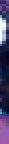




MEDICINAL CHEMISTRY

Medicinal chemistry deals with the design, optimization and development of chemical compounds for use as drugs.



Functional Groups

- Functional groups play a significant role in:
 - Water/lipid solubility
 - Route of administration
 - Ability to interact with the specific biological target
 - Mechanism (mode or method) of action
 - Route of metabolism and elimination
 - Duration of action
 - Susceptibility for specific therapeutic situations
 - Tendency to cause adverse effects or drug interactions
- These concepts that should always be considered when examining a drug molecule:
 - Every atom within the structure belongs to some functional group.
 - Within a drug molecule, some functional groups may be more "important" than others. The opposite may be true for a different drug molecule.
 - Altering functional groups can enhance activity, increase absorption, decrease adverse effects, and provide other therapeutic benefits.
 - These major chemical properties that need to be analyzed for every functional group:
 - Electrostatic effect:** The components that comprise the overall electronic effect of a functional group are induction and resonance.
 - Measured by a functional group's ability to donate its electrons to adjacent atoms or functional groups
 - Solubility effects:** Overall solubility is a composite sum of all the functional groups found as part of a drug molecule.
 - Size effect:** Each functional group has a finite size and some dimensions; this contributes to the overall conformation and thus the 3-D shape of a given drug.
 - The three major chemical properties combined need to be considered when evaluating the overall pharmacodynamic and pharmacokinetic properties of any given drug molecule.

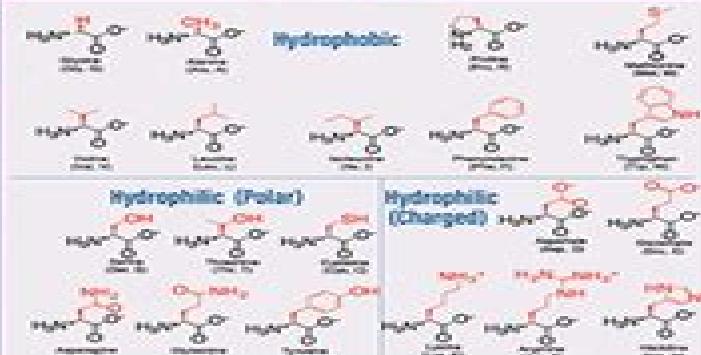
ELECTRONEGATIVITY: KEY POINTS

- C, O, Cl, and N are the most electronegative elements.
- O will always attract electrons to it, unless it is attached to a F.
- All the halogens (F, Cl, Br, and I) as well as O and N will attract electrons away from C.
- C will slightly attract electrons away from H (inductive effect).
- The difference in electronegativity causes a dipole.

Solubility

- Universal water and/or lipid solubility of a drug molecule affects its route(s) of administration, distribution within the body, metabolism, duration of action, and route(s) of elimination.

Amino Acids



pH & pK_a

pH

- pH = $-\log[H^+]$
- Refers to the solution, not a functional group
- Indicates how many " H^+ " there are in the solution
- ICN: pH of 0.1M HCN
- pH = $-\log(0.1) = -(-1) = 1$
- ICN: pH of 0.0001M HCN
- pH = $-\log(0.0001) = -(-4) = 4$

Acid Strength (pK_a)

- Property of functional groups
- Affected by size and electronic effects
- Can be used to compare the relative acidity of functional groups
 - Rule 1: Lower pK_a value → stronger acid (wants to lose the H⁺)
 - Rule 2: Higher pK_a value → stronger conjugate base/weak acid (wants to gain the H⁺)

pK_a

- Low pK_a: Reaction is to the right
- High pK_a: Reaction is to the left

$$pK_a = -\log(K_a)$$



Henderson-Hasselbach equation:

$$pH = pK_a + \log \frac{[A^-]}{[HA]}$$

- Used to calculate the:
 - pH change in buffered solutions
 - pH change in the molar ratio of salt to acid concentrations needed to prepare a buffer solution at a certain pH
 - Percent ionization of a functional group at a certain solution pH

ICN: Fluoroprotein's functional group has a pK_a of 4.5, so it must be carboxylic acid. Will it be protonated or deprotonated if it is in the urine at pH 5.5?



$$1.0 = \log \frac{[CN^-]}{[HCN]}$$

$$10 = \frac{[CN^-]}{[HCN]}$$

Answers: More deprotonated

- The protonation state affects:
 - The charge of a functional group (+ or -)

Medicinal Chemistry Study Guide

Elias Hudson Bartley

Medicinal Chemistry Study Guide:

Medicinal Chemistry of Drugs Affecting Cardiovascular and Endocrine Systems M. O. Faruk Khan,2024-02-19

The primary objective of this 4 volume book series is to educate PharmD students on the subject of medicinal chemistry. The book set serves as a reference guide to pharmacists on aspects of the chemical basis of drug action. Medicinal Chemistry of Drugs Affecting Cardiovascular and Endocrine Systems is the third volume of the series. This volume features 8 chapters focusing on a comprehensive account of drugs affecting both the cardiovascular system and the endocrine functions. The volume informs readers about the medicinal chemistry of relevant drugs which includes the mechanism of drug action, detailed structure activity relationships and metabolism. Topics covered include drugs that affect the renin angiotensin system, calcium channel blockers, diuretics, hematological agents, anticoagulants, thrombolytic and antiplatelet agents, antidiabetics, antihistamines, proton pump inhibitors and therapeutic hormones. Each chapter also offers case studies and self assessments to facilitate discussion and learning. The book equips students with a scientific foundation to competently evaluate, recommend and counsel patients and health care professionals regarding the safe, appropriate and cost effective use of medications. Students and teachers will also be able to integrate the knowledge presented in the book and apply medicinal chemistry concepts to understand the pharmacodynamics and pharmacokinetics of therapeutic agents in the body. The information offered by the book chapters will give readers a strong neuropharmacology knowledge base required for a practicing pharmacist. Readership: PharmD pharmacology students and teachers

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of medicinal chemistry as well as how and why these concepts are essential to therapeutic decisions. The book emphasizes functional group analysis and the basics of drug structure evaluation. In a systematic fashion learn how to identify and evaluate the functional groups that comprise the structure of a drug molecule and their influences on solubility absorption acid base character binding interactions and stereochemical orientation. Relevant Phase I and Phase II metabolic transformations are also discussed for each functional group. Key features include Discussions on the roles and characteristics of organic functional groups including the identification of acidic and basic functional groups. How to solve problems involving pH pKa and ionization salts and solubility drug binding interactions stereochemistry and drug metabolism. Numerous examples and expanded discussions for complex concepts. Therapeutic examples that link the importance of medicinal chemistry to pharmacy and healthcare practice. An overview of structure activity relationships SARs and concepts that govern drug design. Review questions and practice problems at the end of each chapter that allow readers to test their understanding with the answers provided in an appendix. Whether you are just starting your education toward a career in a healthcare field or need to brush up on your organic chemistry concepts this book is here to help you navigate medicinal chemistry.

About the Authors

Marc W Harrold BS Pharm PhD is Professor of Medicinal Chemistry at the Mylan School of Pharmacy Duquesne University Pittsburgh PA. Professor Harrold is the 2011 winner of the Omicron Delta Kappa Teacher of the Year award at Duquesne University. He is also the two time winner of the TOPS Teacher of the Pharmacy School award at the Mylan School of Pharmacy. Robin M Zavod PhD is Associate Professor for Pharmaceutical Sciences at the Chicago College of Pharmacy Midwestern University Downers Grove IL where she was awarded the 2012 Outstanding Faculty of the Year award. Professor Zavod also serves on the adjunct faculty for Elmhurst College and the Illinois Institute of Technology. She currently serves as Editor in Chief of the journal Currents in Pharmacy Teaching and Learning.

Basic Concepts in Medicinal Chemistry Marc W. Harrold, Robin M. Zavod, 2023

Designed to help students incrementally build their knowledge of fundamental concepts of medicinal chemistry and their applications to therapeutic decisions it is progressively organized. Specific sections of the text have been updated to make potentially confusing concepts easier to understand. Numerous examples and review questions further reinforce learning and analytical skills. This updated and expanded edition of the popular textbook *Basic Concepts in Medicinal Chemistry* has been enhanced with new subject material numerous self assessment tools and special features to advance and strengthen the learning process.

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A Text-book of medical chemistry Elias Hudson Bartley, 1895

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Table of Contents Medicinal Chemistry Study Guide

1. Understanding the eBook Medicinal Chemistry Study Guide
 - The Rise of Digital Reading Medicinal Chemistry Study Guide
 - Advantages of eBooks Over Traditional Books
2. Identifying Medicinal Chemistry Study Guide
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Medicinal Chemistry Study Guide
 - User-Friendly Interface
4. Exploring eBook Recommendations from Medicinal Chemistry Study Guide
 - Personalized Recommendations
 - Medicinal Chemistry Study Guide User Reviews and Ratings
 - Medicinal Chemistry Study Guide and Bestseller Lists
5. Accessing Medicinal Chemistry Study Guide Free and Paid eBooks
 - Medicinal Chemistry Study Guide Public Domain eBooks
 - Medicinal Chemistry Study Guide eBook Subscription Services
 - Medicinal Chemistry Study Guide Budget-Friendly Options
6. Navigating Medicinal Chemistry Study Guide eBook Formats
 - ePub, PDF, MOBI, and More
 - Medicinal Chemistry Study Guide Compatibility with Devices
 - Medicinal Chemistry Study Guide Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Medicinal Chemistry Study Guide
 - Highlighting and Note-Taking Medicinal Chemistry Study Guide
 - Interactive Elements Medicinal Chemistry Study Guide
8. Staying Engaged with Medicinal Chemistry Study Guide

- Joining Online Reading Communities
- Participating in Virtual Book Clubs
- Following Authors and Publishers Medicinal Chemistry Study Guide

9. Balancing eBooks and Physical Books Medicinal Chemistry Study Guide

- Benefits of a Digital Library
- Creating a Diverse Reading Collection Medicinal Chemistry Study Guide

10. Overcoming Reading Challenges

- Dealing with Digital Eye Strain
- Minimizing Distractions
- Managing Screen Time

11. Cultivating a Reading Routine Medicinal Chemistry Study Guide

- Setting Reading Goals Medicinal Chemistry Study Guide
- Carving Out Dedicated Reading Time

12. Sourcing Reliable Information of Medicinal Chemistry Study Guide

- Fact-Checking eBook Content of Medicinal Chemistry Study Guide
- Distinguishing Credible Sources

13. Promoting Lifelong Learning

- Utilizing eBooks for Skill Development
- Exploring Educational eBooks

14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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