QP Code: 827006 **Reg. No…….**

Eighth Semester B. Pharm Degree Regular/Supplementary Examinations July 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. Explain the effects of lipophilic, steric and electronic parameters in QSAR studies
2. What is *de novo* drug design. Explain the various ligand assembly and design strategies used in *de novo* drug design

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

3. Write a note on force fields used in molecular mechanics and its applications
4. Explain different methods used in pharmacophore modelling
5. Explain energy minimization methods in search of different conformations of a molecule
6. What is molecular dynamics. Explain the methodology and applications of molecular dynamic simulations
7. Explain the different stages involved in rational drug discovery process
8. Write a note on non-classical bioisosteres with examples
9. Explain molecular docking process and its applications

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

10. How a homology modelled protein structure is evaluated
11. What is role of cheminformatics in drug discovery
12. What are the various lead optimization strategies used in drug discovery
13. Explain Hansch Analysis
14. Compare and contrast structure based drug design and ligand based drug design
15. Applications of quantum mechanics in drug design
16. What is Hammett substituent constant and give its significance
17. How metabolic studies are useful in discovering new lead molecules
18. 3D QSAR
19. Enlist various search algorithms used in molecular docking

****