K24U 2898

Reg. No. : .....

Name : .....

V Semester B.Sc. Degree (CBCSS – OBE – Regular/Supplementary/ Improvement) Examination, November 2024
(2020 to 2022 Admissions)
CORE COURSE IN LIFE SCIENCES (ZOOLOGY) AND COMPUTATIONAL BIOLOGY
5B09ZCB : Chemoinformatics and Computational Medicinal Chemistry

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 is similarity search ?
2. Define chemical space.
3. What is the role of chemical indexing in database search methods ?
4. What do you understand by drug absorption in pharmacokinetics ?
5. What do you mean by the steric parameters ?
6. What is a focused library in combinatorial chemistry ?

PART – B

Explain **any 6** of the following. **Each** question carries **2** marks.

7. What are molecular descriptors ? Give two examples of it.
8. What is the significance of 2D and 3D structure searching in chemoinformatics ?
9. Differentiate between drug absorption and drug metabolism.
10. Describe the significance of proximity searching.

P.T.O.

11. Explain the role of SAR in drug design.

12. What is the concept of structural graphs in database searches ?

13. Discuss the mode of action of antimalarial agents.

14. What do you understand by drug receptor interactions ? **(6×2=12)**

PART – C

Write a short essay on **any 4** of the following. **Each** question carries **3** marks.

15. Explain the process of Pharmacophores and Fingerprint in similarity searching.

16. Discuss the history and development of QSAR in drug design.

17. Describe the concept of lipophilicity and its significance in drug design.

18. Explain the principles of drug action and their relevance in pharmacodynamics.

19. What are the different classifications and SAR of antifungal agents ?

20. Discuss the combinatorial library design strategies. **(4×3=12)**

PART – D

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

21. Discuss the process of virtual screening and prediction of ADMET properties.

22. Briefly explain about the classification and mode of action of various antibiotics.

23. Explain the importance of pharmacokinetics in drug development process.

24. Explain the need and scope of chemoinformatics databases in scientific research. **(2×5=10)**

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