# GUJARAT TECHNOLOGICAL UNIVERSITY
## B.PHARM - SEMESTER– 8 EXAMINATION – SUMMER -2023

**Subject Code: 2280006**                                              **Date:26/06/2023**
**Subject Name: Computer Applications in drug discovery**
**Time: 10.30 a.m. to 1.30 p.m.**                                    **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 ligand? Explain the preparation of ligand library for CADD.** | **06** |
| | **(b) Explain in detail about target based CADD.** | **05** |
| | **(c) Differentiate between SBDD and LBDD.** | **05** |
| **Q.2** | **(a) Explain various technique for detection and characterization of binding site.** | **06** |
| | **(b) Which genetic algorithm are used for protein-ligand docking?** | **05** |
| | **(c) Explain various scoring function for evaluation of protein ligand interaction.** | **05** |
| **Q.3** | **(a) Write a note on virtual HTS.** | **06** |
| | **(b) Explain virtual screening using pharmacophore modelling.** | **05** |
| | **(c) Write a note on high resolution docking.** | **05** |
| **Q.4** | **(a) What are physicochemical properties? Explain octanol/water partition.** | **06** |
| | **(b) Explain about 4-D and 5-D QSAR.** | **05** |
| | **(c) Write a note on pharmacophore mapping.** | **05** |
| **Q.5** | **(a) Explain methods for optimization of drug metabolism.** | **06** |
| | **(b) How prediction of human ether-a-go-go related gene binding done?** | **05** |
| | **(c) Describe various software and their application for toxicity prediction.** | **05** |
| **Q. 6** | **(a) Explain binary molecular finger prints.** | **06** |
| | **(b) Describe about 3-D descriptor used for molecular properties.** | **05** |
| | **(c) What is lead compound?  How it can be optimized?** | **05** |
| **Q. 7** | **(a) Explain how to represent small molecules as SMILES.** | **06** |
| | **(b) Write a note on Monte Carlo simulation.** | **05** |
| | **(c) Write a note on 2-D descriptors** | **05** |

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