Reg. No. : ....

Name : ....

V Semester B.Sc. Degree (C.B.C.S.S. – O.B.E. – Regular/Supplementary/ Improvement) Examination, November 2024
(2020 to 2022 Admissions)
CORE COURSE IN LIFE SCIENCES (ZOOLOGY) AND COMPUTATIONAL BIOLOGY
5B10ZCB : Computer Aided Drug Discovery

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. Define the term "Chemical Intuition".

2. What is pharmacophore modelling ?

3. Name two molecular visualization tools.

4. What is molecular mimicry ?

5. Define the term "ADMET".

6. Name two commonly used MD simulation programs in CADD.

PART – B

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

7. Briefly explain about CADD groups.

8. Explain the term "Drug likeliness".

9. Explain the terms : AMBER and GROMACS.

10. Distinguish between 2D and 3D QSAR models.

11. Define search algorithms and scoring functions.

12. What is a force field in MD simulation ?

13. Name the types of virtual screening techniques.

14. Mention the biological tools for molecular modelling and model refinement.

PART – C

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

15. Define molecular docking. Explain rigid docking.

16. Define in detail structure based virtual screening.

17. What is lead compound ? Discuss lead discovery in drug design.

18. What is COMFA and COMSIA ? Explain.

19. Explain various energy minimization techniques in molecular modelling.

20. Discuss on ab initio and semi-empirical methods of molecular energy calculations.

PART – D

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

21. Explain the key principles, types and steps involved in the molecular docking process. Also give an account on the major molecular docking programs.

22. Describe QSAR modelling and its applications in computational drug discovery.

23. Discuss in detail the various stages of drug discovery and development.

24. Explain the significance of molecular superposition and structural alignment in drug discovery.

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