

**THE TAMIL NADU DR. M.G.R. MEDICAL UNIVERSITY**

**[B.PHARM 1223]**

**DECEMBER 2023  
(SEPTEMBER 2023 EXAM SESSION)**

**Sub. Code: 2083**

**B.PHARMACY DEGREE COURSE (SEMESTER EXAMINATIONS)  
PCI Regulation 2017 - SEMESTER VIII  
PAPER IV - COMPUTER AIDED DRUG DESIGN**

***Q.P. Code: 562083***

**Time: Three hours**

**Maximum: 75 Marks**

**I. Elaborate on: Answer any TWO questions. (2 x 10 = 20)**

1. Define Bioisosterism. Explain Bioisosteric replacement with any two case studies.
2. Define Databases and List out its types. Explain any one in detail.
3. Explain in detail about molecular mechanics.

**II. Write notes on: Answer any SEVEN questions. (7 x 5 = 35)**

1. Explain Free Wilson analysis.
2. Write short notes on History and development of QSAR.
3. Explain Quantum mechanics.
4. Write short notes on Chemoinformatics.
5. Explain Molecular Docking.
6. Write short notes on Global conformation minima determination.
7. Explain Pharmacophore based screening.
8. Explain serendipitous drug discovery.
9. Explain *De novo* drug design.

**III. Short answers on: Answer ALL questions. (10 x 2 = 20)**

1. Define Lead.
2. Define Partition coefficient.
3. Define Lipinski's Rule of five.
4. Energy Minimization.
5. Define Drug Likeness.
6. What is Molecular Docking?
7. Define Pharmacophore.
8. Define Drug.
9. Expand COMFA and COMSIA.
10. Expand SAR and QSAR.

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