Pharmaceutical Process Chemistry For Synthesis Rethinking The Routes To Scale Up

A guide to the important chemical engineering concepts for the development of new drugs, revised second edition The revised and updated second edition of Chemical Engineering in the Pharmaceutical Industry offers a guide to the experimental and computational methods related to drug product design and development. The second edition has been greatly expanded and covers a range of topics related to formulation design and process development of drug products. The authors review basic analytics for quantitation of drug product quality attributes, such as potency, purity, content uniformity, and dissolution, that are addressed with consideration of the applied statistics, process analytical technology, and process control. The 2nd Edition is divided into two separate books: 1) Active Pharmaceutical Ingredients (API's) and 2) Drug Product Design, Development and Modeling. The contributors explore technology transfer and scale-up of batch processes that are exemplified experimentally and computationally. Written for engineers working in the field, the book examines in-silico process modeling tools that streamline experimental screening approaches. In addition, the authors discuss the emerging field of continuous drug product manufacturing. This revised second edition: Contains 21 new or revised chapters, including chapters on quality by design, computational approaches for drug product modeling, process design with PAT and process control, engineering challenges and solutions Covers chemistry and engineering activities related to dosage form design, and process development, and scale-

up Offers analytical methods and applied statistics that highlight drug product quality attributes as design features Presents updated and new example calculations and associated solutions Includes contributions from leading experts in the field Written for pharmaceutical engineers, chemical engineers, undergraduate and graduation students, and professionals in the field of pharmaceutical sciences and manufacturing, Chemical Engineering in the Pharmaceutical Industry, Second Edition contains information designed to be of use from the engineer's perspective and spans information from solid to semi-solid to lyophilized drug products.

This volume gives an overview of the applications of organometallic chemistry in process chemistry relevant to the current topics in synthetic chemistry. This volume starts with an introduction on the historical development of organometallics in process chemistry and is followed by chapters dealing with the last five years' development in various organometallic reaction types such as the challenging cross coupling process, construction of 3.1.0 bicycles, pressure and transfer hydrogenations of historically challenging compounds such as esters, utilization of carbon dioxide for making organic compounds by flow process, drug synthesis and metal detection and scavenging in the finished APIs. A chapter by Colacot et.al., is also devoted to the process development and structural understanding of organometallic catalysts with particular emphasis to LnPd(0) catalysts. An academia – industry collaborated chapter on the use of water as a solvent for organometallic processes is included in this book.

Standard medicinal chemistry courses and texts are organized by classes of drugs with an emphasis on descriptions of their biological and pharmacological effects. This book represents a new approach based on physical organic chemical principles and reaction mechanisms that

allow the reader to extrapolate to many related classes of drug molecules. The Second Edition reflects the significant changes in the drug industry over the past decade, and includes chapter problems and other elements that make the book more useful for course instruction. New edition includes new chapter problems and exercises to help students learn, plus extensive references and illustrations Clearly presents an organic chemist's perspective of how drugs are designed and function, incorporating the extensive changes in the drug industry over the past ten years Well-respected author has published over 200 articles, earned 21 patents, and invented a drug that is under consideration for commercialization Medicinal Chemistry: A Look at How Drugs Are Discovered is written for those who are interested in learning how drugs are discovered. Compared to other books on the market, this text takes a different approach by presenting the subject on chemical reaction mechanism terms, which ideally makes the subject matter more interesting and easier to comprehend. The authors describe the drug discovery process, from advancing an initial lead to the approval process, and include drug discovery sources. Additional features: Explains medicinal chemistry on chemical mechanism terms, allowing for a more interesting and easier to comprehend text Includes valuable insights toward the various pathways taken at pharmaceutical industries in drug discoveries Improved by including questions raised and suggestions made from students in the authors' medicinal chemistry classes This book will benefit both upper level undergraduates and graduates studying in the fields of medicinal chemistry and drug discovery, as well as scientists working in the pharmaceutical industry.

An updated overview of the rapidly developing field of green engineering techniques for organic synthesis and medicinal chemistry Green chemistry remains a high priority in modern

organic synthesis and pharmaceutical R&D, with important environmental and economic implications. This book presents comprehensive coverage of green chemistry techniques for organic and medicinal chemistry applications, summarizing the available new technologies, analyzing each technique's features and green chemistry characteristics, and providing examples to demonstrate applications for green organic synthesis and medicinal chemistry. The extensively revised edition of Green Techniques for Organic Synthesis and Medicinal Chemistry includes 7 entirely new chapters on topics including green chemistry and innovation, green chemistry metrics, green chemistry and biological drugs, and the business case for green chemistry in the generic pharmaceutical industry. It is divided into 4 parts. The first part introduces readers to the concepts of green chemistry and green engineering, global environmental regulations, green analytical chemistry, green solvents, and green chemistry metrics. The other three sections cover green catalysis, green synthetic techniques, and green techniques and strategies in the pharmaceutical industry. Includes more than 30% new and updated material—plus seven brand new chapters Edited by highly regarded experts in the field (Berkeley Cue is one of the fathers of Green Chemistry in Pharma) with backgrounds in academia and industry Brings together a team of international authors from academia, industry, government agencies, and consultancies (including John Warner, one of the founders of the field of Green Chemistry) Green Techniques for Organic Synthesis and Medicinal Chemistry, Second Edition is an essential resource on green chemistry technologies for academic researchers, R&D professionals, and students working in organic chemistry and medicinal chemistry.

Presents the most effective catalytic reactions in use today, with a special focus on process intensification, sustainability,

waste reduction, and innovative methods This book demonstrates the importance of efficient catalytic transformations for producing pharmaceutically active molecules. It presents the key catalytic reactions and the most efficient catalytic processes, including their significant advantages over compared previous methods. It also places a strong emphasis on asymmetric catalytic reactions, process intensification (PI), sustainability and waste mitigation, continuous manufacturing processes as enshrined by continuous flow catalysis, and supported catalysis. Active Pharmaceutical Ingredients in Synthesis: Catalytic Processes in Research and Development offers chapters covering: Catalysis and Prerequisites for the Modern Pharmaceutial Industry Landscape; Catalytic Process Design - The Industrial Perspective; Hydrogenation, Hydroformylation and Other Reductions; Oxidation; ; Catalytic Addition Reactions; Catalytic Cross-Coupling Reactions; Catalytic Metathesis Reactions; Catalytic Cycloaddition Reactions: Coming Full-Circle; Catalytic Cyclopropanation Reactions; Catalytic C-H insertion Reactions; Phase Transfer Catalysis; and Biocatalysis. -Provides the reader with an updated clear view of the current state of the challenging field of catalysis for API production -Focuses on the application of catalytic methods for the synthesis of known APIs -Presents every key reaction, including Diels-Alder, CH Insertions, Metal-catalytic coupling-reactions, and many more -Includes recent patent literature for completeness Covering a topic of great interest for synthetic chemists and R&D researchers in the pharmaceutical industry, Active Pharmaceutical Ingredients in Synthesis: Catalytic Processes in Research and Development is a must-read for every synthetic chemist working with APIs. An integrated and insightful look at successful drug synthesis in today's drug discovery market The pharmaceutical industry is unquestionably vibrant today, with drug synthesis making a

vital contribution. Whether in the early developmental stages of identifying and optimizing a lead, or the latter stages of process development and cost-effective scale-up, the ability to design elegant and economical synthetic routes is often a major factor in the eventual viability and commercial success of a drug. Contemporary Drug Synthesis examines how leading researchers and manufacturers have integrated chemistry, biology, pharmacokinetics, and a host of other disciplines in the creation and development of leading drugs. Authored by four of the pharmaceutical industry's most respected scientists, this timely volume: Focuses on the processes that resulted in high-profile drugs including Lipitor, Celebrex, Viagra, Gleevec, Nexium, Claritin, and over a dozen others Provides an in-depth introduction to each drug, followed by a detailed account of its synthesis Organizes the drugs into fourteen therapeutic areas for clarity and ease of use Process chemists provide an essential bridge between chemistry and the marketplace, creating scientifically practical drug processes while never losing sight of the commercial viability of those processes. Contemporary Drug Synthesis meets the needs of a growing community of researchers in pharmaceutical research and development, and is both a useful guide for practicing pharmaceutical scientists and an excellent text for medicinal and organic chemistry students. Process Systems Engineering for Pharmaceutical Manufacturing: From Product Design to Enterprise-Wide Decisions, Volume 41, covers the following process systems engineering methods and tools for the modernization of the pharmaceutical industry: computer-aided pharmaceutical product design and pharmaceutical production processes design/synthesis; modeling and simulation of the pharmaceutical processing unit operation, integrated flowsheets and applications for design, analysis, risk assessment, sensitivity analysis, optimization, design space

identification and control system design; optimal operation, control and monitoring of pharmaceutical production processes; enterprise-wide optimization and supply chain management for pharmaceutical manufacturing processes. Currently, pharmaceutical companies are going through a paradigm shift, from traditional manufacturing mode to modernized mode, built on cutting edge technology and computer-aided methods and tools. Such shifts can benefit tremendously from the application of methods and tools of process systems engineering. Introduces Process System Engineering (PSE) methods and tools for discovering, developing and deploying greener, safer, cost-effective and efficient pharmaceutical production processes Includes a wide spectrum of case studies where different PSE tools and methods are used to improve various pharmaceutical production processes with distinct final products Examines the future benefits and challenges for applying PSE methods and tools to pharmaceutical manufacturing

Designed to provide a comprehensive, step-by-step approach to organic process research and development in the pharmaceutical, fine chemical, and agricultural chemical industries, this book describes the steps taken, following synthesis and evaluation, to bring key compounds to market in a cost-effective manner. It describes hands-on, step-by-step, approaches to solving process development problems, including route, reagent, and solvent selection; optimising catalytic reactions; chiral syntheses; and "green chemistry." Second Edition highlights: • Reflects the current thinking in chemical process R&D for small molecules • Retains similar structure and orientation to the first edition. • Contains approx. 85% new material • Primarily new examples (work-up and prospective considerations for pilot plant and manufacturing scale-up) • Some new/expanded topics (e.g. green chemistry, genotoxins, enzymatic processes) •

Replaces the first edition, although the first edition contains useful older examples that readers may refer to Provides insights into generating rugged, practical, cost-effective processes for the chemical preparation of "small molecules" Breaks down process optimization into route, reagent and solvent selection, development of reaction conditions, workup, crystallizations and more Presents guidelines for implementing and troubleshooting processes

Chemistry and chemical engineering have changed significantly in the last decade. They have broadened their scopeâ€"into biology, nanotechnology, materials science, computation, and advanced methods of process systems engineering and controlâ€"so much that the programs in most chemistry and chemical engineering departments now barely resemble the classical notion of chemistry. Beyond the Molecular Frontier brings together research, discovery, and invention across the entire spectrum of the chemical sciencesâ€"from fundamental, molecular-level chemistry to large-scale chemical processing technology. This reflects the way the field has evolved, the synergy at universities between research and education in chemistry and chemical engineering, and the way chemists and chemical engineers work together in industry. The astonishing developments in science and engineering during the 20th century have made it possible to dream of new goals that might previously have been considered unthinkable. This book identifies the key opportunities and challenges for the chemical sciences, from basic research to societal needs and from terrorism defense to environmental protection, and it looks at the ways in which chemists and chemical engineers can work together to contribute to an improved future.

This book brings together the chemical strategies used in the optimisation of organic reactions and processes, and highlights the practical and technological options available.

This book offers: an encyclopedic treatment of organic chemistry from an industrial, process research and development, and manufacturing point of view plenty of examples to illustrate the scope and limitation of the strategies a comprehensive index organised by topic, reaction type, and reagent an extensive literature survey. This is an essential and comprehensive guide for experienced practitioners of chemical process research and development, fresh recruits to chemical industry R&D divisions, and academics who are interested in interacting with the chemical industry, optimising their synthetic strategies, and enriching the field of atom economy.

Separation Methods in Drug Synthesis and Purification

There is a need to explain that generic versions of a drug may not be manufactured by the same process as brand-name drugs and that the different processes may have dramatically different environmental impacts. Two global forces are at odds today—the push for "greener" processes and the push for lower drug prices. This book brings this conflict into sharp focus by discussing in detail the published process chemistry for top-selling small molecule drugs. Providing insights about process route selection, choice of reagents, and reaction conditions, Pharmaceutical Process Chemistry for Synthesis guides process chemists in identifying best processes for manufacturing these blockbuster drugs as they lose patent protection. Further, it highlights the strategies and methodology that might be useful for expediting the process research and development of the blockbusters of the future. Written from a refreshingly objective perspective, this book is essential for process chemists who need to devise practical syntheses for increasingly complex drugs in a constantly decreasing time frame.

As pharmaceutical companies strive to develop safer

medicines at a lower cost, they must keep pace with the rapid growth of technology and research methodologies. Defying the misconception of process chemistry as mere scale-up work, Process Chemistry in the Pharmaceutical Industry, Vol. 2: Challenges in an Ever Changing Climate explores novel applications of synthetic, physical, and analytical chemistry in drug discovery and development. It offers an accurate depiction of the most up-to-date process research and development methods applied to synthesis, clinical trials, and commercializing drug candidates. The second installment in this progressive series, this volumereviews the latest breakthroughs to advance process chemistry, including asymmetric synthesis, crystallization, morphology, enzymatic intervention, green chemistry, macromolecules (monoclonal antibodies, biological molecules, polymers), enantioselectivity, organometallic chemistry, process analytical tools, chemical engineering controls, regulatory compliance, and outsourcing/globalization. It explores new approaches to synthetic processes, examines the latest safety methods and experiment design, and suggests realistic solutions to problems encountered in manufacturing and process development. Significant topics include atom economy, ease of synthesis, instrumentation, automization, quality control, cost considerations, green practices, and future trends. Jointly edited by the founder/president of Delphian Pharmaceuticals and the director of Chemical R&D at Pfizer, this book brings together contributions byreputed scientists, technologists, engineers, and professors from leading academic institutions, such as the Imperial College, UK, the University of Tokyo, ETH, Switzerland, the International University at Bermen, Germany, and the University of Connecticut, USA, and from principal pharmaceutical companies that include Merck, Bristol Myers Squibb, Pfizer, Novartis, Eli Lilly, Astrazeneca and DSM.

This book provides a comprehensive, step-by-step approach to organic process research and development in the pharmaceutical, fine chemical, and agricultural chemical industries. Process R&D describes the steps taken, following synthesis and evaluation, to bring key compounds to market in a cost-effective manner. More people are being hired for work in this area as increasing numbers of drug candidates are identified through combinatorial chemistry and high-throughput screening. The book is directed to industrial (primarily organic) chemists, and academicians (particularly those involved in a growing number of start-up companies) and students who need insight into industrial process R&D. Current books do not describe hands-on, step-by-step, approaches to solving process development problems, including route, reagent, and solvent selection; optimising catalytic reactions; chiral syntheses; and "green chemistry." "Practical Process Research and Development" will be a valuable resource for researchers, managers, and graduate students. Provides insights into generating rugged, practical, cost-effective processes for the chemical preparation of "small molecules" Breaks down process optimization into route, reagent and solvent selection, development of reaction conditions, workup, crystallizations and more Includes over 100 tips for rapid process development Presents guidelines for implementing and troubleshooting processes
Covering the whole area of process chemistry in the pharmaceutical industry, this monograph provides the essential knowledge on the basic chemistry needed for future development and key industrial techniques, as well as morphology, engineering and regulatory compliances. Application-oriented and well structured, the authors include recent examples of excellent industrial production of active pharmaceutical ingredients.

Synthesis of Best-Seller Drugs is a key reference guide for all those involved with the design, development, and use of the best-selling drugs. Designed for ease of use, this book provides detailed information on the most popular drugs, using a practical layout arranged according to drug type. Each chapter reviews the main drugs in each of nearly 40 key therapeutic areas, also examining their classification, novel structural features, models of action, and synthesis. Of high interest to all those who work in the captivating areas of biologically active compounds and medicinal drug synthesis, in particular medicinal chemists, biochemists, and pharmacologists, the book aims to support current research efforts, while also encouraging future developments in this important field. Describes methods of synthesis, bioactivity and related drugs in key therapeutic areas Reviews the main drugs in each of nearly 40 key therapeutic areas, also examining their classification, novel structural features, models of action, and more Presents a practical layout designed for use as a quick reference tool by those working in drug design, development and implementation

This comprehensive workbook helps readers become familiar with the structures and synthetic challenges associated with nearly 300 essential medicines and gain the skills needed for pharmaceutical development. Highlights nearly three

hundred medicines on the latest World Health Organization (WHO) Model List of Essential Medicines and their manufacturing routes Features exercises that equip students with the skills necessary to solve similar real-world problems Includes a retrosynthetic analysis for each commodity chemical and supplies an extensive list of key journal and information sites and a library of reagents, solvents, and conditions for many common organic reactions

Offers a compendium of information on retrosynthesis and process chemistry, featuring innovative "reaction maps" showing synthetic routes of some widely used drugs This book illustrates how the retrosynthetic tool is applied in the Pharmaceutical Industry. It considers and evaluates the many viable synthetic routes that can be used by practicing industrialists, guiding readers through the various steps that lead to the "best" processes and the limits encountered if these are put into practice on an industrial scale of seven key Active Pharmaceutical Ingredient (API). It presents an evaluation of the potential each process has for implementation, before merging the two points of view—of retrosynthesis and process chemistry—in order to show how retrosynthetic analysis assists in selecting the most efficient route for an industrial synthesis of a particular compound whilst giving insight into the industrial process. The book also

uses some key concepts used by process chemists to improve efficiency to indicate the best route to select. Each chapter in Retrosynthesis in the Manufacture of Generic Drugs Selected Case Studies is dedicated to one drug, with each containing information on: worldwide sales and patent status of the Active Pharmaceutical Ingredient (API); structure analysis and general retrosynthetic strategy of the API; first reported synthesis; critical analysis of the processes which have been developed and comparison of the synthetic routes; lessons learned; reaction conditions for Schemes A to X; chemical "highlights" on key reactions used during the synthesis; and references. Drugs covered include: Gabapentin, Clopidogrel, Citalopram and Escitalopram, Sitagliptin, Ezetimibe, Montelukast, and Oseltamivir. Show how the retrosynthetic tool is used by the Pharmaceutical Industry Fills a gap for a book where retrosynthetic analysis is systematically applied to active pharmaceutical ingredients (APIs) Features analyses and methodologies that aid readers in uncovering practical synthetic routes to other drug substances, whether they be NCEs (New Chemical Entities) or generic APIs (Active Pharmaceutical Ingredients) Presents information from both the patent and academic literature for those who wish to use as a basis for further study and thought Features the use of "reaction maps" which display several synthetic processes in the

same scheme, and which allow easy comparisons of different routes that give the same molecule or intermediate. A selection of these maps are available to download from:
https://www.wiley.com/go/santos/retrosynthesis
Retrosynthesis in the Manufacture of Generic Drugs Selected Case Studies is an ideal book for researchers and advanced students in organic synthetic chemistry and process chemistry. It will also be of great benefit to practitioners in the pharmaceutical industry, particularly new starters, and those new to process chemistry.
This text discusses the functions of Process R&D (research and development), which involves the method of transforming a research synthetic procedure into a plant process and the key aspects of a synthesis that must be considered when scaling up a process. Topics consist of: basic principles of chemical development; techniques for the minimization of by-product impurities; criteria for cost-effective synthesis of enantiopure compounds by resolutions; asymmetric synthesis, and "chiral pool" strategy; synthesis for labeling substances with hydrogen or carbon isotopes; and last, licensing.
Synthesis of Essential Drugs describes methods of synthesis, activity and implementation of diversity of all drug types and classes. With over 2300 references, mainly patent, for the methods of synthesis for over 700 drugs, along with the most

widespread synonyms for these drugs, this book fills the gap that exists in the literature of drug synthesis. It provides the kind of information that will be of interest to those who work, or plan to begin work, in the areas of biologically active compounds and the synthesis of medicinal drugs. This book presents the synthesis of various groups of drugs in an order similar to that traditionally presented in a pharmacology curriculum. This was done with a very specific goal in mind – to harmonize the chemical aspects with the pharmacology curriculum in a manner useful to chemists. Practically every chapter begins with an accepted brief definition and description of a particular group of drugs, proposes their classification, and briefly explains the present model of their action. This is followed by a detailed discussion of methods for their synthesis. Of the thousands of drugs existing on the pharmaceutical market, the book mainly covers generic drugs that are included in the WHO's Essential List of Drugs. For practically all of the 700+ drugs described in the book, references (around 2350) to the methods of their synthesis are given along with the most widespread synonyms. Synthesis of Essential Drugs is an excellent handbook for chemists, biochemists, medicinal chemists, pharmacists, pharmacologists, scientists, professionals, students, university libraries, researchers, medical doctors and students, and professionals working in medicinal chemistry. *

Provides a brief description of methods of synthesis, activity and implementation of all drug types * Includes synonyms * Includes over 2300 references
In recent years, a significant amount of progress has been made using green chemistry in the synthesis of synthetically useful compounds and molecules by replacing hazardous chemicals with greener alternatives. However, there is still room for improvement, especially in the pharmaceutical sector where new drugs are being formulated. This book examines green approaches to overcoming hazardous organic transformations. Summarizing recent developments, the book features a detailed description of some of the high impact active pharmaceutical ingredients that have been developed considering green chemistry approaches. It explores the design, engineering and process development and the calculations to account for waste. The book includes strategies to further advance green approaches in the development of generic pharmaceutical industries and features novel, innovative approaches that promote waste-free organic synthesis. This book is of interest to industrialists working in pharmaceuticals and researchers working in green chemistry.
An informative look at the intricacies of today's drug development process Once a discovery organization has identified a potential new drug candidate, it is the daunting task of synthetic organic chemists to

identify the chemical process suitable for preparation of this compound in a highly regulated environment. Only through a multi-layered chemical process that takes into account such factors as safety, environmental considerations, freedom to operate and cost-effectiveness can researchers begin to refine the drug in terms of quality and yield. This book covers both recent advances in the design and synthesis of new drugs, as well as the myriad other issues facing a new drug candidate as it moves through the development process. Utilizing recent case studies, the authors provide valuable insights into the complexities of the process, from designing new synthetic methodologies and applying new automated techniques for finding optimal reaction conditions to selecting the final drug form and formulation. Both novice and active researchers will appreciate the inclusion of chapters on such diverse topics as: * Cross-coupling methods * Asymmetric synthesis * Automation * Chemical Engineering * Application of radioisotopes * Final form selection * Formulations * Intellectual property A wealth of real-world examples and contributions from leading process scientists, engineers, and related professionals make this book a valuable addition to the scientific literature.

Edited by three of the world's leading pharmaceutical scientists, this is the first book on this important and hot topic, containing much previously unpublished

information. As such, it covers all aspects of green chemistry in the pharmaceutical industry, from simple molecules to complex proteins, and from drug discovery to the fate of pharmaceuticals in the environment. Furthermore, this ready reference contains several convincing case studies from industry, such as Taxol, Pregabalin and Crestor, illustrating how this multidisciplinary approach has yielded efficient and environmentally-friendly processes. Finally, a section on technology and tools highlights the advantages of green chemistry. Pharmaceutical process research and development is an exacting, multidisciplinary effort but a somewhat neglected discipline in the chemical curriculum. This book presents an overview of the many facets of process development and how recent advances in synthetic organic chemistry, process technology and chemical engineering have impacted on the manufacture of pharmaceuticals. In 15 concise chapters the book covers such diverse subjects as route selection and economics, the interface with medicinal chemistry, the impact of green chemistry, safety, the crucial role of physical organic measurements in gaining a deeper understanding of chemical behaviour, the role of the analyst, new tools and innovations in reactor design, purification and separation, solid state chemistry and its role in formulation. The book ends with an assessment of future trends and challenges. The

book provides a valuable overview of: both early and late stage chemical development, how safe and scaleable synthetic routes are designed, selected and developed, the importance of the chemical engineering, analytical and manufacturing interfaces, the key enabling technologies, including catalysis and biocatalysis, the importance of the green chemical perspective and solid form issues. The book, written and edited by experts in the field, is a contemporary, holistic treatise, with a logical sequence for process development and mini-case histories within the chapters to bring alive different aspects of the process. It is completely pharmaceutical themed, encompassing all essential aspects, from route and reagent selection to manufacture of the active compound. The book is aimed at both graduates and postgraduates interested in a career in the pharmaceutical industry. It informs them about the breadth of the work carried out in chemical research and development departments, and gives them a feel for the challenges involved in the job. The book is also of value to academics who often understand the drug discovery arena, but have far less appreciation of the drug development area, and are thus unable to advise their students about the relative merits of careers in chemical development versus discovery. The methodologies and technologies adaptable to process chemistry are the focus of this unique book,

as new catalysts, reactions, and methods for the synthesis of functional materials are dealt with in depth for the first time. Those materials take in pharmaceuticals, agrochemicals, functional materials, chemical raw materials, and other substances in the field of process chemistry including green chemistry. Process chemistry underpins the competitiveness of chemical and pharmaceutical industries, but its stagnation is estimated to cause industrial depression and excessive loss. For that reason, chemists focus on process chemistry consistently so that the development of novel and efficient new reactions and technologies provides an essential stimulus. In addition, this volume describes the important development of selected new synthetic devices for process development and the process design for a larger scale, thus furnishing a valuable source for all who are engaged in process chemistry.

Transition metal-catalyzed coupling reactions have a rich history that led to the awarding of the 2010 Nobel Prize in Chemistry to Professors Suzuki, Heck, and Negishi for their pioneering contributions to the field. The coming of age of this active area of research is showcased in this book through case studies in which process chemists from the pharmaceutical industry share their personal experiences developing their own transition metal-catalyzed couplings for the large-scale manufacture

of active pharmaceutical ingredients. Authors from Pfizer, Merck, Boehringer-Ingelheim, Novartis, Amgen, GSK, AstraZeneca, and other companies describe the evolution of robust coupling processes from inception through early and late development, including commercial routes where applicable. This book covers a wide range of coupling transformations while capturing the lessons learned from each process. Every case study details the optimization of at least one transition metal-catalyzed coupling while elaborating on issues such as design of experiments, scalability and throughput, product purification, process safety, and waste management. The important issue of metal removal and the different technologies available to accomplish this goal are also addressed. Finally, a section covers novel technologies for cross-coupling with high potential for future applications on a large scale, such as microwave and flow chemistry as well as green cross-couplings performed in water. With Forewords by Stephen L. Buchwald, Massachusetts Institute of Technology, Trevor Laird, Editor of Organic Process Research and Development and Neal G. Anderson, Anderson's Process Solutions LLC.

Green Sustainable Process for Chemical and Environmental Engineering and Science: Switchable Solvents explores the preparation, properties, chemical processes and applications of this class of

green solvents. The book provides an in-depth overview on the area of switchable solvents in various industrial applications, focusing on the purification and extraction of chemical compounds utilizing green chemistry protocols that include liquid-liquid, solid-liquid, liquid-gas and lipids separation technologies. In addition, it includes recent advances in greener extraction and separation processes. This book will be an invaluable guide to students, professors, scientists and R&D industrial specialists working in the field of sustainable chemistry, organic, analytical, chemical engineering, environmental and pharmaceutical sciences. Provides a broad overview of switchable solvents in sustainable chemical processes Compares the use of switchable solvents as greener solvents over conventional solvents Outlines eco-friendly organic synthesis and chemical processes using switchable solvents Lists various industrial separations/extraction processes using switchable solvents

Here is a practical guide that not only presents insights into the organization and management of the disciplines involved in chemical process development but also provides basic knowledge of these disciplines, enabling process development practitioners to recognize and assimilate them in their work. This book illustrates practical considerations through many examples of the successful direction and integration of the activities

of chemists, analysts, chemical engineers, and biologists, as well as safety, regulatory, and environmental professionals in productive teams. Moreover, this reference provides guidance on: Directing and carrying out specific tasks and courses of action Making and communicating clear and achievable decisions Solving problems on the spot Managing the administrative aspects of chemical process development The author, Dr. Derek Walker, has directed chemical process development work for four decades, combining firsthand chemical synthesis experience with many other disciplines needed to create chemical processes. You will benefit from his advice and unique insights into: Understanding the workings of matrix organizations Defining missions and creating action plans Developing interdisciplinary approaches to problem solving Holding review meetings, revising goals, and motivating staff Prioritizing programs and responses to emergencies In addition, you'll learn how successful chemists, in collaboration with other disciplines, define the best (green) chemistry for process scale-up, including accommodating FDA requirements in the last process steps and addressing safety and environmental matters early in their work. Case studies provide incisive perspective on these issues. A chapter on recognizing and patenting intellectual property emphasizes the importance of comprehensive literature surveys and

understanding invention. A chapter on the future challenges you to think beyond narrow constraints and explore new horizons.

The Art of Drug Synthesis illustrates how chemistry, biology, pharmacokinetics, and a host of other disciplines come together to produce successful medicines. The authors have compiled a collection of 21 representative categories of drugs, from which they have selected as examples many of the best-selling drugs on the market today. An introduction to each drug is provided, as well as background to the biology, pharmacology, pharmacokinetics, and drug metabolism, followed by a detailed account of the drug synthesis. Edited by prominent scientists working in drug discovery for Pfizer Meets the needs of a growing community of researchers in pharmaceutical R&D Provides a useful guide for practicing pharmaceutical scientists as well as a text for medicinal chemistry students An excellent follow-up to the very successful first book by these editors, Contemporary Drug Synthesis, but with all new therapeutic categories and drugs discussed.

This book is aimed at both graduates and postgraduates interested in a career in the pharmaceutical industry by informing them about the breadth of the work carried out in chemical research and development departments. It is also of great value to academics wishing to advise students on the merits of careers in chemical development over

discovery.

Pharmaceutical Process Chemistry for SynthesisRethinking the Routes to Scale-UpJohn Wiley & Sons

Small Molecule Drug Discovery: Methods, Molecules and Applications presents the methods used to identify bioactive small molecules, synthetic strategies and techniques to produce novel chemical entities and small molecule libraries, chemoinformatics to characterize and enumerate chemical libraries, and screening methods, including biophysical techniques, virtual screening and phenotypic screening. The second part of the book gives an overview of privileged cyclic small molecules and major classes of natural product-derived small molecules, including carbohydrate-derived compounds, peptides and peptidomimetics, and alkaloid-inspired compounds. The last section comprises an exciting collection of selected case studies on drug discovery enabled by small molecules in the fields of cancer research, CNS diseases and infectious diseases. The discovery of novel molecular entities capable of specific interactions represents a significant challenge in early drug discovery. Small molecules are low molecular weight organic compounds that include natural products and metabolites, as well as drugs and other xenobiotics. When the biological target is well defined and understood, the rational design of small molecule ligands is possible. Alternatively, small molecule libraries are being used for unbiased assays for complex diseases where a target is unknown or multiple factors contribute to a disease pathology. Outlines modern concepts and

synthetic strategies underlying the building of small molecules and their chemical libraries useful for drug discovery Provides modern biophysical methods to screening small molecule libraries, including high-throughput screening, small molecule microarrays, phenotypic screening and chemical genetics Presents the most advanced chemoinformatics tools to characterize the structural features of small molecule libraries in terms of chemical diversity and complexity, also including the application of virtual screening approaches Gives an overview of structural features and classification of natural product-derived small molecules, including carbohydrate derivatives, peptides and peptidomimetics, and alkaloid-inspired small molecules

Packed with real-world examples, this book illustrates the 12 principles of green chemistry. These diverse case studies demonstrate to scientists and students that beyond the theory, the challenges of green chemistry in pharmaceutical discovery and development remain an ongoing endeavor. By informing and welcoming additional practitioners to this mission, the negative environmental impact of pharmaceutical products will continue to be minimized. Green chemistry is the methodology by which chemical production in this industry can become more efficient, adding environmental stewardship to the noble mission of treating human disease.

The report assesses the current state of chemistry and chemical engineering within the context of drug discovery, disease diagnosis, and disease prevention. Also addressed are chemical and chemical engineering

challenges in pharmaceutical synthesis, delivery, and manufacture.

Updated every five years, the series represents the optimal compromise between currency and a sufficient body of material for cohesive and comprehensive treatment in a monograph. Provides a quick yet thorough overview of the synthetic routines that have been used to access specific classes of therapeutic agents. Materials are organized by chemical class, and syntheses are taken back to available starting materials. Discusses disease state, rational for method of drug therapy, biological activities of each compound and preparation. Coverage also includes those generic pharmaceutical compounds not accorded clinical status. A glossary defines biological terms.

The Practice of Medicinal Chemistry, Fourth Edition provides a practical and comprehensive overview of the daily issues facing pharmaceutical researchers and chemists. In addition to its thorough treatment of basic medicinal chemistry principles, this updated edition has been revised to provide new and expanded coverage of the latest technologies and approaches in drug discovery. With topics like high content screening, scoring, docking, binding free energy calculations, polypharmacology, QSAR, chemical collections and databases, and much more, this book is the go-to reference for all academic and pharmaceutical researchers who need a complete understanding of medicinal chemistry and its application to drug discovery and development. Includes updated and expanded material on systems biology, chemogenomics, computer-

aided drug design, and other important recent advances in the field Incorporates extensive color figures, case studies, and practical examples to help users gain a further understanding of key concepts Provides high-quality content in a comprehensive manner, including contributions from international chapter authors to illustrate the global nature of medicinal chemistry and drug development research An image bank is available for instructors at www.textbooks.elsevier.com

Providing must-have knowledge for the pharmaceutical industry and process chemists in industry, this ready reference offers solutions for saving time and money and supplying -- in a sustainable way -- valuable products. Application-oriented and well structured, each chapter presents successful strategies for the latest modern drugs, showing how to provide very fast bulk quantities of drug candidates. Throughout, the text illustrates how all the key factors are interwoven and dependent on one another in creating optimized methods for optimal products.

Side Reactions in Peptide Synthesis, based on the author's academic and industrial experience, and backed by a thorough review of the current literature, provides analysis of, and proposes solutions to, the most frequently encountered side reactions during peptide and peptidomimetic synthesis. This valuable handbook is ideal for research and process chemists working with peptide synthesis in diverse settings across academic, biotech, and pharmaceutical research and development. While peptide chemistry is increasingly prevalent, common side reactions and their causes are often poorly

understood or anticipated, causing unnecessary waste of materials and delay. Each chapter discusses common side reactions through detailed chemical equations, proposed mechanisms (if any), theoretical background, and finally, a variety of possible solutions to avoid or alleviate the specified side reaction. Provides a systematic examination on how to troubleshoot and minimize the most frequent side reactions in peptide synthesis Gives chemists the background information and the practical tools they need to successfully troubleshoot and improve results Includes optimization-oriented analysis of side reactions in peptide synthesis for improved industrial process development in peptidyl API (active pharmaceutical ingredient) production Answers the growing, global need for improved, replicable processes to avoid impurities and maintain the integrity of the end product. Presents a thorough discussion of critical factors in peptide synthesis which are often neglected or underestimated by chemists Covers solid phase and solution phase methodologies, and provides abundant references for further exploration

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