QP Code: 827006 **Reg. No……**

Eighth Semester B. Pharm Degree Supplementary Examinations
November 2024
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. Explain the various methods of lead discovery and add a note on lead optimization.
2. What is pharmacophore modelling. Explain the fundamental steps in pharmacophore modelling.

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

3. Explain global and local energy minimum conformation. List out various energy minimization methods to generate different conformations of a molecule and explain any one of them.
4. What is Hansch analysis in QSAR. Write the equation and explain.
5. Write a note on natural classic bioisosteres giving examples.
6. Define molecular docking. Classify and explain molecular docking methods.
7. Explain structure based drug design approaches in CADD.
8. Molecular dynamic simulation and its applications.
9. Explain the effects of electronic parameters in QSAR.

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

10. Define 3D QSAR. How it is different from 2D QSAR.
11. Explain homology modelling. Enlist the stages in homology modelling.
12. Explain the binding site identification in molecular docking.
13. What are the various strategies used in *de novo* drug design.
14. Explain bioinformatics. How it is useful in drug discovery.
15. What is a lead molecule in a drug discovery programme. Add a note on criteria to be satisfied for a lead molecule.
16. What are the principles of molecular mechanics.
17. Applications of quantum mechanics in drug design.
18. Taft equation.
19. What are the uses of chemical and pharmaceutical databases in drug discovery.

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