QP Code: 827006 **Reg. No……**

Eighth Semester B. Pharm Degree Supplementary Examinations
December 2023
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. Define molecular docking. Classify and explain different molecular docking methods in detail.
2. Enumerate different physicochemical properties of a molecule and explain the role of various physicochemical parameters of a molecule in QSAR studies.

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

3. Pharmacophore mapping.
4. Explain ligand and structure based drug design.
5. Classify bioisosterism and discuss bioisosteric replacement.
6. Explain the principle involved in molecular dynamic simulations and its applications in drug design.
7. Explain Hansch analysis. Write its advantages and disadvantages.
8. Various methods involved in lead optimization process in rational drug discovery process.
9. What is homology modelling. Explain different steps involved in homology modelling.

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

10. Define 3D QSAR.
11. List out different energy minimization methods used in molecular mechanics.
12. Enumerate different stages involved in rational drug discovery process.
13. COMFA.
14. Write a note on pharmaceutical data bases.
15. Explain the force field used in molecular mechanics.
16. Role of quantum mechanics in drug design.
17. Binding free energy calculation in molecular docking.
18. Write the applications of *de novo* design.
19. Define cheminformatics.

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