Seat No./Enrolment No._____

GUJARAT TECHNOLOGICAL UNIVERSITY

POST GRADUATE DIPLOMA IN BIOINFORMATICS (DB) - SEMESTER - 1 EXAMINATION - WINTER - 2024

Subject Code:1310206 **Date: 03 Jan 2025**

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. How does quantum mechanics contribute to drug design?
2. What is a contour map analysis in 3D-QSAR?
3. What is Free Wilson analysis, and how does it differ from Hansch analysis?
4. Differentiate between global minimum conformation and bioactive conformation.
5. What is the full form of ADMET? Give the reason why is predicting ADMET properties important in drug design.
6. What are the key features typically identified in a pharmacophore?
7. Write a short note on internal 2D structure representations of a small molecule.
8. What techniques can be used for the validation of drug candidates identified through SBDD?
9. Give the advantages of structure-based virtual screening.
10. How does flexible docking differ from rigid docking?

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

1. Describe the integration of structure-based and ligand-based approaches in the context of Computer-Aided Drug Design.
2. Provide a detailed description of the empirical force field and explain its role in calculating the energy of a molecule.
3. Compare and contrast quantitative structure-activity relationship (QSAR) modeling with molecular dynamics simulations in drug design.

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

1. What parameters are typically evaluated in docking studies? Explain.
2. What is fragment-based drug design (FBDD)? How does it differ from traditional drug design?
3. How does pharmacophore-based screening differ from similarity-based methods?

4. Provide a brief overview of the different secondary structures found in proteins. Which secondary structure is the most flexible and commonly located in the active site of a protein?
5. Describe the conjugate gradient method for energy minimization. What makes it more advantageous than the steepest descent method when dealing with large molecules?
6. How does SMILES notation improve upon other line notations, such as Wiswesser line notation, based on the information it encodes? Please explain.
7. How can genomic and proteomic data contribute to the discovery of novel drug targets? Please explain in detail.
8. What advantages does molecular dynamics offer over molecular mechanics calculations? Provide a brief explanation.

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