Rajiv Gandhi University of Health Sciences, Karnataka

VIII Semester B. Pharm Degree Examination – 21-Nov-2023

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 various physicochemical parameters of QSAR with examples.

   OR

   Elaborate De Novo drug designing giving emphasis on various approaches involved.

2. Elaborate Analog based drug designing giving emphasis on objectives and categories of analog designing.

SHORT ESSAYS **7 x 5 = 35 Marks**

3. What properties a lead compound should possess to develop as an orally active compound.

   OR

   Discuss Hammett's substituent constant and Taft's steric constant and its role in predicting biological activity.

4. Explain the role of Pharmacophore.

   OR

   Discuss various databases used in drug design and discovery.

5. What is molecular docking? Explain rigid docking.
6. Write a short note on energy minimization.
7. Discuss global minima.
8. Write a note on the role of bioinformatics in the drug discovery process.
9. Explain various parameters of molecular mechanics.

SHORT ANSWERS **10 x 2 = 20 Marks**

10. Mention any two advantages of free Wilson analysis.
11. **Define COMFA**
12. Explain Hansch analysis.
13. Compare SAR and QSAR.
14. Define COMSIA with its two applications.
15. Explain Lipinski rule of 5.
16. Define cheminformatics and mention its two applications.
17. **Give Examples of drugs discovered through serendipity.**
18. How are ADME databases are obtained?
19. Define Local minima.

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