

Rajiv Gandhi University of Health Sciences, Karnataka

VIII Semester B. Pharm Degree Examination – 18-Jun-2024

Time: Three Hours

Max. Marks: 75

COMPUTER AIDED DRUG DESIGN

Q.P. CODE: 5039

Your answers should be specific to the questions asked

Draw neat labeled diagrams wherever necessary

All the Questions are compulsory

LONG ESSAYS

2 x 10 = 20 Marks

1. What is QSAR? Explain the Hansch analysis and Free Wilson analysis
OR
Discuss the various Stages of drug discovery and development
2. Define pharmacophore and discuss concept of pharmacophore mapping and pharmacophore based Screening

SHORT ESSAYS

7 x 5 = 35 Marks

3. Explain in brief about the quantum mechanical approach in drug design
OR
Define and Classify bio-isosters and Explain bio-isosterism approach with examples
4. Give an account of brief history and development of QSAR
OR
Write an elaborative note on De novo drug design with example
5. Define Molecular docking and enlist various steps involved in the flexible docking
6. Explain the role of molecular mechanics in drug design
7. Discuss about similarity based methods used in virtual screening
8. Define Chemoinformatics? Explain steps involved in chemical data curation
9. Write a note on various energy minimization techniques used in molecular modeling study

SHORT ANSWERS

10 x 2 = 20 Marks

10. What is bio-informatics?
11. Define partition coefficient and log P
12. Define Random screening and Non-random screening
13. What is drug likeliness? Explain
14. Compare SAR versus QSAR
15. Write a note on importance of biochemical databases
16. What is Conformational Analysis and give its applications
17. Enlist two ADME databases
18. Give two methods of lead optimization
19. Expand COMFA and COMSIA
