computer Application In Drug Discovery****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) Write in brief about various approaches to drug discovery. | 06 |
| | (b) Write a note on representation of small molecules as “SMILES”. | 05 |
| | (c) Explain in brief about target databases for Computer Aided Drug Discovery. | 05 |
| Q.2 | (a) Explain various methods for binding site detection and characterization and discuss Pocket matching in detail. | 06 |
| | (b) Discuss about empirical scoring functions. | 05 |
| | (c) Write note on high resolution docking. | 05 |
| Q.3 | (a) Discuss about multitarget inhibitors using common pharmacophore model. | 06 |
| | (b) Write a note on binding site characterization. | 05 |
| | (c) Discuss about comparative modeling in preparation of target. | 05 |
| Q.4 | (a) Discuss various Toxicity Prediction Software Packages and Algorithms. | 06 |
| | (b) Write note on binary molecular fingerprints. | 05 |
| | (c) Discuss about pharmacophore algorithms and software packages. | 05 |
| Q.5 | (a) Write a note on importance of various drug design approaches in drug discovery. | 06 |
| | (b) Write note on 4D and 5D descriptors. | 05 |
| | (c) Write method of selection of optimal descriptors in ligand based CADD. | 05 |
| Q. 6 | (a) Explain how ligand libraries were prepared for CADD? | 06 |
| | (b) Explain structure based virtual high throughput screening. | 05 |
| | (c) Discuss about Monte Carlo Search with metropolis criterion. | 05 |
| Q.7 | (a) Enlist methods to identify protein binding sites and explain geometric method. | 06 |
| | (b) Explain how ligand libraries were prepared for CADD? | 05 |
| | (c) Explain genetic algorithms in SBDD | 05 |
