GUJARAT TECHNOLOGICAL UNIVERSITY

POST GRADUATE DIPLOMA IN BIOINFORMATICS SEMESTER - 1 WINTER 2022 EXAMINATION

Subject Code:1310206   **Date:7 Jan 2023**
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. BLAST and how it can be used as a Homology and similarity search tool?
2. Describe Genbank sequence format with example?
3. In Ramachandran plot, the values of the dihedral angle ψ(psi) is based on rotation around which bond?
4. ProSA web-server.
5. Importance of sequence identity and query coverage in homology modeling.
6. Uncompetitive inhibition.
7. Use of Procheck tool
8. Docking and how it is useful in computational based drug discovery
9. Swiss modeler.
10. Protein tertiary structure database.

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

1. What is Homology Modeling? Describe its importance. Describe model building using phyre web server.
2. Describe the type of protein structure validation software. Briefly describe Ramachandran Plot.
3. Describe the different methods of enzyme inhibition. How to identify an active site when substrate binding activity is known.

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

1. Briefly describe structure based and fragment based drug designing.
2. What is sequence homology? Describe the importance of BLAST in Homology modeling.
3. Describe Errat plot briefly.
4. Molecular complementarity in Computational Docking
5. Shed light on molecular Flexibility in Protein-Ligand Docking
6. Describe any 3 type of sequence format.

7. Describe the Phyre2 result briefly.
8. What do you mean by template structure in homology modeling? Describe its importance. Describe the Factor (template) affecting the Homology Modeling.