QP Code: 827006 **Reg. No…….**

Eighth Semester B. Pharm Degree Supplementary Examinations
November 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. Define and classify QSAR with their advantages. Elaborate on the multi-parametric approach to QSAR as enunciated by Hansch.
2. Define Molecular Docking. Classify and explain different docking methods.

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

3. Explain about Lipinski's rule of five
4. Fragment based de novo drug designing.
5. Global energy minimum conformation
6. Explain in detail homology modelling and the method adopted for the generation of the 3D structure of a protein.
7. Hammet equation and steric effects.
8. Discuss about the structure based in silico virtual screening.
9. Explain COMFA and COMSIA

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

10. Brief about the role of computer applications in lead discovery.
11. Role of computers in lead optimization"
12. Lipophilicity effect with an example.
13. Write the advantages of free Wilson analysis.
14. Differentiate bioinformatics and cheminformatics.
15. Classify bioisosterism.
16. What are energy minimization methods.
17. What are docking components.
18. Define simulation.
19. Applications of Quantum Mechanics in drug design

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