

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 afflicate its moutor's air administrations distribution within the 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

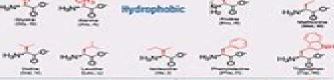
 The addition of a sterically bulky functional group can:
- Increase selectivity for its biological target
- Enhance blading interactions with its biological target Cause fiscorable alterations in the rate of metabolisms
- The acidio-basic nature of a drug molecule influences its chemical, pharmaceutical, 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 memoryalizati bondo.
- 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
100	Corbonythe sold	Aridar	2.5-3
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
· · · · ·	Sullines	Neide	0-2
e o f on	- F-0-	Action	1.5-2.5 (Seet plansplane) 6.5-7.5 (second plansplane) 2-3 (Seet plansplane) 7-9 (second plansplane)
1	-	Desir	9-10 (offer performance)
oi.	Anton	t-	2 f (other protections)
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	.	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. $p(0) = -\log_2(0, 1) = -(-1) = 1$ EX: pell of 0.0001 MHT 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.

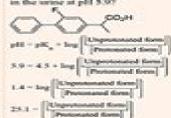
$$pK_{a} = \log(K_{a})$$

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

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 if it is in the sering at pHI 5.97



Autowayer Morey umprotomotod The protonation state affects:

The charge of a functional group (n or -)

Medicinal Chemistry Study Guide

SJ Ball

Medicinal Chemistry Study Guide:

Fundamentals of Medicinal Chemistry and Drug Metabolism M. O. Faruk Khan, Ashok Philip, 2018-06-01 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 chemical basis of drug action This first volume of the series is comprised of 8 chapters focusing on basic background information about medicinal chemistry It takes a succinct and conceptual approach to introducing important fundamental concepts required for a clear understanding of various facets of pharmacotherapeutic agents drug metabolism and important biosynthetic pathways that are relevant to drug action Notable topics covered in this first volume include the scope and importance of medicinal chemistry in pharmacy education a comprehensive discussion of the organic functional groups present in drugs and information about four major types of biomolecules proteins carbohydrates lipids nucleic acids and key heterocyclic ring systems. The concepts of acid base chemistry and salt formation and their applications to the drug action and design follow thereafter These include concepts of solubility and lipid water partition coefficient LWPC isosterism stereochemical properties mechanisms of drug action drug receptor interactions critical for pharmacological responses of drugs and much more Students and teachers will be able to integrate the knowledge presented in the book and apply medicinal chemistry concepts to understand the pharmacodynamics Oxford IB Study Guides: Chemistry for the IB Diploma Geoff and pharmacokinetics of therapeutic agents in the body Neuss, 2014-10-02 This comprehensive Study Guide reinforces all the key concepts for the 2014 syllabus ensuring students develop a clear understanding of all the crucial topics at SL and HL Breaking concepts down into manageable sections and with diagrams and illustrations to cement understanding exam preparation material is integrated to build student confidence and assessment potential Directly linked to the new Oxford Chemistry Course Book to extend and sharpen comprehension this book supports maximum achievement in the course and assessment Fully comprehensive and matched to the new 2014 syllabus Concise and focused approach simplifies complex ideas building truly confident understanding Clear and explanatory style uses plenty of visuals to make each concept accessible easing comprehension Build a strong foundation of assessment skills strengthening potential with integrated exam questions Develop assessment confidence drawing on thorough assessment support and advice Clear and straightforward lan 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 Organic Chemistry Fundamentals Study Guide Speedy Publishing, 2014-11-26 In order to fully understand any subject the fundamentals must be understood and kept in the back of the mind Organic Chemistry is one of the most difficult subjects a college student can take especially if they are not a Chemistry major A lot goes into the fundamentals of the subject That is why an Organic Chemistry Fundamentals book can be so helpful to a student When studying the material if the student discovers they do not understand something they can reference the book and continue with studying in no time at all Having a reference book is the key to success in an Organic Chemistry class **Study Guide for Clinical Procedures** for Medical Assistants - E-Book Kathy Bonewit-West, 2022-10-12 Learn how to think critically and perform competently in the clinical setting Correlating to chapters in Clinical Procedures for Medical Assistants 11th Edition this study guide provides additional activities review questions and exercises designed to prepare you to work in a modern medical office Content aligns to the new 2022 medical assisting educational competencies and provides procedure checklists and video evaluations to help you track your mastery of clinical skills This essential companion provides the practice you need to prepare for a successful career in the fast paced world of medical assisting Critical thinking activities with realistic situations help students analyze and apply what they we learned with games role playing situations crossword puzzles and independent study questions Focus on competency mastery includes worksheets to practice key skills and evaluation forms to assess proficiency Assignment sheets at the beginning of chapters help students stay organized and document their progress NEW 2022 CAAHEP medical assisting competencies throughout represent the latest educational standards NEW Updated content addresses changes in the medical record nutritional guidelines OSHA standards for infection control and prevention emergency preparedness and more REVISED Self assessment opportunities allow students to perform quick comprehension checks including pre tests post tests and key term assessments **Medicinal Chemistry of Drugs Affecting the Nervous** System M. O. Faruk Khan ,Ashok E. Philip,2020-09-24 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 the Nervous System is the second volume of the

series and it presents 8 chapters focusing on a comprehensive account of drugs affecting the nervous system The volume informs readers about the medicinal chemistry of relevant drugs which includes the mechanism of drug action detail structure activity relationships and metabolism as well as clinical significance of drugs affecting autonomic and central nervous system Chapters in this volume cover cholinergic drugs adrenergic drugs antipsychotics antidepressants sedatives hypnotics anxiolytics antiepileptic drugs anesthetics and antiparkinsonian drugs respectively Students and teachers will 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 Study Guide for Brunner & Suddarth's Textbook of Medical-Surgical Nursing Janice L. Hinkle, 2025-08-28 Make the most of what you learn in Brunner Suddarth's Textbook of Medical Surgical Nursing 16th Edition with this easy to use study companion Updated to reflect the latest textbook material this study guide provides everything you need to assess your understanding and practice applying your knowledge preparing you for success in class on the NCLEX exam and in nursing practice Medical Laboratory Technician Certification Study Guide 2025-2026 Lucas Blade Hebert, Master Laboratory Science Ace Your Certification Ready to excel in your MLT or MLS certification exam This comprehensive review guide provides everything you need to succeed from fundamental concepts to advanced clinical applications 700 Practice Questions Test your knowledge across all laboratory disciplines with detailed explanations that reinforce learning 26 Complete Chapters Master Hematology Chemistry Microbiology Immunology Blood Banking and more with systematic easy to follow content Real Clinical Cases Apply your knowledge through authentic laboratory scenarios that mirror actual practice High Yield Review Focus your study time on the most frequently tested concepts with targeted review sections Test Taking Strategies Learn proven techniques to maximize your performance on examination day From basic laboratory principles to complex diagnostic challenges this guide builds the knowledge and confidence you need for certification success Perfect for MLT and MLS candidates laboratory science students and practicing professionals seeking continuing education Transform your preparation Achieve your Study Guide for Today's Medical Assistant - E-Book Kathy Bonewit-West, Sue Hunt, Edith certification goals Applegate, 2014-07-30 Use this study tool to master the content from your Today's Medical Assistant Clinical Administrative Procedures 2nd Edition textbook Corresponding to the chapters in the textbook by Kathy Bonewit West Sue Hunt and Edith Applegate this study guide helps you understand and apply the material with practical exercises activities flashcards checklists review questions and more Chapter assignment tables at the beginning of chapters guide you through textbook and study guide assignments and make it easy to track your progress Laboratory assignment tables list the procedures in each chapter including study guide page number references and indicate the procedures shown on the DVDs A pretest and posttest in each chapter measure your understanding with 10 true false questions Key term assessments include exercises to

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exercises strengthen your comprehension of key concepts Multiple choice questions help you prepare for classroom and board exams Workplace application exercises promote critical thinking and job readiness before you enter practice Internet exercises offer ideas for expanded and project based learning NEW Content aligns to 2022 medical assisting educational competencies NEW Advanced Clinical Skills unit features three new chapters on IV therapy radiology basics and radiology positioning to support expanded medical assisting functions NEW Coverage of telemedicine enhanced infection control related to COVID 19 and catheterization NEW Procedures address IV therapy limited scope radiography applying a sling and coaching for stool collection EXPANDED Information on physical medicine and rehabilitation EXPANDED Content on specimen collection including wound swab nasal and nasopharyngeal collections BIOS Instant Notes in Chemistry for Biologists Julie Fisher, John Arnold, 2003-09-25 Instant Notes in Chemistry for Biologists is a concise book for undergraduates who have a limited background in chemistry This book covers the main concepts in chemistry provides simple explanations of chemical terminology and illustrates underlying principles and phenomena in the life sciences with clear biological examples Building on the success of the first edition the second edition has been fully revised and updated and comprises new sections on water as a biological solvent inorganic molecules and biological macromolecules **Fove's Principles of Medicinal** Chemistry Marc W. Harrold, Kimberly Beck, Victoria F. Roche, S. William Zito, Thomas L. Lemke, David A. Williams, 2025-08-26 Maintaining its status as the gold standard in medicinal chemistry education Foye's Principles of Medicinal Chemistry 9th Edition presents a renewed focus on the fundamental concepts that form the backbone of this critical discipline This latest edition helmed by new senior editors Marc Harrold and Kim Beck continues the text's legacy of excellence while streamlining content for today s pharmacy students and practitioners Expert contributions from experienced educators research scientists and clinicians clarify the chemical basis of drug action emphasizing the structure activity relationships physicochemical pharmacokinetic properties and metabolic profiles of the most commonly used drugs Catalog of Copyright Entries. Third Current Catalog National Library of Medicine (U.S.),1979 First multi Series Library of Congress. Copyright Office, 1971 year cumulation covers six years 1965 70 **Applied Medical Chemistry** Lawrence Wolff, 1885

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