**STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086**
**(For candidates admitted from the academic year 2019 – 2020 & thereafter)**

**M. Sc. DEGREE EXAMINATION, NOVEMBER 2023**
**BIOINFORMATICS**
**THIRD SEMESTER**

**COURSE : CORE**
**PAPER : MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGN**
**SUBJECT CODE : 19BI/PC/MC34**
**TIME : 3 HOURS MAX. MARKS: 100**

**SECTION – A**

**ANSWER ALL QUESTIONS (20 x 1 = 20)**

1. In molecular modeling, what are Potential Energy Surfaces, and how are they used?
2. How torsion angle potentials are incorporated into force fields?
3. Define Van der Waals interactions and provide an example of their significance in molecular modeling.
4. Describe the role of Electrostatic Potential in molecular interactions. How does it influence non-bonded interactions?
5. What is the importance of Hydrogen Bonding in molecular modelling? Provide examples of hydrogen bonding terms.
6. Differentiate between derivative and non-derivative energy minimization methods. When might one be preferred over the other?
7. Define long range forces.
8. Define the significance of saddle point.
9. Describe the general approach for molecular simulation.
10. Define Gibbs Ensemble.
11. Describe the principles of Molecular Dynamics using a simple model. How does it simulate molecular motion?
12. Explain the significance of incorporating solvent effects into Molecular Dynamics simulations at constant temperature and pressure.
13. Discuss the concept of conformational changes observed from Molecular Dynamics simulations.
14. Elaborate Microcanonical ensemble?
15. What is a trajectory in molecular dynamics?
16. Define Protein Structure Prediction. Explain the process of Secondary Structure Prediction and its applications.
17. Differentiate between Homology modeling and ab initio methods in protein structure prediction. When is each approach suitable?
18. Discuss the tools and techniques used for protein structural visualization and geometry optimization.
19. How does the Ramachandran Plot serve as a tool for structure validation in molecular modeling?
20. What is Molecular Docking, and how does it contribute to Structure-Based Drug Design? Describe the steps involved in lead identification and optimization.

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## SECTION – B

**ANSWER ANY FOUR QUESTIONS (4 x 10 = 40)**

21. Explain the significance of using different molecular representations in molecular modelling.
22. Discuss the challenges and strategies for incorporating solvent effects into Molecular Dynamics simulations at constant temperature and pressure.
23. Explain the concepts of calculation of simple thermodynamic properties.
24. Describe the essential components of a Molecular Dynamics simulation using continuous potential. Explain how this approach can be used to study the motion of molecules.
25. Explain the principles and methodologies involved in predicting secondary protein structures. Discuss the limitations and accuracy of these predictions in real-world applications.
26. Elaborate on the steps involved in structure-based drug design using molecular docking. Explain how this approach aids in target discovery, lead identification, and optimization.
27. Discuss the principles of Quantitative Structure-Activity Relationship (QSAR) and 3D pharmacophore identification in drug design. Explain their significance and provide examples of their applications in drug discovery.

**ANSWER ANY TWO OF THE FOLLOWING IN DETAIL (2 x 20=40 )**

28. Molecular modeling relies on various representations, coordinate systems, and potential energy surfaces. Explain the significance of each of these components in molecular mechanics. How do they collectively contribute to our understanding of molecular behavior and interactions? Provide specific examples to illustrate their applications.
29. Compare and contrast derivative and non-derivative energy minimization methods used in molecular modeling. Discuss the mathematical principles underlying each method and their practical applications. Provide insights into scenarios where one method might be preferred over the other.
30. Comment on molecular mechanics and explain the different force fields.
31. Ligand-based drug design approaches play a vital role in drug discovery. Explain the principles and applications of lead designing, High Throughput Screening (HTS), and the use of chemical libraries in ligand-based drug design. Discuss how ADME prediction contributes to the success of drug candidates. Provide examples of successful drug design projects that utilized these approaches.

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