Rajiv Gandhi University of Health Sciences, Karnataka

VIII Semester B. Pharm Degree Examination – 11-Nov-2024

Time: Three Hours **Max. Marks: 75 Mark**

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 lead compound? How lead compounds are generated and developed in drug discovery?

   OR

   Define and classify Molecular docking and discuss various steps involved in the flexible docking.

2. Discuss Hammett's Substituent constant and Taft's steric constant and give their importance.

SHORT ESSAYS

7 x 5 = 35 Marks

3. What is analog Based Drug Design? Explain with suitable examples.

   OR

   Discuss the role of quantum mechanical approach in drug design.

4. Explain bioisosteric replacement method in drug design with an example.

   OR

   Give an account of brief history and development of QSAR.

5. Discuss the importance Cheminformatics in drug design.
6. Enlist the various databases applications in drug design?
7. Explain various energy minimization techniques used in molecular modeling.
8. Discuss the various steps involved in pharmacophore based virtual screening.
9. Explain the various parameters of molecular mechanics in drug design.

SHORT ANSWERS

10 x 2 = 20 Marks

10. Define Bioisosterism with examples.
11. Enlist 1D and 2D descriptors of QSAR.
12. Define partition coefficient and log P.
13. What is lead optimization?
14. Give the application of 3D QSAR.
15. What is drug likeliness? Explain.
16. List out biochemical databases.
17. What is Conformational Analysis and give its applications.
18. Define local minima.
19. Give the importance of various ADME properties in drug design.