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

[LM 947] MAY 2018 **Sub. Code: 2947**

M.PHARM. DEGREE EXAMINATION
(PCI New regulations 2016)
SEMESTER-II
BRANCH–II – PHARMACEUTICAL CHEMISTRY – MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code : 262947

Time : Three hours **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. a) The log P values for benzene, chlorobenzene and Benzamide are 2.13, 2.84 and 0.64 respectively. Calculate the log P value of m-Chlorobenzamide.

   b) Explain in detail the different physiochemical parameters that affect Biological activity.

2. a) Discuss in detail the docking of agents on HIV protease and DHFR.
   b) Discuss in detail 3D-QSAR approaches and contour Map analysis.

II. Write notes on: **(7 x 5 = 35)**

1. Briefly explain Craig plot.
2. Write a short note on Comparative Molecular Field Analysis (CoMFA).
3. What is Free-Wilson approach to QSAR? Give an example.
4. Discuss the statistical methods used in QSAR analysis.
5. Briefly explain Lipinsky's Rule of five.
6. Write a short note on De Novo drug design.
7. What is pharmacophore mapping? Give an example.

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

[LN 947] NOVEMBER 2018 **Sub. Code: 2947**

M.PHARM. DEGREE EXAMINATION
(PCI New regulations 2016)
SEMESTER-II
BRANCH–II – PHARMACEUTICAL CHEMISTRY – MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code : 262947

Time : Three hours **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. Elaborate on the multi-parametric approach to QSAR as enunciated by Hansch.

2. a) The Hammett substituent constant (σ x) for a given substituent (X) on benzoic acid is defined by the following equation.

$$\sigma x = \log \frac{K_x}{K_H} = \log K_x - \log K_H$$

(Where K_H is value for the un-substituted benzoic acid)
Comment on the value of σ x when the substituents are:
a) Electron with drawing b) Electron donating

b) Explain in detail Homology modeling and the method adopted for the generation of the 3D structure of a protein.

II. Write notes on: **(7 x 5 = 35)**

1. Distinguish between Rigid docking, Flexible docking and Extra precision docking.
2. Write a short note on Topliss Decision Tree for aromatic substituents in deciding on newer analogues with improved biological activity.
3. Write briefly on stages in automated de novo design in CADD.
4. Write a short note on Virtual screening techniques.
5. Discuss molecular docking of agents inhibiting HMGCoA.
6. Discuss the important aspect of pharmacophore modeling.
7. Write a short note on global energy minimization.

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

[LO 947] MAY 2019 **Sub. Code: 2947**

M.PHARM. DEGREE EXAMINATION
(PCI New regulations 2016)
SEMESTER-II
BRANCH–II – PHARMACEUTICAL CHEMISTRY – MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code : 262947

Time : Three hours **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. a) Explain briefly various protocols used in *In-silico* virtual screening techniques.
   b) Explain the utilization of conformational search used in pharmacophore mapping.

2. a) Enumerate various statistical approaches utilized in QSAR analysis.
   b) Enumerate briefly about the discovery of acetyl and butyryl choline esterase inhibitors based on docking studies.

II. Write notes on: **(7 x 5 = 35)**

1. Brief out on quantum mechanical approach.
2. Write a note on the agents acting on the enzyme, HIV protease.
3. Explain how changes in log of values affect biological activity?
4. Elaborate on similarity based methods used in virtual screening.
5. Explain what is Cralg's plot?
6. Write a note on the importance of prediction and analysis of ADMET properties in drug design.
7. Write a note on drug receptor interactions.

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

[LP 947] NOVEMBER 2019 **Sub. Code: 2947**

M.PHARM. DEGREE EXAMINATION
(PCI New regulations 2016)
SEMESTER-II
BRANCH–II – PHARMACEUTICAL CHEMISTRY – MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code : 262947

Time : Three hours **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. Explain various physico chemical parameters involved in the study of Quantitative Structure Activity Relationship.

2. a) Write a note on various energy minimization techniques used in molecular modelling study.
   b) Explain briefly about the molecular modelling approaches in the discovery of DHFR inhibitors

II. Write notes on: **(7 x 5 = 35)**

1. Write a note on 3D-QSAR approach.
2. Brief out on ligand based drug design.
3. State the Lipinski's rule of five and explain the importance of the parameters in drug discovery.
4. Write a note on 3D structure alignment.
5. Explain De Novo drug design.
6. Brief out on PLS & CoMFA analysis.
7. Brief out on fragment based drug design.

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

[LQ 0121] JANUARY 2021 Sub. Code: 2947

(APRIL 2020 EXAM SESSION)

M.PHARMACY DEGREE EXAMINATION

SEMESTER-II (PCI New regulations 2016)

PHARMACEUTICAL CHEMISTRY – MPC

PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code : 262947

Time : Three hours **Answer ALL Questions** **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. Discuss in detail the molecular and quantum mechanics in drug design.

2. a) Discuss in detail 3D-QSAR approaches and contour map analysis.
   b) Explain homology modeling and the method adopted for the generation of the 3D structure of a protein.

II. Write notes on: **(7 x 5 = 35)**

1. Briefly explain the Hammett equation parameters.
2. Discuss the statistical methods used in QSAR analysis.
3. Write a short note on global energy minimization.
4. Explain the physico chemical parameters that affect biological activity.
5. Write short note on De Nova drug design.
6. Short notes on pharmacophore mapping.
7. Explain insilico virtual screening protocols.

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

[MPHARM 0921] SEPTEMBER 2021 Sub. Code: 2947
(OCTOBER 2020 EXAM SESSION)

M.PHARMACY DEGREE EXAMINATION
SEMESTER-II (PCI New regulations 2016)
PHARMACEUTICAL CHEMISTRY - MPC
PAPER III – COMPUTER AIDED DRUG DESIGN
Q.P. Code : 262947

Time : Three hours **Answer ALL Questions** **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. a) Explain briefly on various strategies utilized in homology modeling.
   b) Discuss briefly on various QSAR analysis methods in relation to biological activity.

2. a) Elaborate briefly on the strategic approaches on structure based and ligand based *In-silico* virtual screening protocols.
   b) Explain about the techniques utilized in De Novo drug design.

II. Write notes on: **(7 x 5 = 35)**

1. Write a brief note on the types of docking.
2. Brief on the development of HMG–CoA reductase inhibitors using molecular modeling strategies.
3. Give an account on CoMFA and CoMSIA methods in 3D QSAR studies.
4. Write a note on molar refractivity.
5. Brief a note on pharmacophore mapping techniques.
6. Derive Hammet substituent constant and explain the changes in its value related to electronic parameters.
7. Compare and contrast between global minimum conformation and bioactive conformation.

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

[M.PHARM 0922] **SEPTEMBER 2022** **Sub. Code: 2947**
(APRIL 2022 EXAM SESSION)

M.PHARMACY DEGREE EXAMINATION
SEMESTER - II (PCI New regulations 2016)
PHARMACEUTICAL CHEMISTRY - MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code : 262947

Time : Three hours **Answer ALL Questions** **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. Explain Fragment based drug design.

2. a) Differentiate between rigid docking and flexible docking.
   b) Brief out on ligand-based drug design.

II. Write notes on: **(7 x 5 = 35)**

1. Explain in detail the partition coefficient property of the molecules with examples.
2. Write a short note on Comparative Molecular Field Analysis (CoMFA).
3. Note on the applications of quantum mechanics in drug design.
4. Briefly explain Lipinsky's Rule of five.
5. Write a short note on global energy minimization.
6. What do you mean by ADMET? Discuss the importance of ADMET property prediction in drug design.
7. Write a note on the agents acting on the enzyme, Choline esterase.

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

[M.PHARM 0423] APRIL 2023 Sub. Code: 2947
(OCTOBER 2022 EXAM SESSION)

M.PHARMACY DEGREE EXAMINATION
SEMESTER - II (PCI New regulations 2016)
PHARMACEUTICAL CHEMISTRY - MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code: 262947

Time : Three hours **Answer ALL Questions** **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. Give an account of QSAR studies and their implications.

2. Explain in detail the homology modeling used for the generation of the 3D structure of a protein.

II. Write notes on: **(7 x 5 = 35)**

1. Brief about drug-receptor interaction in docking study.
2. Give a detailed explanation of de-novo drug design.
3. Explain comparison between Global minimum conformation and bioactive conformation.
4. Enumerate the structure-based in-silico virtual screening protocols.
5. Note on Hansch analysis.
6. Explain conformational search used in pharmacophore mapping.
7. Write about molecular mechanics.

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

[M.PHARM 0823] **AUGUST 2023** **Sub. Code: 2947**
(APRIL 2023 EXAM SESSION)

M.PHARMACY DEGREE EXAMINATION
SEMESTER - II (PCI New Regulations 2016)
PHARMACEUTICAL CHEMISTRY - MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code: 262947

Time : Three hours **Answer ALL Questions** **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. Theoretical and Experimental approaches for calculating QSAR parameters.

2. A. Design two agents each for both cholinesterases (Acetyl and butyryl).
   B. Steps to determine ADME properties of a molecule.

II. Write notes on: **(7 x 5 = 35)**

1. Bioactive conformation of an active molecule.
2. Discuss the force fields operating under MOLECULAR MECHANICS.
3. Fragment based drug designing.
4. Types of drug – receptor interactions.
5. 2D Pharmacophore screening.
6. Frame equations for QSAR applying 2D parameter.
7. Drugs designed based on homology techniques.

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

[M.PHARM 1223] DECEMBER 2023 Sub. Code: 2947
(OCTOBER 2023 EXAM SESSION)

M.PHARMACY DEGREE EXAMINATION
SEMESTER - II (PCI New Regulations 2016)
PHARMACEUTICAL CHEMISTRY - MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code: 262947

Time: Three hours **Answer ALL Questions** **Maximum: 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. a) Discuss in detail Denova drug design.
   b) Write the methods used in the energy minimization of molecules.

2. Write a note on various steps involved in pharmacophore mapping and its features.

II. Write notes on: **(7 x 5 = 35)**

1. Enumerate the Taft steric parameter.
2. Discuss different statistical approaches used in QSAR.
3. A brief note on quantum mechanics.
4. Brief out on fragment-based drug design.
5. Write a note on the agents acting on the enzyme Dihydrofolate reductase.
6. Discuss homology modeling.
7. Explain in detail physiochemical parameters that affect biological activity.

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

[M.PHARM 0524] MAY 2024 Sub. Code: 2947
(APRIL 2024 EXAM SESSION)

M.PHARMACY DEGREE EXAMINATION
SEMESTER - II (PCI New Regulations 2016)
PHARMACEUTICAL CHEMISTRY - MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code: 262947

Time: Three hours **Answer ALL Questions** **Maximum: 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. Applications of contour map and statistical techniques in quantitative designing of a new molecule as a probable drug candidate.

2. A) Types of docking methods their advantages and disadvantages.
   B) Quantum mechanics and Global minimum of a conformer.

II. Write notes on: **(7 x 5 = 35)**

1. Log P, Taft and Hammet equation.
2. Virtual Screening Techniques.
3. Free Wilson and Hansch analysis.
4. DeNovo design.
5. Topliss Decison Tree.
6. Homology modeling for finding 3D structure of a protein.
7. Types of Pharmacophore based screening.

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

[M.PHARM 0425] **APRIL 2025** **Sub. Code: 2947**

M.PHARMACY DEGREE EXAMINATION
SEMESTER - II (PCI New Regulations 2016)
PHARMACEUTICAL CHEMISTRY - MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code: 262947

Time: Three hours **Answer ALL Questions** **Maximum: 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. Explain the details in physiochemical of Hammet and lipophilicity parameters.

2. a) Explain the insilico drug design and virtual screening techniques.
   b) Discuss in detail the docking of agents on HIV protease and DHFR.

II. Write notes on: **(7 x 5 = 35)**

1. What is free-Wilson approach to QSAR? Give an example.
2. Discuss the statistical method used in QSAR analysis.
3. Write note on molecular mechanics in drug design.
4. Short note on homology modeling and generation of 3D structure of protein.
5. Discuss the important aspect of pharmacophore modeling.
6. Short note on Denovo drug design.
7. Short note on Hansch Analysis.

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

[M.PHARM 1025] **OCTOBER 2025** **Sub. Code: 2947**

M.PHARMACY DEGREE EXAMINATION
SEMESTER - II (PCI New Regulations 2016)
PHARMACEUTICAL CHEMISTRY - MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code: 262947

Time: Three hours **Answer ALL Questions** **Maximum: 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. a) Explain different types of Docking.
   b) Write briefly flexible docking and extra precision docking.

2. Elaborate pharmacophore mapping and virtual screening.

II. Write notes on: **(7 x 5 = 35)**

1. Explain various physiochemical parameters in QSAR.
2. Write short notes on rigid docking.
3. Explain the stages in automated de-novo design in CADD.
4. Write Hansch analysis.
5. Write prediction and analysis of ADMET properties in drug design.
6. Discuss in detail 3D-QSAR approaches and contour map analysis.
7. Discuss molecular docking of agents inhibiting choline esterase.

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