BRAINWARE UNIVERSITY

Term End Examination 2025-2026
Programme – M.Sc.(BI)-2025
Course Name – Computer-Aided Drug Design
Course Code - MBI27503 (T)
(Semester II)

Full Marks : 40 **Time : 2:0 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

(Multiple Choice Type Question) 1 x 10=10

1. *Choose the correct alternative from the following :*

(i) Differential gene expression analysis mainly supports which stage?

a) Clinical validation b) Target identification
c) Drug formulation d) Lead optimization

(ii) Early ADMET prediction helps to:

a) Increase chemical diversity b) Reduce late-stage drug failure
c) Improve docking accuracy d) Identify molecular targets

(iii) In docking workflows, why are ligands often converted to MOL2 format?

a) For accurate atom types and partial charges b) For protein folding analysis
c) For sequence annotation d) For secondary structure prediction

(iv) Missing residues in protein structures must be corrected because they:

a) Distort binding site geometry b) Reduce file size
c) Affect ligand flexibility d) Change primary sequence

(v) Which visualization representation in PyMOL is best for observing protein–ligand interactions?

a) Sequence view b) Line plot
c) Histogram d) Stick or surface model

(vi) Why is Chimera particularly useful for comparing experimental and predicted structures?

a) It removes water molecules b) It predicts ADMET properties
c) It performs docking automatically d) It provides structure alignment and comparison tools

(vii) Why should AlphaFold models be interpreted cautiously for multi-protein complexes?

a) They may not represent quaternary interactions accurately b) They lack atomic coordinates
c) They are computationally expensive d) They are low resolution

(viii) Which ensemble maintains constant number of particles, volume, and temperature?

a) NPT
b) NVT
c) Grand canonical
d) NVE

(ix) Why are periodic boundary conditions used in MD simulations?

a) To mimic an infinite system
b) To increase protein rigidity
c) To stabilize ligands
d) To reduce atom count

(x) How does integration of FBDD and de novo design enhance drug discovery?

a) It combines fragment efficiency with creative molecule generation
b) It avoids docking
c) It eliminates experiments
d) It reduces chemical diversity

Group-B

(Short Answer Type Questions) 3 x 5=15

2. Describe the role of lead optimization in the drug discovery pipeline. (3)
3. Demonstrate the role of docking scores in ranking compounds during virtual screening. (3)
4. Examine how RMSF analysis helps identify flexible regions in proteins. (3)
5. Differentiate between structure-based and ligand-based drug design approaches. (3)
6. Justify the selection of MOL2 format over PDB format for ligand docking. (3)

OR

Critically analyze the use of AlphaFold models in drug discovery studies. (3)

Group-C

(Long Answer Type Questions) 5 x 3=15

7. Analyze the principles and applications of MM-PBSA and MM-GBSA methods. (5)
8. Explain the principles of computer-aided drug design and discuss its role in modern drug discovery. (5)
9. Evaluate the principles and computational framework of de novo drug design. (5)

OR

Assess the impact of weak fragment binding on the overall success of fragment-based workflows. (5)

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