Journal Of Medicinal Chemistry

Indoles continue to be of great interest to the pharmaceutical industry and at the current time several thousand specific new derivatives are reported annually. Research has been driven by the wide range of indole derivatives which occur in nature and through the biological activity of many indole derivatives, of both natural and synthetic origin.This book provides a systematic guide to the most useful and important reactions in the field for both synthesis and synthetic modification of the indole ring. While including the most recently developed and promising methods, it also updates informationavailable on classical methods to give the reader an up-to-date and comprehensive view of the subject. The methods are illustrated by procedures drawn from the literature and by tables including examples chosen to indicate both the scope of applicabilityand variations in methodology. The organization of the book is based on the retrosynthetic concept of identifying the bond(s) formed in the reaction, which in turn identifies potential starting materials. Includes systematic summaries of the most important methods for the construction of indoles from aromatic precursors Discusses methods for preparing indoles by annelation of pyrroles Covers methods for adding or modifying substituent groups, including methods for introducing the tryptamine and tryptophan side-chainsExamines reduction/oxidation reactions that are specific for indoles Considers use of cycloaddition reactions for synthetic elaboration of indoles

Medicinal chemistry and pharmacology are closely associated fields, and the use of natural products for their medicinal properties is ever-growing. The study of drugs from natural products and their effects on the living body are explored in this volume. The book looks into the research, discovery, and characterization of chemicals that exhibit biological effects. Providing an informative compilation of research, valuable case studies, and reviews of existing literature in the area, the book focuses on the ethnobotanical uses of natural products and phytochemicals for health care, including applications for diabetes, ulcers, wound healing, chronic alcoholism, hemorrhoidal treatment, cancer mitigation, pain management, immunotherapy, and more.

Written with the practicing medicinal chemist in mind, this is the first modern handbook to systematically address the topic of bioisosterism. As such, it provides a ready reference on the principles and methods of bioisosteric replacement as a key tool in preclinical drug development. The first part provides an overview of bioisosterism, classical bioisosteres and typical molecular interactions that need to be considered, while the second part describes a number of molecular databases as sources of bioisosteric identification and rationalization. The third part covers the four key methodologies for bioisostere identification and replacement: physicochemical properties, topology, shape, and overlays of protein-ligand crystal structures. In the final part, several real-world examples of bioisosterism in drug discovery projects are discussed. With its detailed descriptions of databases, methods and real-life case studies, this is tailor-made for busy industrial researchers with little time for reading, while remaining easily accessible to novice drug developers due to its systematic structure and introductory section.

Current discoveries and research into bioactive naturalproducts Medicinal Chemistry of Bioactive Natural Products provides amuch-needed survey of bioactive natural products and theirapplications in medicinal chemistry. This comprehensive referencefeatures

*articles by some of the world's leading scientists in thefield on discovery, structure elucidation, and elegant syntheticstrategies--developed for natural products--with an emphasis on thestructure activity relationship of bioactive natural products. Thetopics have been carefully chosen on the basis of relevance tocurrent research and to importance as clinicially usefulagents. Rather than attempting to be a comprehensive encyclopedia ofbioactive natural products, Medicinal Chemistry of BioactiveNatural Products guides the reader to the key developments in thefield. By providing not only practical detail but a historicalperspective on the chemistry and biology of the compounds underconsideration, the book serves as a handy resource for researchersin their own work developing pharmaceuticals, and as an inspiringintroduction for young scientists to the dynamic field of bioactivenatural products research. Enhanced by examples with updated research results, the discussioncovers such topics as: * The chemistry and biology of epothilones * Vancomycin and other glycopeptide antibiotic derivates * Antitumor and other related activities of Taxol and itsanalogs * The antimalarial properties of the traditional Chinese medicine,Quinghaosu (artemisinin) * Huperzine A: A natural drug for the treatment of Alzheimer'sdisease * The medicinal chemistry of ginkgolides from Ginkgo biloba * Recent progress in Calophyllum coumarins as potent anti-HIVagents * Plant-derived anti-HIV agents and analogs * Chemical synthesis of annonaceous acetogenins and theirstructurally modified mimics*

Accounts in Drug Discovery

Synthesis of Heterocycles in Contemporary Medicinal Chemistry

New Developments in Medicinal Chemistry

Medicinal Organometallic Chemistry

Computational methods are transforming the work of chemical and pharmaceutical laboratories. Increasingly faster and more exact simulation algorithms have made quantum chemistry a valuable tool in the search for active substances. Written by a team of leading international quantum chemists, this book is aimed at both beginners as well as experienced users of quantum chemical methods. All commonly used quantum chemical methods are treated here, including Density Functional Theory, quantum and molecular mechanical approaches. Numerous examples illustrate the use of these methods for dealing with problems in pharmaceutical practice, whether the study of inhibitor binding, identifying the surface load of active substances or deriving molecular descriptors using quantum chemical tools. For anyone striving to stay ahead in this rapidly evolving field. Backed by leading authorities, this is a professional guide to successful compound screening in pharmaceutical research and chemical biology, including the chemoinformatic tools needed for correct data evaluation. Chapter authors from leading pharmaceutical companies as well as from Harvard University discuss such factors as chemical genetics, binding, cell-based and biochemical assays, the efficient use of compound libraries and data mining using cell-based assay results. For both academics and professionals in the pharma and biotech industries working on small molecule screening.

Medicinal Chemistry begins with the history of the field, starting from the serendipitous use of plant preparations to current practice of design- and target-based screening methods. Written from the perspective of practicing medicinal chemists, the text covers key drug discovery activities such as pharmacokinetics and patenting, as well as the classes and structures of drug target (receptors, enzymes, nucleic acids, and protein-protein and lipid interactions) with numerous examples of drugs acting at each type. Selected therapeutic areas include drugs to treat cancer, infectious diseases, and central nervous system disorders. Throughout the book, historical and current examples illustrate the progress to market and case studies explore the applications of concepts discussed in the text. Each chapter features a Journal Club, as well as review and application questions to enhance and test comprehension. This textbook is ideal for upper-level undergraduates and graduate students taking a one-semester surv course on medicinal chemistry and/or drug discovery, as well as scientists entering the pharmaceutical industry.
Medicinal Chemistry: An Introduction, Second Edition provides a comprehensive, balanced introduction to this evolving and multidisciplinary area of research. Building on the success of the First Edition, this edition has been completely revised and updated to include the latest developments in the field. Written in an accessible style, Medicinal Chemistry: An Introduction, Second Edition carefully explains fundamental principles, assuming little in the way of prior knowledge. The book focuses on the chemical principles used for drug discovery and design covering physiology and biology where relevant. It opens with a broad overview of the subject with subsequent chapters examining topics in greater depth. From the reviews of the First Edition: "It contains a wealth of information in a compact form" ANGEWANDTE CHEMIE, INTERNATIONAL EDITION "Medicinal Chemistry is certainly a text I would chose to teach from for undergraduates. It fills a unique niche in the market place." PHYSICAL SCIENCES AND EDUCATIONAL REVIEWS

Proceedings of 10th World Congress on Medicinal Chemistry & Drug Design 2018

European Journal of Medicinal Chemistry

High-Throughput Screening in Drug Discovery

Medicinal Chemistry of Anticancer Drugs

An Introduction

This volume provides an introduction to medicinal chemistry. It covers basic principles and background, and describes the general tactics and strategies involved in developing an effective drug.

The Practice of Medicinal Chemistry, 2E, is a single-volume source on the practical aspects of medicinal chemistry. The successful first edition was nicknamed "The Bible" by medicinal chemists, and the second edition has been updated, expanded and refocused to reflect developments over the last decade. Emphasis is put on how medicinal chemists conduct their search for and design of new drug entities. In contrast to competing books, it focuses on the chemistry rather than pharmacological concepts or descriptions of the various therapeutic classes of drugs. Most medicinal chemists

working in the pharmaceutical industry are organic synthetic chemists who must acquire a strong knowledge of medicinal chemistry as they enter the industry. This book aims to be their practical handbook - a complete guide to the drug discovery process. * The only book available dealing with the practical aspects of medicinal chemistry * Serves as a complete guide to the drug discovery process, from conception of the molecules to drug production * Updated chapters devoted to the discovery of new lead compounds, including combinatorial chemistry

The series Topics in Heterocyclic Chemistry presents critical reviews on present and future trends in the research of heterocyclic compounds. Overall the scope is to cover topics dealing with all areas within heterocyclic chemistry, both experimental and theoretical, of interest to the general heterocyclic chemistry community. The series consists of topic related volumes edited by renowned editors with contributions of experts in the field. All chapters from Topics in Heterocyclic Chemistry are published Online First with an individual DOI. In references, Topics in Heterocyclic Chemistry is abbreviated as Top Heterocycl Chem and cited as a journal.

The authors of this guide are experts on the use of microwaves for drug synthesis as well as having much experience in teaching courses held under the auspices of the American Chemical Society and the IUPAC. In this handy source of information for any practicing synthetic chemist they focus on common reaction types in medicinal chemistry, including solid-phase and combinatorial methods. They consider the underlying theory, latest developments in microwave applications and include a variety of examples from recent literature, as well as less common applications that are equally relevant for organic and medicinal chemists. An indispensable reference for researchers with an affinity to modern methods.

Measurement and Prediction

Proceedings of 6th World Congress on Medicinal Chemistry and Drug Design 2017

Journal of Medicinal Chemistry : Volume 8

Journal of Medicinal Chemistry

Medicinal Chemistry of Bioactive Natural Products

Medicinal chemistry is a complex topic. Written in an easy to follow and conversational style, Basic Concepts in Medicinal Chemistry focuses on the fundamental concepts that govern the discipline 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.

The inspiration provided by biologically active natural products to conceive of hybrids, congeners, analogs and unnatural variants is discussed by experts in the field in 16 highly informative chapters. Using well-documented studies over the past decade, this timely monograph demonstrates the current importance and future potential of natural products as starting points for the development of new drugs with improved properties over their progenitors. The examples are chosen so as to represent a wide range of natural products with therapeutic relevance among others, as anticancer agents, antimicrobials, antifungals, antisense nucleosides, antidiabetics, and analgesics. From the content: * Part I: Natural Products as Sources of Potential Drugs and Systematic Compound Collections * Part II: From Marketed Drugs to Designed Analogs and Clinical Candidates * Part III: Natural Products as an Incentive for Enabling Technologies * Part IV: Natural Products as Pharmacological Tools * Part V: Nature: The Provider, the Enticer, and the Healer

This is Volume 1: Drug Discovery, of Burger's Medicinal Chemistry and Drug Discovery, 6th Edition. This new volume contains critical new chapters on Virtual Screening, Bioinformatics and Chemical Information Computing Systems in Drug Discovery. To purchase the entire 6 volume set, please refer to ISBN 0-471-37032-0. For a complete list of articles and contributors as well as FREE sample chapters from this new 6th Edition please visit: www.mrw.interscience.wiley.com/bmcdd

Medicinal Chemistry of Anticancer Drugs, Second Edition, provides an updated treatment from the point of view of medicinal chemistry and drug design, focusing on the mechanism of action of antitumor drugs from the molecular level, and on the relationship between chemical structure and chemical and biochemical reactivity of antitumor agents. Antitumor chemotherapy is a very active field of research, and a huge amount of information on the topic is generated every year. Cytotoxic chemotherapy is gradually being supplemented by a new generation of drugs that recognize specific targets on the surface or inside cancer cells, and resistance to antitumor drugs continues to be investigated. While these therapies are in their infancy, they hold promise of more effective therapies with fewer side effects. Although many books are available that deal with clinical aspects of cancer chemotherapy, this book provides a sorely needed update from the point of view of medicinal chemistry and drug design. Presents information in a clear and concise way using a large number of figures Historical background provides insights on how the process of drug discovery in the anticancer field has evolved Extensive references to primary literature

Green Approaches in Medicinal Chemistry for Sustainable Drug Design
Scaffold Hopping in Medicinal Chemistry
Textbook of Drug Design and Discovery, Third Edition
Bioisosteres in Medicinal Chemistry
Molecular Drug Properties

The most comprehensive source of the latest information in drug discovery and medicinal chemistry BURGER'S MEDICINAL CHEMISTRY AND DRUG DISCOVERY, FIFTH EDITION, Volume 2: Therapeutic Agents Renowned for its incisive, systematic examination of the new classes of drugs, Burger's Medicinal Chemistry and Drug Discovery provides professionals with thorough, yet selective access to drug chemistry information in a convenient format. Volume 2 outlines the newest generation of drugs with the potential for controlling cardiovascular, gastrointestinal, and tubercular disease. These include: * Cholinergics and anticholinergics * Gastric proton pump inhibitors * Cardiac drugs and antihypertensive agents * Diuretic and urcosuric agents * Aminoglycoside, macrolide, glycopeptide, and other antibacterial antibiotics * Antimycobacterial and antifungal agents The behavior of each drug class is explored in terms of pathophysiology of the disease state, molecular mechanism of action, pharmacokinetics, toxicity, drug metabolism, and structure activity relationships. Special attention is given to fertile areas of further research. Burger's Medicinal Chemistry and Drug Discovery, Volume 2 is an essential reference for medical professionals and researchers working today. Burger's Medicinal Chemistry, Fifth Edition consists of five volumes: Volume 1: Principles and Practice (0-471-57556-9) 1995 " . . . an essential addition to the libraries of any medicinal chemist . . . an outstanding work . . . highly praised as a fountain of information in drug studies and research."--Journal of Medicinal Chemistry * Volume 2: Therapeutic Agents (0-471-57557-7) 1996 * Volume 3: Therapeutic Agents (0-471-57558-5) 1996 * Volume 4: Therapeutic Agents (0-471-57559-3) 1997 * Volume 5: Therapeutic Agents (0-471-57560-7) 1997

Advances in knowledge and technology have revolutionized the process of drug development, making it possible to design drugs for a given target or disease. Building on the foundation laid by the previous three editions, Smith and Williams Introduction to the Principles of Drug Design and Action, Fourth Edition includes the latest informatio

Building on the success of the previous editions, Textbook of Drug Design and Discovery has been thoroughly revised and updated to provide a complete source of information on all facets of drug design and discovery for students of chemistry, pharmacy, pharmacology, biochemistry, and medicine. The book follows drug design from the initial lead identification through optimization and structure-activity relationship with reference to the final processes of clinical evaluation and registration. Chapters investigate the design of enzyme inhibitors and drugs for particular cellular targets such as ion channels and receptors, and also explore specific classes of drug such as peptidomimetics, antivirals and anticancer agents. The use of gene technology in pharmaceutical research, computer modeling techniques, and combinatorial approaches are also included.

June 07-08, 2017 Milan,. Italy Key Topics : Medicinal Chemistry, Synthetic Organic Chemistry, Drug Design and Drug

Development, CADD (Computer Aided Drug Design), Bioorganic and Medicinal Chemistry, Pharmacology and toxicology, BioInorganic Chemistry, Organometallic Chemistry, Radiopharmaceuticals, Chemical Biology, Anticancer agents in Medicinal Chemistry, Pharmaceutical Industry, Clinical Pharmacology, Pharmaceutical Sciences, Bioisostere, Analytical Chemistry, Nanomedicine, Stereochemistry, Pharmacovigilance,

Medicinal and Biological Inorganic Chemistry

Molecular Biology in Medicinal Chemistry

Indoles

Smith and Williams' Introduction to the Principles of Drug Design and Action

Quantum Medicinal Chemistry

This readily comprehensible book explains the identification of molecular targets via cellular assays, reporter genes or transgenic models, as well as surveying recent advances in the synthesis, separation and analysis of drugs. A special section is devoted to molecular genetics methods. With its examination of these novel methods and generous practical advice, this is essential reading for all pharmaceutical chemists, molecular biologists and medical researchers using molecular methods to study drugs and their action.

Provides a thorough overview of the role of fluorine in pharmaceutical science and development Includes chapters on fluorinated analogues of natural products, fluorinated amino acids and peptides, and derivatives of sugars Classifies marketed and in-development fluorinated pharmaceuticals according to their therapeutic classes

The book provides a current overview and comprehensive compilation for medicinal chemists that discusses the effects of aiming for multiple targets on the entire drug development process. The result is a broad survey of current and future strategies for drug selectivity in medicinal chemistry with theoretical but also practical aspects. Different strategies are presented and evaluated, such as various design approaches, merged multiple ligands, discovery technologies and a broad range of successful examples of unselective drugs taken from all major disease areas. With its wide-ranging view of an emerging new paradigm in drug development, this handbook is of prime importance for every medicinal and pharmaceutical chemist.

June 14-15, 2018 Barcelona,Spain Key Topics : Medicinal Chemistry, Pharmaceutical Sciences, Drug Design and Drug Development, CADD (Computer Aided Drug Design), Bioorganic and Medicinal Chemistry, Pharmacology and toxicology, Anticancer agents in Medicinal Chemistry, Analytical Chemistry, Pharmaceutical Industry, Organic Chemistry, Clinical Pharmacology, Evolution of Organic and Medicinal Chemistry in Pharma, Organic and Medicinal Chemistry Technologies for Drug

Discovery, QSAR (Quantitative Structure-Activity Relationship) Fragment-Based Drug Design, Applications of Organic and Medicinal Chemistry in Drug Discovery, Market Dynamics, Conclusions and Future Trends, Medicinal Plants,

Drug Selectivity

Adventures in Medicinal Chemistry

Natural Products in Medicinal Chemistry

Basic Concepts in Medicinal Chemistry

Name Reactions in Heterocyclic Chemistry

Covers important name reactions relevant to heterocyclic chemistry The field of heterocyclic chemistry has long presented a specialchallenge for chemists. Because of the enormous amount and varietyof information, it is often a difficult topic to cover forundergraduate and graduate chemistry students, even in simplifiedform. Yet the chemistry of heterocyclic compounds and methods fortheir synthesis form the bedrock of modern medicinal chemical andpharmaceutical research. Thus there is a great need for highquality, up-to-date, and authoritative books on heterocyclicsynthesis helpful to both the professional research chemist as wellas the advanced student. Name Reactions in Heterocyclic Chemistry provides aone-stop repository for this important field of organic chemistry.The primary topics include three- and four-membered heterocycles,five-membered heterocycles including indoles, furans, thiophenes,and oxazoles, six-membered heterocycles including quinolines,isoquinolines, and pyrimidines, and other heterocycles. Each name reaction is summarized in seven sections: Description Historical perspective Mechanism Variations and improvements Synthetic utility Experimental References Authored by a team of world-renowned contributors - some of whomhave discovered the very reactions they describe - NameReactions in Heterocyclic Chemistry represents astate-of-the-art resource for students and researchers alike.

Contents: Gérard Jaouen, Nils Metzler-Nolte : Introduction ; Stéphane GIBAUD and Gérard JAOUEN: Arsenic - based drugs: from Fowler's solution to modern anticancer chemotherapy; Ana M. Pizarro, Abraha Habtemariam and Peter J. Sadler : Activation Mechanisms for Organometallic Anticancer Complexes; Angela Casini, Christian G. Hartinger, Alexey A. Nazarov, Paul J. Dyson : Organometallic antitumour agents with alternative modes of action; Elizabeth A. Hillard, Anne Vessières, Gerard Jaouen : Ferrocene functionalized endocrine modulators for the treatment of cancer; Megan Hogan and Matthias Tacke : Titanocenes - Cytotoxic and Anti-Angiogenic

Chemotherapy Against Advanced Renal-Cell Cancer; Seann P. Mulcahy and Eric Meggers : Organometallics as Structural Scaffolds for Enzyme Inhibitor Design; Christophe Biot and Daniel Dive : Bioorganometallic Chemistry and Malaria; Nils Metzler-Nolte : Biomedical applications of organometal-peptide conjugates; Roger Alberto : Organometallic Radiopharmaceuticals; Brian E. Mann : Carbon Monoxide - an essential signaling molecule.

Burger's Medicinal Chemistry, Drug Discovery and Development Explore the freshly updated flagship reference for medicinal chemists and pharmaceutical professionals The newly revised eighth edition of the eight-volume Burger's Medicinal Chemistry, Drug Discovery and Development is the latest installment in this celebrated series covering the entirety of the drug development and discovery process. With the addition of expert editors in each subject area, this eight-volume set adds 35 chapters to the extensive existing chapters. New additions include analyses of opioid addiction treatments, antibody and gene therapy for cancer, blood-brain barrier, HIV treatments, and industrial-academic collaboration structures. Along with the incorporation of practical material on drug hunting, the set features sections on drug discovery, drug development, cardiovascular diseases, metabolic diseases, immunology, cancer, anti-Infectives, and CNS disorders. The text continues the legacy of previous volumes in the series by providing recognized, renowned, authoritative, and comprehensive information in the area of drug discovery and development while adding cutting-edge new material on issues like the use of artificial intelligence in medicinal chemistry. Included: Volume 1: Methods in Drug Discovery, edited by Kent D. Stewart Volume 2: Discovering Lead Molecules, edited by Kent D. Stewart Volume 3: Drug Development, edited by Ramnarayan S. Randad and Michael Myers Volume 4: Cardiovascular, Endocrine, and Metabolic Diseases, edited by Scott D. Edmondson Volume 5: Pulmonary, Bone, Immunology, Vitamins, and Autocoid Therapeutic Agents, edited by Bryan H. Norman Volume 6: Cancer, edited by Barry Gold and Donna M. Huryn Volume 7: Anti-Infectives, edited by Roland E. Dolle Volume 8: CNS Disorders, edited by Richard A. Glennon Perfect for research departments in the pharmaceutical and biotechnology industries, Burger's Medicinal Chemistry, Drug Discovery and Development can be used by graduate students seeking a one-stop reference for drug development and discovery and deserves its place in the libraries of biomedical research institutes, medical, pharmaceutical, and veterinary schools.

This e-book series is recommended for readers who are interested in or work with current theoretical and experimental research in medicinal chemistry, with an emphasis on computer aided-

drug design and organic synthesis for therapeutic purposes. The e-book series encompasses the multidisciplinary field of medicinal chemistry which overlaps the knowledge of chemistry, physics, biochemistry, biology and pharmacology. The second volume of the series contains the following topics: -Current State-of-the-Art for Virtual Screening and Docking Methods -Estimating Protein-Ligand Binding Affinity by NMR -ADME/Tox Predictions in Drug Design -Bioisosteric Replacements in Drug Design

Case Studies in Medicinal Chemistry

Burger's Medicinal Chemistry, Drug Discovery and Development, 8 Volume Set

The Practice of Medicinal Chemistry

Medicinal Chemistry

Burger's Medicinal Chemistry and Drug Discovery, Drug Discovery

Accounts in Drug Discovery describes recent case studies in medicinal chemistry with a particular emphasis on how the inevitable problems that arise during any project can be surmounted or overcome. The Editors cover a wide range of therapeutic areas and medicinal chemistry strategies, including lead optimization starting from high-throughput screening "hits" as well as rational, structure-based design. The chapters include "follow-ons" and "next generation" compounds that aim to improve upon first-generation agents. This volume surveys the range of challenges commonly faced by medicinal chemistry researchers, including the optimization of metabolism and pharmacokinetics, toxicology, pharmaceutics and pharmacology, including proof-of-concept in the clinic for novel biological targets. The case studies include medicinal chemistry stories on recently approved and marketed drugs, but also chronicle "near-misses," i.e. exemplary compounds that may have proceeded well into the clinic but for various reasons did not result in a successful registration. As the vast majority of projects fail prior to registration, much can be learned from such narratives. By sharing a wide range of drug discovery experiences and information across the community of medicinal chemists in both industry and academia, the Editors believe that these accounts will provide insights into the art of medicinal chemistry as it is currently practiced and will help to serve the needs of active medicinal chemists.

This first systematic overview for more than a decade is tailor-made for the medicinal chemist. All the chapters are written by experienced drug developers and include practical examples from real drug candidates. Following an introduction to global drug properties and their impact on

drug research, screening and combinatorial chemistry libraries, this handbook demonstrates the best and fastest way to estimate those properties most relevant for the efficiency and pharmacokinetic performance of a drug molecule: lipophilicity,solubility, electronic properties and conformation.

This first systematic treatment of the concept and practice of scaffold hopping shows the tricks of the trade and provides invaluable guidance for the reader's own projects. The first section serves as an introduction to the topic by describing the concept of scaffolds, their discovery, diversity and representation, and their importance for finding new chemical entities. The following part describes the most common tools and methods for scaffold hopping, whether topological, shape-based or structure-based. Methods such as CATS, Feature Trees, Feature Point Pharmacophores (FEPOPS), and SkelGen are discussed among many others. The final part contains three fully documented real-world examples of successful drug development projects by scaffold hopping that illustrate the benefits of the approach for medicinal chemistry. While most of the case studies are taken from medicinal chemistry, chemical and structural biologists will also benefit greatly from the insights presented here.

Journal of Medicinal ChemistryJournal of Medicinal ChemistryEuropean Journal of Medicinal ChemistryThe Ups and Downs in Drug DesignAdventures in Medicinal ChemistryCRC Press

Medicinal Chemistry of Nucleic Acids

Bioorganic and Medicinal Chemistry of Fluorine

Journal of Medicinal Chemistry: Open Access : Volume 7

Progress in Medicinal Chemistry

The Ups and Downs in Drug Design

The Ups and Downs in Drug Design: Adventures in Medicinal Chemistry highlights the necessity for an integrative approach in medicinal chemistry and chemical biology. As medicinal chemistry is not a monolithic science, it is important to emphasize the other various disciplines that are required for successful drug design. This book presents the author’s own personal experience in this field and describes the "ups" and "downs" that come with drug discovery. It is an excellent companion text for graduate and postgraduate students who would like further insight into the parameters of drug design, including the challenges that come with the project. Key Features Illustrates "real-life" examples in medicinal chemistry Integrates the use of physical, chemical, and biological concepts that are important in drug design Highlights the "ups" and "downs" that come with drug discovery Aims to inspire students

who may be struggling with the challenges and thought process in drug design Intends to be an excellent companion text for graduate and postgraduate students

Complete, up-to-date coverage of the broad area of nucleic acid chemistry and biology Assembling contributions from a collection of authors with expertise in all areas of nucleic acids, medicinal chemistry, and therapeutic applications, Medicinal Chemistry of Nucleic Acids presents a thorough overview of nucleic acid chemistry—a rapidly evolving and highly challenging discipline directly responsible for the development of antiviral and antitumor drugs. This reliable resource delves into a multitude of subject areas involving the study of nucleic acids—such as the new advances in genome sequencing, and the processes for creating RNA interference (RNAi) based drugs—to assist pharmaceutical researchers in removing roadblocks that hinder their ability to predict drug efficacy. Offering the latest cutting-edge science in this growing field, Medicinal Chemistry of Nucleic Acids includes: In-depth coverage of the development and application of modified nucleosides and nucleotides in medicinal chemistry A close look at a large range of current topics on nucleic acid chemistry and biology Essential information on the use of nucleic acid drugs to treat diseases like cancer A thorough exploration of siRNA for RNAi and the regulation of microRNA, non-coding RNA (ncRNA), a newly developing and exciting research area Thorough in its approach and promising in its message, Medicinal Chemistry of Nucleic Acids probes the new domains of pharmaceutical research—and exposes readers to a wealth of new drug discovery opportunities emerging in the dynamic field of nucleic acid chemistry.

Edited by two experts working at the pioneering pharmaceutical company and major global player in hormone-derived drugs, this handbook and reference systematically treats the drug development aspects of all human nuclear receptors, including recently characterized receptors such as PPAR, FXR and LXR. Authors from leading pharmaceutical companies around the world present examples and real-life data from their own work.

The book provides a detailed state-of-the-art overview of inorganic chemistry applied to medicinal chemistry and biology. It covers the newly emerging field of metals in medicine and the future of medicinal inorganic chemistry. It is an essential reading for every researcher and student in medicinal and bioinorganic chemistry.

Burger's Medicinal Chemistry and Drug Discovery, Therapeutic Agents

Methods and Principles in Medicinal Chemistry

Microwaves in Organic and Medicinal Chemistry

An Evolving Concept in Medicinal Chemistry

Natural Products Pharmacology and Phytochemicals for Health Care

Extensive experimentation and high failure rates are a well-recognised downside to the drug discovery process, with the resultant high levels of inefficiency and waste producing a negative environmental impact. Sustainable and Green Approaches in Medicinal Chemistry reveals how medicinal and green chemistry can work together to directly address this issue. After providing essential context to the growth of green chemistry in relation to drug discovery in Part 1, the book goes on to identify a broad range of practical methods and synthesis techniques in Part 2. Part 3 reveals how medicinal chemistry techniques can be used to improve efficiency, mitigate failure and increase the environmental benignity of the entire drug discovery process, whilst Parts 4 and 5 discuss natural products and microwave-induced chemistry. Finally, the role of computers in drug discovery is explored in Part 6. Identifies novel and cost effective green medicinal chemistry approaches for improved efficiency and sustainability Reflects on techniques for a broad range of compounds and materials Highlights sustainable and green chemistry pathways for molecular synthesis

Nuclear Receptors as Drug Targets

An Introduction to Medicinal Chemistry