Seat No.: _____ Enrolment No._____

GUJARAT TECHNOLOGICAL UNIVERSITY

POST GRADUATE DIPLOMA IN BIOINFORMATICS (DB) - SEMESTER - 1 EXAMINATION - WINTER - 2023

Subject Code:1310206 Date: 20 Dec 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. What do you understand by SMILE notation.

2. Write a short note on the importance of electrostatic interactions in the protein folding process.

3. Write a short note on the knowledge-based fold recognition method of protein tertiary structure prediction.

4. Write a short note on combinatorial chemistry and its role in de novo drug design.

5. Write a short note on the hit to lead optimization process and its significance.

6. Write a short note on the importance of various chemical databases and their application in CADD.

7 Write a short note of Lipinski's rule of 5. Why is it considered important in the drug screening process.

8 Explain the role of hydrogen bonds instability of various rigid secondary structural components of a protein.

9 Write a short note on the significance of pharmacokinetics and pharmacodynamics of a drug molecule in the drug discovery process.

10. Write a short note on various drug receptor interactions.

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

1. What do you understand by structure-based drug design? Describe in detail the process of receptor centric design. What are limitations of molecular docking and how can you refine the results of molecular docking?

2. Define Force field, elaborate the equation of a force field in terms of bonded and non-bonded parameters for calculation of energy of a molecule.

3. Explain in detail pharmacophore-based drug design process. How do you think it would be useful in case identification of a new drug molecule for a disease X where drug resistance is a major hurdle in treatment.

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

1.	What are the various 2D molecular descriptors of a molecule that can be used to develop a QSAR equation.	**5**
2.	Why is energy minimization required for molecules? Describe the various steps of energy minimization.	**5**
3.	Early Computer representations of molecules started with line notations in text only systems, which contained all the necessary information about its structure. For an ethane molecule apply any one of the internal 2D computer representations to describe its structure.	**5**
4.	Explain and elaborate with the help of an example the difference between 3D database searching and Virtual screening. Why is one preferred over the other?	**5**
5.	Explain the basic principle of Molecular Dynamics simulation. Why are molecular dynamics simulation calculations with respect to drug receptor interactions considered to be more reliable than molecular docking calculations	**5**
6.	What do you understand by secondary structure prediction of a protein. Give examples of any two tools used for prediction of secondary structure of a given protein sequence.	**5**
7	Explain and elaborate with the help of an example the difference between 3D database searching and Virtual screening. Why is one preferred over the other?	**5**
8	Why do you think target identification is the most important step in the drug discovery process. What are the various considerations to be taken care of during target identification?	**5**

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