K23U 1158

Reg. No. : .....

Name : .....

IV Semester B.Sc. Degree (CBCSS-OBE-Regular/Supplementary/ Improvement) Examination, April 2023
(2020 Admission Onwards)
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. Hairpin arrays
2. Collagen helix
3. Techniques of Geometry optimization
4. Interaction potential of proteins
5. Energy Minimization
6. Lipid Bilayers.

PART – B

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

7. Parallel and anti-parallel combinations.
8. Classical alpha helix.
9. Fragment libraries
10. In vitro membrane protein environments.

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11. Self-assembly systems.
12. Brownian dynamics MD simulations.
13. Treatment of long-range forces.
14. Turns and loops.

PART – C

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

15. Detergents and their use in membrane proteins.
16. Free energy calculations.
17. Quantum mechanical methods.
18. Principle and applications of X-Ray Crystallography.
19. Monte Carlo method of molecular modelling.
20. Quaternary structure.

PART – D

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

21. Protein Data Bank format.
22. GROMACS
23. Give an overview on the prediction of secondary structure of proteins with suitable computational biology tools.
24. Ab initio prediction methods in molecular modeling.

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