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

[B.PHARM 0524] **MAY 2024** **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. Briefly explain Comparative Molecular Similarity Indices Analysis (COMSIA), the 3-Dimensional Quantitative Structure Activity Relationship approach (3D-QSAR).
2. Describe Molecular docking and its importance in drug discovery.
3. Explain Bioinformatics and Chemoinformatics briefly.

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

1. Random screening.
2. Lead discovery based on clinical observation.
3. Rational approaches for lead discovery based on Traditional medicine.
4. Different types of Physiochemical parameters involved in Quantitative Structure Activity Relationship (QSAR).
5. Pharmacophore mapping.
6. Pharmaceutical databases.
7. Difference between Molecular mechanics and Quantum mechanics.
8. Fore fields used in Molecular modeling.
9. Monte Carlo simulation in Molecular dynamics.

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

1. What is Computer Aided Drug Design?
2. Mention any two lead optimization techniques.
3. Examples for drug discovery based on Drug metabolism.
4. Molecular descriptors.
5. Applications of Molecular modeling.
6. Scoring in docking.
7. Chemoinformatics.
8. Algorithms in docking.
9. Global conformational minima.
10. De novo drug design.

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