

Rajiv Gandhi University of Health Sciences, Karnataka
VIII Semester B. Pharm Degree Examination – 24-Jun-2022

Time: Three Hours

Max. Marks: 75 Marks

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. Classify bio-isosterism approach with examples. Discuss of bio-isosterism replacement strategy with one case study.

OR

Describe the theoretical determination of partition coefficient and electronic parameters in QSAR.

2. Define the term pharmacophore. Explain about the pharmacophore mapping suitable example.

SHORT ESSAYS

7 x 5 = 35 Marks

3. Write a note on Random and non-random screening.

OR

Differentiate molecular mechanics and Quantum mechanics.

4. Define the term virtual screening. Explain the concept.

OR

Define Chemoinformatics? Explain steps involved in chemical data curation.

5. Write a note on different stages of drug discovery.
6. Discuss the parameters of Hansch and Free Wilson analysis.
7. Discuss various methods for determination of energy minimization.
8. Define molecular docking. Explain rigid docking.
9. Write note on ADME databases.

SHORT ANSWERS

10 x 2 = 20 Marks

10. Define lead molecule.
11. Give two methods of lead optimization
12. Taft's steric constant.
13. Expand COMFA and COMSIA.
14. Define global minima.
15. Enumerate the applications of QSAR
16. List out the various chemical database.
17. Lipinski's rule of five.
18. What is bio-informatics?
19. Enlist any two biochemical database'.
