

M. Sc. DEGREE EXAMINATION, NOVEMBER 2022  
BIOINFORMATICS  
THIRD SEMESTER

COURSE : CORE  
PAPER : MOLECULAR MODELING AND COMPUTER AIDED DRUG  
DESIGN  
TIME : 3 HOURS

MAX. MARKS: 100

SECTION – A

ANSWER ALL QUESTIONS

(20 x 1 = 20)

1. Define potential energy surface.
2. Define force field.
3. What is a coordinate system?
4. What are long range forces?
5. Brief about Verlet algorithm.
6. What are Gibbs free energy and change in Gibbs energy?
7. Define ensemble.
8. Define the periodic boundary conditions.
9. Why do we need to minimise energy?
10. What is the difference between dynamics and Monte Carlo simulation?
11. Define ADMET.
12. Define a pharmacophore?
13. What is *ab initio* modelling?
14. How a chemical library can be constructed?
15. Mention two protein visualization tools.
16. Differentiate leads and hits.
17. Expand QSAR.
18. How the modelled protein structure can be validated?
19. Write brief notes on any two molecular descriptors.
20. Justify the need for selecting a potential target for molecular docking.

SECTION – B

ANSWER ANY FOUR QUESTIONS

(4 x 10 = 40)

21. Explain the coordinate systems and detail their types.
22. Enumerate the significance of force fields and why different force fields are needed for effective structure analysis.
23. How molecular thermodynamic properties are explored during protein structure analysis?
24. List out the advantages of Monte Carlo simulation.
25. How effective the pharmacophore modelling in the field of drug discovery?.
26. Describe the ways of protein structure prediction methodologies.
27. Explain the methods involved in loop refinement and geometry optimization.

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

28. Discuss in detail about Energy Minimization and their applications in structural bioinformatics.
29. Explain the concepts of molecular dynamics. Elaborate in detail the various algorithms involved.
30. Appreciate “structure based drug design” and explain various strategies.
31. How “molecular descriptors” are exploited in QSAR. Also elaborate the significance of QSAR.

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