17801

BRAINWARE UNIVERSITY

Term End Examination 2024-2025
Programme – M.Pharm(PC)-2024
Course Name – Computer Aided Drug Design
Course Code - MPC203T
(Semester II)

Full Marks : 75 **Time : 3:0 Hours**

[The figure in the margin indicates full marks. Candidates are required to give their answers in their own words as far as practicable.]

Group-A
(Short Answer Type Questions) 5 x 5=25

1. Ennumerate the steps involved in QSAR. (5)
2. Explain the advantages and limitations of homology modeling in drug discovery. (5)
3. Illustrate on the application of Free Wilson analysis. (5)
4. Mention the various steps involved in drug discovery process. (5)
5. Summarize the significance of pharmacophore mapping in drug discovery. (5)

OR

Summarize the role of virtual screening help for identifying potential drug candidates. (5)

Group-B
(Long Answer Type Questions) 10 x 5=50

6. Explain the various validation techniques, such as re-docking, cross-docking, and using experimental binding data. (10)
7. Enumerate on the statistical methods for QSAR. (10)
8. Explain the process of lead optimization in drug design and how do medicinal chemists modify molecular properties to enhance drug performance. (10)
9. Write the concept of de novo drug design in silico and how do computational techniques generate entirely new chemical structures with desired pharmacological properties. (10)

OR

Write the differences between ligand-based and structure-based virtual screening approaches. (10)

10. Summarize how homology modeling is applied in drug discovery. (10)

OR

Summarize the role of in silico ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) prediction in virtual screening and how does evaluating ADMET properties early in the screening process influence the selection of drug candidates. (10)

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