K23U 2593

Reg. No. : .....

Name : .....

V Semester B.Sc. Degree (CBCSS – OBE – Regular/Supplementary/ Improvement) Examination, November 2023
(2020 – 2021 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. What are the key stages in the drug discovery and development process ?
2. Explain the concept of pharmacophore modeling in drug discovery.
3. What is the purpose of structure-based virtual screening in computational drug discovery ?
4. Describe the main components of the molecular docking process.
5. Name two commonly used molecular dynamics simulation programs in computational drug discovery.
6. Briefly explain the difference between 2D QSAR and 3D QSAR in drug discovery.

PART – B

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

7. Explain the concept of "Molecular Mimicry" and its relevance in drug discovery.
8. Discuss the role of "Chemical Intuition" in the drug discovery process.

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9. Highlight some contributions and achievements of CADD groups in the field of drug discovery.

10. Discuss the significance of model visualization in drug discovery.

11. What are ADMET studies and why are they crucial in drug discovery ?

12. Describe the steps involved in designing a QSAR experiment.

13. Explain the importance of validating force fields and programs in molecular dynamics simulations.

14. Name and briefly explain some major docking programs and utilities used in drug discovery.

PART – C

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

15. Discuss the importance of molecular superposition and structural alignment in molecular modeling. Provide examples of how these techniques are used in drug discovery.

16. How can computational biology tools and statistical models assist in the prediction of ADMET properties ?

17. Explain the significance of search algorithms and scoring functions in molecular docking.

18. Discuss the strengths and limitations of major molecular dynamics simulation programs like AMBER and GROMACS.

19. Provide examples of how QSAR modeling has been applied in real-world drug discovery scenarios.

20. Explore the world of molecular dynamics simulations, covering topics such as force fields, computational requirements and the simulation process.

PART – D

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

21. Discuss the role of rational approaches in drug discovery. How do these approaches leverage computational tools and techniques to enhance the efficiency of the drug development process ? Provide examples.

22. Discuss the fundamental concepts of force fields, computational requirements and the simulation process. How are these simulations applied to gain insights into drug-receptor interactions and other biological processes ?

23. Describe the key principles, types and steps involved in the molecular docking process. Provide insights into how it helps in identifying potential drug-receptor interactions.

24. Explain the significance of molecular superposition and structural alignment in drug discovery. How do these techniques aid in the identification of potential drug candidates ? Discuss their applications in real-world scenarios.
