# GUJARAT TECHNOLOGICAL UNIVERSITY

## POST GRADUATE DIPLOMA IN BIOINFORMATICS SEMESTER - 1 WINTER 2021 EXAMINATION

**Subject Code:1310206**                                    **Date:15 Mar 2022**

**Subject Name:Computer Aided Drug Designing**

**Time:10:30 AM TO 01:00 PM**                          **Total Marks: 70**

**Instructions:**
1. **Attempt all questions.**
2. **Make suitable assumptions wherever necessary.**
3. **Figures to the right indicate full marks.**
4. **Draw neat and clean diagrams as required**

**Q.1**       **Write a note on following**                                    **(Marks-10X2=20)**

1. Protein-ligand docking
2. MODELLER
3. AutoDock and AutoDock vina
4. Homology model validation tools
5. ADME properties
6. Lipophilicity parameter
7. Quantum Mechanics
8. RMSD and RMSF
9. Forcefield
10. Lipinski's rule of five

**Q.2**       **Answer the following (Any 2 out of 3)**                   **(Marks-2X10=20)**

1. Define rational drug design. Explain lead identification and lead optimization process in detail.
2. What are pharmacophores? Give an account of the structure-based and ligand-based pharmacophore design?
3. Discuss *in silico* structure prediction methods with emphasis on homology modelling.

**Q.3**       **Answer the following  (Any 6 out of 8)**                  **(Marks-6X5=30)**

1. Explain energy minimization and utility in biomolecule optimization.
2. What are 2DQSAR descriptors? Discuss on electronic descriptors
3. Discuss molecular dynamics simulations in evaluating conformational stability of a biomolecule
4. Discuss molecular modelling approaches for structure optimization
5. Discuss briefly on COMFA and CoMSIA
6. Explain circumstances one need to implement de novo drug design in their drug discovery projects.
7. Give a brief account of computer-aided antibody design to enhance binding affinity of a known antibody.
8. Discuss briefly on various molecular docking software

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