



K24U 0857

Reg. No. : .....

Name : .....

**IV Semester B.Sc. Degree (CBCSS-OBE-Regular/Supplementary/  
Improvement) Examination, April 2024  
(2020 to 2022 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** or **3** sentences. **Each** question carries **1** mark.

(6×1=6)

1. X-Ray crystallography
2. PDB
3. Leucine-Rich  $\alpha/\beta$  Folds
4. Folded Leafs
5. Molecular Dynamics (MD)
6. Lipid bilayers.



PART – B

Explain about **any six** of the following. **Each** question carries **2** marks.

(6×2=12)

7. NMR spectroscopy.
8.  $\alpha/\beta$  and  $\alpha + \beta$ -Class Folds.
9. Give a brief account of the prediction of primary, secondary and tertiary structure of proteins with suitable computational biology tools.
10. AMBER.

P.T.O.



11. Newtonian approach in MD.
12. Free energy calculations in MD.
13. List out any four computational tools for molecular modeling.
14. Homology modelling.

PART – C

Write short essay on **any four** of the following. **Each** question carries **3** marks.

**(4×3=12)**

15. Roots of Molecular Modelling in Molecular Mechanics.
16. Name the Classes in Protein Architecture.
17. Parallel and Anti-parallel combinations of  $\beta$ -Class Folds.
18. Write an account on any two Molecular dynamics packages.
19. Systematic search procedures in Conformational analysis.
20. What are the three main aspects of Generation of 3D Coordinates in molecular modelling ?

PART – D

Write essay on **any two** of the following. **Each** question carries **5** marks.

**(2×5=10)**

21. Write an essay on Protein Structure Hierarchy.
  22. Describe about membrane protein simulations.
  23. Discuss the procedures of conformational analysis in molecular modelling.
  24. Write an essay on energy minimizing procedures in molecular modelling.
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