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

[BPHARM 0422] **APRIL 2022** **Sub. Code: 2083**
(SEPTEMBER 2021 SESSION)

B.PHARMACY DEGREE COURSE (SEMESTER EXAMINATIONS)
PCI Regulation 2017 SEMESTER VIII
PAPER VII - 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. Elaborate the stages of *Denovo* drug design.
2. Explain Random and Non-random screening methods.
3. Explain the Biosteric replacement strategies with ring replacement.

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

1. Tafts steric constant (Es).
2. Discuss Clinical studies with the phases of clinical trials.
3. What is Bioisosterism? Classify them with examples.
4. Illustrate Linear Hansch model.
5. Explain Free-Wilson approach.
6. Applications of Pharmacophore.
7. Write a brief note on Flexible Docking.
8. ADME and biochemical Databases.
9. Explain Energy minimization method-non derivative method.

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

1. Rigid Docking.
2. Analog design and its goals.
3. What is COMFA?
4. Verloop Steric Parameter.
5. SAR Vs QSAR.
6. What is Partition Coefficient?
7. Post marketing monitoring.
8. *Invitro, Invivo* and *Silico* assays.
9. Structure of Isoniazid and Chloramphenicol.
10. Structure based virtual screening.

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

[BPHARM 1022] **OCTOBER 2022** **Sub. Code: 2083**
(MARCH 2022 SESSION)

B.PHARMACY DEGREE COURSE (SEMESTER EXAMINATIONS)
PCI Regulation 2017 - SEMESTER VIII
PAPER VII - 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. Explain Pharmacophore mapping and concept-based screening.
2. Discuss Lead optimization with their characters. Explain the methods of optimization.
3. Explain the principle of quantum mechanics and its methods.

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

1. Enumerate the properties determined by the researchers for preclinical studies.
2. Explain the methodology of 3D QSAR.
3. Explain the determination of Partition Coefficient.
4. Write short notes on rigid docking.
5. What is bio informatics? Give its applications.
6. Write a brief note on computer aided drug design.
7. Explain briefly Chemical databases.
8. Conformational analysis-history and process.
9. Explain the phases of drug development.

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

1. Objectives of QSAR.
2. Hansch's equation.
3. LBVS
4. What is bioisosterism?
5. Molecular modeling method with flow chart.
6. What is molecular mechanics?
7. Advantages and disadvantages of Semiempirical method.
8. Manual docking.
9. Write the formula used to calculate number of conformations.
10. Define drug likeness and the methods for its assessment.

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

[B.PHARM 0323] MARCH 2023 Sub. Code: 2083
(SEPTEMBER 2022 EXAM SESSION)

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. Explain Analog Based Drug Design.
2. Explain steps involved in *De novo* Drug Design.
3. Explain the Rational approaches to Lead Discovery.

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

1. Explain the concept of Drug likeness Screening.
2. Explain Rigid Docking.
3. Explain Pharmacophore Mapping.
4. Explain Hansch Analysis.
5. Explain Conformational Analysis.
6. Explain methods of Energy Minimisation.
7. Explain stages of drug discovery.
8. Explain COMFA and COMSIA.
9. Explain Global conformational minima determination.

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

1. Define Bioisosterism with example.
2. List out chemoinformatic databases.
3. Define Molecular Mechanics.
4. Differentiate SAR Vs QSAR.
5. Expand LUMO and HOMO.
6. Tafts steric constant.
7. Define flexible docking.
8. Define Lipinski's Rule of five.
9. Define Quantum mechanics.
10. List out the advantages of Computer aided drug designing.

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

[B.PHARM 0823] AUGUST 2023 Sub. Code: 2083
(MARCH 2023 EXAM SESSION)

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.

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

[B.PHARM 1223] DECEMBER 2023 Sub. Code: 2083
(SEPTEMBER 2023 EXAM SESSION)

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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