

**VINAYAKA MISSION'S RESEARCH FOUNDATION  
(Deemed to be University) , SALEM**

**B.PHARM. DEGREE EXAMINATION – October 2021  
Eighth Semester**

**COMPUTER AIDED DRUG DESIGN**

Time : Three hours

Maximum: 75 marks

I. Write essays on any **TWO** questions: (2 x 10 = 20)

1. Explain the concept of Quantitative structure activity relationship (QSAR). Enlist the different QSAR parameters.
2. Classify bio-isosterism approach with examples. Discuss about bio-isosterism replacement strategy with one case study.
3. Define and classify Molecular docking and discuss various steps involved in the flexible docking.

II. Write short answers on any **SEVEN** questions: (7 x 5 = 35)

4. Explain the role of Pharmacophore.
5. What is analog Base Drug Design? Explain with suitable examples.
6. Discuss Comparative Molecular Field Analysis (CoMFA).
7. Discuss the importance of predication and analysis of ADME properties in drug design.
8. Briefly explain quantum mechanical approach in drug design.
9. Give a brief account of drug protein docking.
10. Methods to identify drug binding casket.
11. Explain CADD in pharmaceutical industry.
12. Explain few methods of determination of Partition coefficient.

III. Write short notes on : (10 x 2 = 20)

13. De nova drug design.
14. Define Partition coefficient.
15. COMSIA.
16. Cheminformatics.
17. SAR.
18. Serendipitous.
19. What is drug design?
20. Pharmaceutical databases.
21. Global minima.
22. CADD.