

KATHMANDU UNIVERSITY
End Semester Examination
January/February, 2025

Level : B.Tech.

Year : IV

Time : 2 hrs. 30mins.

Course : BIOT 413

Semester : I

F. M. : 40

09 FEB 2025

SECTION "C"

[4 Q. × 6 = 24 marks]

Attempt ANY FOUR questions.

1. Explain the process of Allosteric modulation. Describe the effect of the different modulators with representative figures. [3+3]
2. Describe the components of pharmacophore model. Give examples on how pharmacophore models are used in structure based and ligand based techniques. [3+3]
3. Explain the various key steps of drug design implemented in structure based approaches with representative examples. [6]
4. Explain the methods for handling protein flexibility during molecular docking. [6]
5. Why molecular dynamics is required even after performing molecular docking? Explain the generic results obtained from a MD simulation. [2+4]

SECTION "D"

[8 Q. × 2 = 16 marks]

Attempt ANY EIGHT questions.

6. Explain competitive antagonism.
7. Why do the torsional angles of Glycine and Proline do not confirm with Ramachandran Plot?
8. Which protein structure prediction methods are used if there is no homologous structure available to compare?
9. How do hydrophobic interactions drive the protein folding process?
10. Explain the terms Resolution, R-factor, Temperature factor and Occupancy as they appear in PDB website.
11. With examples, explain the prediction of biological activity using QSAR.
12. Differentiate between ligand-ensemble and fragmentation methods for introducing ligand flexibility.
13. Explain the components of force fields used for molecular mechanics.
14. How Area Under the Curve is used to assess bioavailability?

