

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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[LN 947]

NOVEMBER 2018

Sub. Code: 2947

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**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 ( $\sigma_x$ ) 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  $\sigma_x$  when the substituents are:

- a) Electron withdrawing      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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**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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**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  
(OCTOBER 2020 EXAM SESSION)

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 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 Hammett 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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