QP Code: 827006 **Reg. No…….**

Eighth Semester B. Pharm Degree Regular Examinations May 2022
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 Hansch analysis and discuss how it can be used in predicting biological activity.
2. Discuss in detail about various parameters used in QSAR.

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

3. Lipinsky's rule of five, explain.
4. Applications of free Wilson analysis in drug design.
5. Discuss about the various energy minimization techniques.
6. Describe about the scoring techniques in molecular docking.
7. Discuss the history of drug discovery.
8. Explain Hammett equation and Steric effects
9. Narrate the concept of pharmacophore based virtual screening.

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

10. Role of computer applications in lead optimization.
11. Electronic effect with an example.
12. Write the limitations of free Wilson analysis.
13. Define pharmacophore.
14. Define molecular mechanics.
15. Define molecular docking.
16. How can you identify the binding sites.
17. Give the applications of quantum mechanics.
18. Define bioinformatics.
19. List out any two ADME and pharmaceutical data bases.

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