

GUJARAT TECHNOLOGICAL UNIVERSITY**B.PHARM - SEMESTER- 8 EXAMINATION – SUMMER-2024****Subject Code:BP807TT****Date: 13/05/2024****Subject Name: Computer Aided Drug Design****Time: 10.30 a.m. to 1.30 p.m.****Total Marks: 80****Instructions:**

1. Attempt any five questions.
2. Make suitable assumptions wherever necessary.
3. Figures to the right indicate full marks.

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| Q.1 | (a) | Explain various rational approaches for lead discovery. | 06 |
| | (b) | Explain various physicochemical parameters of QSAR with examples. | 05 |
| | (c) | Define Bioinformatics. Mention applications of bioinformatics. | 05 |
| Q.2 | (a) | Define and classify Molecular docking and discuss various steps involved in the flexible docking. | 06 |
| | (b) | Discuss Comparative Molecular Field Analysis (CoMFA) | 05 |
| | (c) | Write a note ADME databases. | 05 |
| Q.3 | (a) | Define and Classify bio-isosterism approach with examples. Discuss of bio-isosterism replacement strategy with one case study. | 06 |
| | (b) | What is a lead molecule? Discuss the various stages involved in identification of a lead molecule. | 05 |
| | (c) | Write a note on Random and non-random screening. | 05 |
| Q.4 | (a) | What is QSAR? Explain the Hansch analysis and Free Wilson analysis in brief. | 06 |
| | (b) | Write a note on various energy minimization techniques used in molecular modeling study. | 05 |
| | (c) | Explain the process of global conformational minima determination | 05 |
| Q.5 | (a) | What is automated De Novo design? Explain various stages involved in De Novo drug design. | 06 |
| | (b) | Define and explain in brief about direct and indirect molecular modeling. | 05 |
| | (c) | What is analog Based Drug Design? Explain with suitable examples. | 05 |
| Q. 6 | (a) | Explain Pharmacophore mapping and its applications. | 06 |
| | (b) | Write a note on Chemoinformatics. | 05 |
| | (c) | What is serendipitous drug discovery. Explain in detail with examples | 05 |
| Q.7 | (a) | Discuss Hammett's Substituent constant and Taft's steric constant and give their importance. | 06 |
| | (b) | Discuss in detail about COMSIA | 05 |
| | (c) | Explain the concept of molecular mechanics in drug design. | 05 |