

Rajiv Gandhi University of Health Sciences, Karnataka

VIII Semester B. Pharm Degree Examination – 29-Nov-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. Explain Hansch analysis and Free Wilson analysis along with its advantages and disadvantages.

OR

Explain the stages of drug discovery and development.

2. Discuss the different types of lead discovery. Explain and discovery based on clinical observation with examples.

SHORT ESSAYS

7 x 5 = 35 Marks

3. Explain Hammett's and Taft's constants of QSAR.

OR

Explain *de novo* drug design.

4. Discuss concept of pharmacophore mapping.

OR

Write note on ADME databases.

5. Discuss importance of quantum mechanics in drug design.
6. Define bio-isosterism? Classify bio-isosterism with examples.
7. Write a note on Conformational analysis.
8. Explain different methods in determination of energy minimization.
9. Define bioinformatics? Explain its application in drug discovery.

SHORT ANSWERS

10 x 2 = 20 Marks

10. Mention the electronic parameters used in QSAR studies
11. Mention the steric parameters used in QSAR.
12. Expand COMFA and COMSIA.
13. Define random and non-random screening.
14. Define global and local minima.
15. Lipinski's rule of five.
16. Define lead optimization.
17. Define Chemeinformatics.
18. Enlist biochemical database's.
19. Application of chemical database's.
