K25U 0958

Reg. No. : .....

Name : .....

IV Semester B.Sc. Degree (C.B.C.S.S. – O.B.E. – Regular/Supplementary/ Improvement) Examination, April 2025
(2020 to 2023 Admissions)
CORE COURSE IN LIFE SCIENCES (ZOOLOGY) AND COMPUTATIONAL BIOLOGY
4B05 ZCB : Biomolecular Modelling and Simulations

Time : 3 Hours Max. Marks : 40

PART – A

Write about **each** of the following in **2** to **3** sentences. **Each** question carries **1** mark. **(6×1=6)**

1. Define PDB format.
2. Alpha helix.
3. Types of β-sheets
4. Homology modelling.
5. Membrane proteins.
6. Force field in molecular modelling.

PART – B

Explain about **any six** of the following. **Each** question carries **2** marks. **(6×2=12)**

7. What are the key differences between alpha-class and beta-class protein folds ?
8. Explain the concept of geometry optimization in molecular modelling.
9. What are detergent micelles, and why are they used in membrane protein studies ?
10. What is Quaternary structure ? Give example of a protein with quaternary structure.

P.T.O.

11. Explain the concept of a protein fold.

12. Write down the importance of lipid bilayers in molecular modelling.

13. Discuss the importance of computational biology tools in predicting protein structures.

14. Explain the concept of free energy calculations in molecular dynamics simulations.

PART – C

Write short essay on **any four** of the following. **Each** question carries **3** marks. **(4×3=12)**

15. Describe the historical perspective of molecular modelling and its roots in molecular mechanics.

16. Describe the concept of molecular electrostatic potential and its importance in understanding protein structures.

17. Describe the hierarchical structure of proteins.

18. What are the key steps in converting 2D structural data into a 3D model ?

19. Explain the concept of alpha/beta barrels.

20. Discuss the importance of membrane protein simulations in understanding biological processes.

PART – D

Write essay on **any two** of the following. **Each** question carries **5** marks. **(2×5=10)**

21. Explain the concept of molecular dynamics simulations and its applications in computational biology. Discuss the limitations of molecular dynamics simulations.

22. Discuss various molecular dynamics packages and their functionalities.

23. Describe the energy minimization procedures used in molecular modelling.

24. Explain the basic molecular dynamics algorithm and its application in simulating macromolecules. Describe the difference between Newtonian and Brownian dynamics.

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