

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

[B.PHARM 0823]

**AUGUST 2023
(MARCH 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. Enlist the different phases of Case studies. Explain Captopril.
2. Explain Serendipitous drug discovery.
3. Explain Ligand based (LBVS) and Structure based (SBVS) techniques in detail.

II. Write notes on: Answer any SEVEN questions.

(7 x 5 = 35)

1. Hammett Substituent Constant.
2. Role of Chemo informatics in modern drug discovery.
3. Molecular docking.
4. Write a brief note on Non-clinical activities.
5. Concept of Pharmacophore mapping.
6. Biochemical databases.
7. Monte-Carlo method in conformational searching.
8. Energy minimization method- derivative method.
9. Explain CoMFA and CoMSIA.

III. Short answers on: Answer ALL questions.

(10 x 2 = 20)

1. Molecular refractivity.
2. Name the two drugs discovered without Lead.
3. SNPs- single nucleotide polymorphism.
4. LUDI programme.
5. Advantages and disadvantages of QSAR.
6. Free wilson approach equation.
7. Difference between molecular and quantum mechanics.
8. ADME Databases.
9. What is Lipinskis rule of five?
10. Give examples of Amide group Bioisosteres.
