

# MEDICINAL CHEM

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 Right notlability
- Route of administration.
- Ability to interact with the specific biological target.
- Mochanism (mode or method) of action
- Route of metabolism and elimination
- Duration of action
- Suitability for specific thempeutic situations
- Tendency to course adverse effects or drug interactions Three concepts that should always be considered when examining a drug molecule:
- I. Every atom within the structure belongs to some functional atoms.
- 2. Within a drug molecule, some functional groups may be more "important" than others. The opposite may be true for a different drug molecule.
- 3. Altering functional groups can enhance activity, increase advorption, decrease adverse effects, and provide other the appearing beauties.
- Three major chemical proporties that need to be analyzed for every functional group:
- 1. Electronic effect: The components that comprise the overall electronic effect of a functional group are induction manufic attenues and continues of
- a. Measured by a functional group's ability to donate its electrons to adjacent atoms or functional groups 2. Solubility effect: Overall solubility is a composite sum of
- all the functional groups found as part of a drug molecule. 3. Storic effects Each functional group has a finite size
  - and storic dimension; 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 evaluation the overall pharmacodynamic and pharmacokinetic properties of any given-drug molecule.

#### ELECTRONEGATIVITY: KEY POINTS

- . E.D.CL and Name the most electromagative element O will always attract electrons to it, unless it is attached to a fi-
- . All the halogens (I, O), Br, and () as well as O and 6 will attract electrons away
- C will slightly attract electrons away from it (inductive effect).
- . The difference in electronogativity causes a dipole.

#### Solubility

 Overall water and/or lipid solubility of a drug molecule affligate its moutor's and administrations, distribution to other than body, metabolism, duration of action, and route(s) of climintelligent.

- Toronto too Serveror
- Hydrophobicity (a.k.a. lipophilicity): How waterdistilling (i.e., oil-liking) a drug molecule is
- Hydrophilicity (a.k.a. lipophobicity): How waterfilting (i.e., oil-distribute) a drug molocule is
- . The contribution to solubility by a functional group may be increased or decreased depending upon adjacent groups.
- Water soluble functional groups:
  - Enhance water solubility; often referred to as hydrophillie groups.
  - The two major properties that contribute to water solubility:
  - Whether the group is or can be loaded. © Either positive (+) or negative (-)
  - EX: Quaternary amine—no matter what pH the molecule finds itself in, it will always have a + charge.
  - The group's ability to hydrogen bond with water

- Size & Steric Dimension

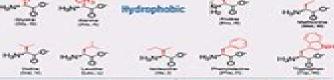
  The addition of a sterically bulky functional group can:
- Increase selectivity for its biological target
- Enhance blading interactions with its biological target Cause fiscorable alterations in the rate of metabolisms
- The acidio-basic nature of a drug molecule influences its chemical, pharmaceutical, and therapeutic proporties.
- . If a functional group can be isolated at a certain pH, its water solubility will increase.
- While this helps the gastrointestinal (GI) tract dissolve the molecule, the unionized form (without a charge) is better for passage through the lipid membrane.
- Ionization: Equilibrium process that allows for functional groups to form electrostatic interactions with target receptors, transport proteins, enzymes, and other endogenous biological targets.
  - Electrostatic (a.k.a ionic) interactions are the strongest memory about boards.
- Drug molecules can interact with plasma proteins dustriallly via electrostatics).
  - This sequesters them from metabolic/elimination pathways and extends the duration of action.
- The human serum allbumin is a major transporter of drug molecules but is nonspecific. It generally binds acid drug molecules to a greater extent than basic drug molecules.
  - Albumin also binds hydrophobic compounds more tightly than hydrophilic ones.
- What if you are taking two different drugs and both contain. an acidic functional group?
- Plasma protein displacement interactions one occur.
- This could grounly affect the half-life of the drug, particularly when the drug is 90% plasma protein bound.

- · Drug molecules that are highly looked are more water soluble, so they need less metabolism to be eliminated.
- There are specific transport proteins of certain organic acids within the renal tubules that actively secrete acidic moleemilione.
  - From the plasma to the urine
  - . This decreases the half-life of the drug molecules.
  - From the urine to the plasma.
  - This increases the half-life of the drug molecules.

#### Acidic & Basic Functional Groups

Executional I	-	-	phi, Name
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iji.	() observations)	Airtidae	45-45
25-	Bullimanuka	Artiflet	5-10
-1280	Mr Studilling Statem	Acides	3-6
	Yetronides	Neidle	4.5-6
000	Should	Acidia	7-10
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and the same of th	Bettern	Bloom	3-4 Cellus promiserant
and the same	Disposition of the last of the	Blanck	7.5-8.5 (allos protessatores)
- T.	Amirbine	Beerle	30-11 (other protosotion)
- , -	Consider	David,	12-13 (other protonultion)
& C	<b>.</b>	State of	1-5 Calles protessations)

#### Amino Acids







#### pH & pK

#### phil - - Acquirt |

- Refers to the solution, not a functional group
- Indicates how many "free" III's there are in the solution
- HEX: plit of 0.1 M H.  $p(0) = -\log_2(0, 1) = -(-1) = 1$ EXI pell of 0.0004 MIT p01 = -(1-1) = -(10000.0) = -(-1) = 4

#### Acid Strength (pK\_)

- · Property of functional groups Afflocted by steric and electronic
- Can be used to compare the relative acidity of functional groups Rule Is Lower pK value -stronger acid (wants to lose One 10 h
- Rule 2: Higher pK, value -stronger conjugate base/weakor sould (wants to gain the H )

#### + 18" + A" - THAN

- Low pK : Reaction is to the
- High p.K., : Reaction is to the Lord St.

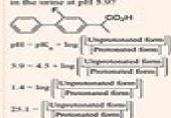
$$pK_{a} = \log(K_{a})$$

$$[pt^{*}][A^{*}]$$

BUA Hersdorson-Hussielbidch ogusti part or part, or long. Unpresented from Proteind from

- Used to calculate the:
- pHI change in buffered solu-Berger.
- pHI change in the motor ratio of salt to acid concentrations needed to prepare a buffler sobuttom at a cortain pill
- Percent ionization of a fenctional group at a certain soluthem pitt

EX: Fluibiposition's functional group. has a pK, of 4.5, so it must be carbooxidis sold. Will it be primary protonated or improtonated iff it is im the serine at pHI 5.97



Autowayer Morey umprotomotod The protonation state affects:

The charge of a functional group (n or -)

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**Ying-Ying Zheng** 

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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, 2001 These tutorials focus on the basic chemical concepts which govern drug action and are meant to serve as a review for the sequence of Biomedical Science Therapeutics courses PHBMS 422 PHBMS 427 These concepts are first introduced in the stand alone Medicinal Chemistry course PHBMS 421 taught in the Fall semester of the PIV year and should not be foreign to those who have completed this course It is the expectation of the author that each student understands and masters these concepts since he she is expected to apply these concepts and understand how they relate to the drugs and drug classes discussed in the BMS T modules

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Chemistry, 2024-04-02 Introduction to Medicinal Chemistry serves as a comprehensive guide to exploring the dynamic and evolving field of medicinal chemistry Written with precision and expertise this book provides a practical journey into the principles and applications underpinning the development of pharmaceutical agents With a focus on the intersection of chemistry and medicine the text delves deeply into the molecular mechanisms controlling drug action emphasizing the importance of understanding structure activity relationships This book highlights the complexities of drug design synthesis and optimization through the fundamental concepts of medicinal chemistry. It meets the needs of both novice learners and experienced practitioners in the field offering a balanced mix of theoretical foundations and practical applications Readers will find explanations on the chemical basis of various diseases identification of drug targets and design of molecules with therapeutic potential Notably the author uses a clear writing style which highlights complex concepts and facilitates an intuitive understanding of the subject matter The inclusion of case studies and real world examples further enhances the practical relevance of the book fostering a deeper appreciation for the role of medicinal chemistry in modern health care Introduction to Medicinal Chemistry stands as an indispensable resource for students researchers and professionals seeking a holistic understanding of the principles of drug discovery and development Its broad coverage and accessible approach make it an invaluable tool for those wishing to unravel the secrets of medicinal chemistry and contribute to the advancement of pharmaceutical science The American Journal of the Medical Sciences, 1871 A Reader's Guide to Contemporary Literature William Swan Sonnenschein, 1896 A Treatise on nervous and mental diseases Landon Carter Gray, 1893 **A Text-book of Physiology** Sir Michael Foster, 1891 Readers' Guide to Periodical Literature, 1913

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