QP Code: 827006 **Reg. No……**

Eighth Semester B. Pharm Degree Regular/Supplementary Examinations March 2025
Computer Aided Drug Design
(2017 Scheme)

Time: 3 Hours **Max. Marks: 75**

- ***Answer all questions to the point neatly and legibly • Do not leave any blank pages between answers • Indicate the question number correctly for the answer in the margin space***
- ***Answer all parts of a single question together • Leave sufficient space between answers***
- ***Draw diagrams wherever necessary***

Essays **(2x10=20)**

1. Enlist the various parameters of QSAR. Explain Hansch & Free Wilson analysis for QSAR with its advantages & disadvantages.
2. Explain the various stages involved in drug discovery.

Short Notes **(7x5=35)**

3. Explain the molecular docking procedures involved in rigid docking.
4. Explain the various methods involved in energy minimization.
5. Explain various databases used in drug design and discovery.
6. Explain homology modeling of proteins.
7. Explain Hammet's substituent constant and Taft's steric constant, and its role in predicting biological activity.
8. Explain the de novo drug design.
9. Explain Bioisosteric replacement with examples.

Answer Briefly **(10x2=20)**

10. Role of computer applications in lead discovery.
11. Define COMFA
12. What is binding free energy in docking.
13. Define pharmacophore.
14. List the docking components.
15. Write a note on history of drug discovery.
16. Define COMSIA.
17. Application of molecular dynamic simulations.
18. Pharmacophore mapping.
19. Application of cheminformatics in drug design.

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