BRAINWARE UNIVERSITY

Term End Examination 2025-2026
Programme – M.Sc.(BI)-2025
Course Name – Cheminformatics and Drug Discovery
Course Code - MBI20405
(Semester II)

Full Marks : 60 **Time : 2:30 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 15=15

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

(i) Choose the software tool primarily used for the interconversion of over 100 chemical file formats?
a) PyMOL b) RDKit
c) ChemDraw d) Open Babel

(ii) Name the database that is maintained by the NCBI and contains Substance, Compound, and BioAssay sections?
a) ChEMBL b) DrugBank
c) ZINC d) PubChem

(iii) Recall the term describing a graphical representation of molecules in three dimensions.
a) Molecular graphics b) Fingerprint
c) Descriptor d) Topology

(iv) Indicate the purpose of CONECT records in a PDB file.
a) Store energy values b) Define symmetry
c) Specify bonding connectivity d) Indicate atom charge

(v) Interpret the function of temperature (B) factors in PDB files.
a) Measure bond strength b) Indicate atomic charge
c) Reflect atomic mobility d) Define residue type

(vi) Analyze why multiple visualization tools are used in modelling workflows.
a) Cost reduction b) File redundancy
c) Different tools offer complementary analysis d) Standardization

(vii) Identify the force field designed to cover the entire periodic table.
a) AMBER b) CHARMM
c) UFF d) OPLS

(viii) Apply molecular mechanics to calculate thermodynamic properties.
a) Orbital energies b) Enthalpy and free energy

c) UV spectra d) HOMO–LUMO gap

(ix) Evaluate when force-field parametrization becomes necessary.

a) All simulations b) Never required
c) Novel or unusual chemistries d) Only proteins

(x) Apply non-bonded interaction principles to identify which force-field term best represents hydrogen-bond-driven stabilization when modelling ethanol in water.

a) Dispersion interaction b) Electrostatic interaction
c) Bond stretching d) Torsional interaction

(xi) Determine the role of feature tolerance in pharmacophore models.

a) Fix atom types b) Control charge
c) Allow spatial flexibility d) Define topology

(xii) Analyze how pharmacophore features influence virtual screening selectivity.

a) Filter molecules by interaction patterns b) Encode topology
c) Store coordinates d) Predict ADMET

(xiii) Identify the graphical model used in Egan's Egg.

a) Radar plot b) PCA plot
c) LogP vs TPSA plot d) ROC curve

(xiv) Interpret the output of SwissADME bioavailability radar.

a) Binding affinity b) Target selectivity
c) Overall drug-likeness profile d) Toxicity score

(xv) Evaluate why Imatinib is considered a landmark in rational drug design.

a) Viral target b) High toxicity
c) Targeted kinase inhibition strategy d) Rapid approval

Group-B

(Short Answer Type Questions) 3 x 5=15

2. Explain the role of bonded terms in molecular mechanics force fields. (3)
3. Design a basic workflow for generating energy parameters for a small organic compound using molecular modelling. (3)
4. Define a pharmacophore in the context of drug discovery. (3)
5. Apply the Hill System to explain how elements are ordered when writing an empirical formula for organic and inorganic compounds. (3)
6. Analyze the role of ADMET modelling in reducing late-stage drug failure. (3)

OR

Analyze how computational PK/PD models support dose optimization in drug development. (3)

Group-C

(Long Answer Type Questions) 5 x 6=30

7. Explain the types of experimental data stored in the CSD and analyze how CSD data can be used to derive geometric constraints and conformational preferences for molecular modelling. (5)
8. Describe the principles of molecular graphics and discuss their role in visualizing and interpreting 3-D molecular structures. (5)
9. Evaluate the strengths and limitations of classical force fields compared to quantum mechanical methods. (5)
10. A drug discovery project aims to explore chemical space beyond known scaffolds for a GPCR target. Design a pharmacophore-driven screening workflow using databases such as Pharmit or ZINCPharmer. (5)
11. Explain the importance of the Tanimoto coefficient in cheminformatics. (5)
12. Evaluate the significance of chemical clustering and list three common methods. (5)

OR

Analyze the technological prospects of cheminformatics in the post-silicon era. (5)

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