QP Code: 827006 **Reg. No……**

Eighth Semester B. Pharm Degree Regular/Supplementary Examinations July 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 various stages involved in rational drug discovery process in detail.
2. What is molecular docking. Explain the various types and stages of molecular docking studies.

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

3. Write the principle involved in quantum mechanics. Name two methods used and explain any one of them.
4. Explain π substituent constant as an important parameter in QSAR studies.
5. Explain on ligand based drug design approaches in CADD.
6. What are classical and non-classical bioisosteres. Give examples.
7. Explain the protocol for homology modelling and its evaluation.
8. Explain how bioinformatics is useful in new drug discovery.
9. Pharmacophore mapping and its applications.

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

10. Hammet Equation.
11. Global energy minimum conformation.
12. COMFA and COMSIA.
13. Applications of molecular dynamic simulations.
14. Free Wilson analysis in QSAR.
15. Explain the form force field.
16. Taft equation.
17. What are the uses of *de novo* methods in structure based drug design.
18. Enumerate different energy minimization methods and in molecular mechanics.
19. Explain the scoring function used in molecular docking.

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