NG ESSAY (Answer any Three)   **3 X 10 = 30 Marks**

1. Explain different experimental and theoretical approaches for the determination of physicochemical parameters.

2. Discuss about the agents acting on DHFR and HIV protease enzymes.

3. How do you predict ADMET properties of small molecules and what is their importance in drug design?

4. What is pharmacophore? Explain the concept, mapping and modeling of pharmacophore.

SHORT ESSAY (Answer any Nine)   **9 X 5 = 45 Marks**

5. Enlist various methods used for calculation of partition co-efficient. Explain any one method.

6. Explain historical development of QSAR.

7. Discuss the relationship between Hansch and Free Wilson analysis.

8. What are the primary requirements to carry out a 3D QSAR study?

9. Explain the role of contour map analysis in 3D QSAR.

10. Discuss the role of quantum mechanics in drug design.

11. Discuss in brief about fragment-based drug design.

12. Define molecular docking and discuss the different methods of molecular docking.

13. Discuss in detail about Virtual screening techniques.

14. Explain briefly about modeling and generation of 3D structure of proteins.

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