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BRAINWARE UNIVERSITY

Term End Examination 2025-2026

Programme – M.Pharm(PC)-2025

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. Enumerate on the application of Hammett equation. (5)
2. Illustrate on the application of Free Wilson analysis. (5)
3. Explain schematically the steps for construction of QSAR model using OECD guideline. (5)
4. Summarise the various factors contributing to drug discovery. (5)
5. Propose a workflow integrating COMFA and COMSIA analysis for rational drug design. (5)

OR

Justify how does virtual screening accelerate the process of drug discovery. (5)

Group-B

(Long Answer Type Questions)

10 x 5=50

6. Explain the mechanism of action of dihydrofolate reductase (DHFR) inhibitors in cancer therapy. (10)
7. Explain the concept of homology modeling in structural biology and how is it used to predict the 3D structure of a protein. (10)
8. Enumerate on the development of QSAR model. (10)
9. Summarize the limitations and challenges of homology modeling. (10)

OR

- Summarize the challenges of false positives/false negatives in virtual screening and what strategies are employed to reduce the occurrence of false predictions and improve the accuracy of the screening process. (10)
10. Write the concept of in silico drug design and its significance in modern drug discovery. (10)

OR

Write the concept of virtual screening (VS) in drug discovery and how does it aid in identifying potential lead compounds. (10)
