Blood Brain Barrier In Drug Discovery Optimizing Brain Exposure Of Cns Drugs And Minimizing Brain Side Effects For Peripheral Drugs

Optimization in Drug Discovery **Static and Dynamic Properties of Liquids** Optimizing the "Drug-Like" Properties of Leads in Drug Discovery High-Throughput Lead Optimization in Drug Discovery **Pharmacokinetic Optimization in Drug Research** *Optimization of Pharmaceutical R&D Programs and Portfolios* Drug-like Properties: Concepts, Structure Design and Methods *Peptide-based Drug Discovery* **Dose Optimization in Drug Development** *Industrialization of Drug Discovery Optimization in Drug Discovery Computer Applications in Drug Discovery and Development* **The Medicinal Chemist's Guide to Solving ADMET Challenges** Optimization of Pharmaceutical R&D Programs and Portfolios Optimization in Medicine and Biology Blood-Brain Barrier in Drug Discovery **Translational Medicine** Pharmaceutical Drug Product Development and Process Optimization **Lead Optimization for Medicinal Chemists Drug Discovery for Leishmaniasis Lead Generation Optimization in Drug Discovery** Early Drug Development, 2 Volume Set *Nanoscale Fabrication, Optimization, Scale-up and Biological Aspects of Pharmaceutical Nanotechnology* **New Methods and Approaches Toward Lead Optimization and Drug Discovery** *Optimization in Drug Discovery High Throughput Screening Methods Physicochemical and Biomimetic Properties in Drug Discovery* Oral Formulation Roadmap from Early Drug Discovery to Development Advanced Drug Formulation Design to Optimize Therapeutic Outcomes Ant Colony Optimization **Computational Methods for GPCR Drug Discovery** Transporters in Drug Development NMR of Biomolecules *Artificial Intelligence in Drug Discovery* **Optimization in Computational Chemistry and Molecular Biology The Agile Approach to Adaptive Research** *Physicochemical and Biomimetic Properties in Drug Discovery* **Inhaled Medicines Recent Highlights in the Discovery and Optimization of Crop Protection Products**

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Drug-like Properties: Concepts, Structure Design and Methods Apr 24 2022 Of the thousands of novel compounds that a drug discovery project team invents and that bind to the therapeutic target, typically only a fraction of these have sufficient ADME/Tox properties to become a drug product. Understanding ADME/Tox is critical for all drug researchers, owing to its increasing importance in advancing high quality candidates to clinical studies and the processes of drug discovery. If the properties are weak, the candidate will have a high risk of failure or be less desirable as a drug product. This book is a tool and resource for scientists engaged in, or preparing for, the selection and optimization process. The authors describe how properties affect in vivo pharmacological activity and impact in vitro assays. Individual drug-like properties are discussed from a practical point of view, such as solubility, permeability and metabolic stability, with regard to fundamental understanding, applications of property data in drug discovery and examples of structural modifications that have achieved improved property performance. The authors also review various methods for the screening (high throughput), diagnosis (medium throughput) and in-depth (low throughput) analysis of drug properties. * Serves as an essential working handbook aimed at scientists and students in medicinal chemistry * Provides practical, step-by-step guidance on property fundamentals, effects, structure-property relationships, and structure modification strategies * Discusses improvements in pharmacokinetics from a practical chemist's standpoint

Oral Formulation Roadmap from Early Drug Discovery to Development Jun 02 2020 Detailing formulation approaches by stage of discovery to early development, this book gives a “playbook” of practical and efficient strategies to formulate drug candidates with the least chance of failing in clinical development. • Comes from contributing authors with experience developing formulations on the frontlines of the pharmaceutical industry • Focuses on pre (or non-) clinical and early stage development, the phases where most compounds are used in drug research • Features case studies to illustrate practical challenges and solutions in formulation selection • Covers regulatory filing, drug metabolism and physical and chemical properties, toxicology formulation, biopharmaceutics classification system (BCS), screening approaches, early stage clinical formulation development, and outsourcing

Lead Optimization for Medicinal Chemists Apr 12 2021 Small structural modifications can significantly affect the pharmacokinetic properties of drug candidates. This book, written by a medicinal chemist for medicinal chemists, is a comprehensive guide to the pharmacokinetic impact of functional groups, the pharmacokinetic optimization of drug leads, and an exhaustive collection of pharmacokinetic data, arranged according to the structure of the drug, not its target or indication. The historical origins of most drug classes and general aspects of modern drug discovery and development are also discussed. The index contains all the drug names and synonyms to facilitate the location of any drug or functional group in the book. This compact working guide provides a wealth of information on the ways small structural modifications affect the pharmacokinetic properties of organic compounds, and offers plentiful, fact-based inspiration for the development of new drugs. This book is mainly aimed at medicinal chemists, but may also be of interest to graduate students in chemical or pharmaceutical sciences, preparing themselves for a job in the pharmaceutical industry, and to healthcare professionals in need of pharmacokinetic data.

Early Drug Development, 2 Volume Set Dec 09 2020 This one-stop reference systematically covers key aspects in early drug development that are directly relevant to the discovery phase and are required for first-in-human studies. Its broad scope brings together critical knowledge from many disciplines, ranging from process technology to pharmacology to intellectual property issues. After introducing the overall early development workflow, the critical steps of early drug development are described in a sequential and enabling order: the availability of the drug substance and that of the drug product, the prediction of pharmacokinetics and -dynamics, as well as that of drug safety. The final section

focuses on intellectual property aspects during early clinical development. The emphasis throughout is on recent case studies to exemplify salient points, resulting in an abundance of practice-oriented information that is usually not available from other sources. Aimed at medicinal chemists in industry as well as academia, this invaluable reference enables readers to understand and navigate the challenges in developing clinical candidate molecules that can be successfully used in phase one clinical trials.

Optimization of Pharmaceutical R&D Programs and Portfolios May 26 2022 Very little has been published on optimization of pharmaceutical portfolios. Moreover, most of published literature is coming from the commercial side, where probability of technical success (PoS) is treated as fixed, and not as a consequence of development strategy or design. In this book there is a strong focus on impact of study design on PoS and ultimately on the value of portfolio. Design options that are discussed in different chapters are dose-selection strategies, adaptive design and enrichment. Some development strategies that are discussed are indication sequencing, optimal number of programs and optimal decision criteria. This book includes chapters written by authors with very broad backgrounds including financial, clinical, statistical, decision sciences, commercial and regulatory. Many authors have long held executive positions and have been involved with decision making at a product or at a portfolio level. As such, it is expected that this book will attract a very broad audience, including decision makers in pharmaceutical R&D, commercial and financial departments. The intended audience also includes portfolio planners and managers, statisticians, decision scientists and clinicians. Early chapters describe approaches to portfolio optimization from big Pharma and Venture Capital standpoints. They have stronger focus on finances and processes. Later chapters present selected statistical and decision analysis methods for optimizing drug development programs and portfolios. Some methodological chapters are technical; however, with a few exceptions they require a relatively basic knowledge of statistics by a reader.

Advanced Drug Formulation Design to Optimize Therapeutic Outcomes May 02 2020 This title demonstrates how advanced formulation designs and delivery technologies can be used to improve drug efficacy and treatment outcomes in particular therapeutic categories or disease states. It discusses nanoparticle systems for cancer treatments, and also presents cutting edge immono-regulation agents for transplantation and the local targ

Optimization in Drug Discovery Sep 05 2020 Recent reports of drug attrition rates have revealed that a significant number of drug candidates fail in the later stage of clinical development due to absorption, distribution, metabolism, elimination and toxicity issues. Lead optimization in drug discovery, a process of attempting to uncover and correct these defects, is highly beneficial in lowering the cost and time to develop therapeutic drugs by reducing drug candidate failures in development. This book provides the assays utilized in drug discovery to rapidly screen for compounds with favorable drug-like properties. A total of 25 chapters, contributed by many experts in the field, cover a wide spectrum of subjects including physicochemical properties, absorption, plasma binding, metabolism, drug interactions, and toxicity, making this an essential book for all pharmacologists and pharmaceutical scientists.

Blood-Brain Barrier in Drug Discovery Jul 16 2021 Focused on central nervous system (CNS) drug discovery efforts, this book educates drug researchers about the blood-brain barrier (BBB) so they can affect important improvements in one of the most significant – and most challenging – areas of drug discovery. • Written by world experts to provide practical solutions to increase brain penetration or minimize CNS side-effects • Reviews state-of-the-art in silico, in vitro, and in vivo tools to assess brain penetration and advanced CNS drug delivery strategies • Covers BBB physiology, medicinal chemistry design principles, free drug hypothesis for the BBB, and transport mechanisms including passive diffusion, uptake/efflux transporters, and receptor-mediated processes • Highlights the advances in modelling BBB pharmacokinetics and dynamics relationships (PK/PD) and physiologically-based pharmacokinetics (PBPK) • Discusses case studies of successful CNS and non-CNS drugs, lessons learned and paths to the market

Ant Colony Optimization Mar 31 2020 An overview of the rapidly growing field of ant colony optimization that describes theoretical findings, the major algorithms, and current applications. The complex social behaviors of ants have been much studied by science, and computer scientists are now finding that these behavior patterns can provide models for solving difficult combinatorial optimization problems. The attempt to develop algorithms inspired by one aspect of ant behavior, the ability to find what computer scientists would call shortest paths, has become the field of ant colony optimization (ACO), the most successful and widely recognized algorithmic technique based on ant behavior. This book presents an overview of this rapidly growing field, from its theoretical inception to practical applications, including descriptions of many available ACO algorithms and their uses. The book first describes the translation of observed ant behavior into working optimization algorithms. The ant colony metaheuristic is then introduced and viewed in the general context of combinatorial optimization. This is followed by a detailed description and guide to all major ACO algorithms and a report on current theoretical findings. The book surveys ACO applications now in use, including routing, assignment, scheduling, subset, machine learning, and bioinformatics problems. AntNet, an ACO algorithm designed for the network routing problem, is described in detail. The authors conclude by summarizing the progress in the field and outlining future research directions. Each chapter ends with bibliographic material, bullet points setting out important ideas covered in the chapter, and exercises. Ant Colony Optimization will be of interest to academic and industry researchers, graduate students, and practitioners who wish to learn how to implement ACO algorithms.

Optimization in Drug Discovery Oct 31 2022 Thoroughly revised and updated, Optimization in Drug Discovery: In Vitro Methods, Second Edition presents a wide spectrum of in vitro assays including formulation, plasma binding, absorption and permeability, cytochrome P450 (CYP) and UDP-glucuronosyltransferases (UGT) metabolism, CYP inhibition and induction, drug transporters, drug-drug interactions via assessment of reactive metabolites, genotoxicity, and chemical and photo-mutagenicity assays. Written for the Methods in Pharmacology and Toxicology series, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible protocols, and tips on troubleshooting and avoiding known pitfalls. Expert authors have developed and utilized these in vitro assays to achieve “drug-like” characteristics in addition to efficacy properties and good safety profiles of drug candidates. Comprehensive and up-to-date, Optimization in Drug Discovery: In Vitro Methods, Second Edition aims to guide researchers down the difficult path to successful drug discovery and development.

Translational Medicine Jun 14 2021 Translational Medicine: Optimizing Preclinical Safety Evaluation of Biopharmaceuticals provides scientists responsible for the translation of novel biopharmaceuticals into clinical trials with a better understanding of how to navigate the obstacles that keep innovative medical research discoveries from becoming new therapies or even making it to clinical trials. The book includes sections on protein-based therapeutics, modified proteins, oligonucleotide-based therapies, monoclonal antibodies, antibody–drug conjugates, gene and cell-based therapies, gene-modified cell-based therapies, combination products, and therapeutic vaccines. Best practices are defined for efficient discovery research to facilitate a science-based, efficient, and predictive preclinical development program to ensure clinical efficacy and safety. Key Features: Defines best practices for leveraging of discovery research to facilitate a development program Includes general principles, animal models, biomarkers, preclinical toxicology testing paradigms, and practical applications Discusses rare diseases Discusses "What-Why-When-How" highlighting different considerations based upon product attributes. Includes special considerations for rare diseases About the Editors Joy A. Cavagnaro is an internationally recognized expert in preclinical development and

regulatory strategy with an emphasis on genetic medicines.. Her 40-year career spans academia, government (FDA), and the CRO and biotech industries. She was awarded the 2019 Arnold J Lehman Award from the Society of Toxicology for introducing the concept of science-based, case-by-case approach to preclinical safety evaluation, which became the foundation of ICH S6. She currently serves on scientific advisory boards for advocacy groups and companies and consults and lectures in the area of preclinical development of novel therapies. Mary Ellen Cosenza is a regulatory toxicology consultant with over 30 years of senior leadership experience in the biopharmaceutical industry in the U.S., Europe, and emerging markets. She has held leadership position in both the American College of Toxicology (ACT) and the International Union of Toxicology (IUTOX) and is also an adjunct assistant professor at the University of Southern California where she teaches graduate-level courses in toxicology and regulation of biologics.

High-Throughput Lead Optimization in Drug Discovery Jul 28 2022 A Single Source on Parallel Synthesis for Lead Optimization The end of the previous millennium saw an explosion in the application of parallel synthesis techniques for making compounds for high-throughput screening. Over time, it became clear that more thought in the design phase of library development is necessary to generate high quality hits. More recently, the use of parallel synthesis techniques has shifted to applications beyond screening collections. Exploring the nuances of this technology, High-Throughput Lead Optimization in Drug Discovery describes the application of parallel synthesis to lead optimization and the design and synthesis of targeted libraries. Examine Case Studies that Cover a Range of Different Biological Targets Featuring real-world examples and contributions from well-known scientists, the book explores the shift to conducting parallel lead optimization in-house while outsourcing most of the screening libraries synthesis. It includes more than 15 case studies that encompass a range of biological targets for application in different therapeutic areas. The text contains examples of solid and solution-phase techniques for the synthesis of directed libraries. The chapter authors explain the design principles they used to direct the choice of templates and diversity elements. Speed Up Drug Discovery and the Hit-to-Lead Process Focusing on the application of combinatorial chemistry to medicinal chemistry, this volume compiles a series of optimization projects that give you a snapshot of successes and challenges in the use of parallel synthesis for lead optimization. It explores how this technology, when applied to library design, can speed up drug discovery.

High Throughput Screening Methods Aug 05 2020 High throughput screening remains a key part of early stage drug and tool compound discovery, and methods and technologies have seen many fundamental improvements and innovations over the past 20 years. This comprehensive book provides a historical survey of the field up to the current state-of-the-art. In addition to the specific methods, this book also considers cultural and organizational questions that represent opportunities for future success. Following thought-provoking foreword and introduction from Professor Stuart Schreiber and the editors, chapters from leading experts across academia and industry cover initial considerations for screening, methods appropriate for different goals in small molecule discovery, newer technologies that provide alternative approaches to traditional miniaturization procedures, and practical aspects such as cost and resourcing. Within the context of their historical development, authors explain common pitfalls and their solutions. This book will serve as both a practical reference and a thoughtful guide to the philosophy underlying technological change in such a fast-moving area for postgraduates and researchers in academia and industry, particularly in the areas of chemical biology, pharmacology, structural biology and assay development.

New Methods and Approaches Toward Lead Optimization and Drug Discovery Oct 07 2020

Pharmaceutical Drug Product Development and Process Optimization May 14 2021 Pharmaceutical manufacturers are constantly facing quality crises of drug products, leading to an escalating number of product recalls and rejects. Due to the involvement of multiple factors, the goal of achieving consistent product quality is always a great challenge for pharmaceutical scientists. This volume addresses this challenge by using the Quality by Design (QbD) concept, which was instituted to focus on the systematic development of drug products with predefined objectives to provide enhanced product and process understanding. This volume presents and discusses the vital precepts underlying the efficient, effective, and cost effective development of pharmaceutical drug products. It focuses on the adoption of systematic quality principles of pharmaceutical development, which is imperative in achieving continuous improvement in end-product quality and also leads to reducing cost, time, and effort, while meeting regulatory requirements. The volume covers the important new advances in the development of solid oral dosage forms, modified release oral dosage forms, parenteral dosage forms, semisolid dosage forms, transdermal drug, delivery systems, inhalational dosage forms, ocular drug delivery systems, nanopharmaceutical products, and nanoparticles for oral delivery.

NMR of Biomolecules Dec 29 2019 NMR is one of the most powerful methods for imaging of biomolecules. This book is the ultimate NMR guide for researchers in the biomedical community and gives not only background and practical tips but also a forward looking view on the future of NMR in systems biology.

Optimization in Medicine and Biology Aug 17 2021 Thanks to recent advancements, optimization is now recognized as a crucial component in research and decision-making across a number of fields. Through optimization, scientists have made tremendous advances in cancer treatment planning, disease control, and drug development, as well as in sequencing DNA, and identifying protein structures. Optimization in Medicine and Biology provides researchers with a comprehensive, single-source reference that will enable them to apply the very latest optimization techniques to their work. With contributions from pioneering international experts this volume integrates strong foundational theory, good modeling techniques, and efficient and robust algorithms with relevant applications Divided into two sections, the first begins with mathematical programming techniques for medical decision making processes and demonstrates their application to optimizing pediatric vaccine formularies, kidney paired donation, and the cost-effectiveness of HIV programs. It also presents recent advances in cancer treatment planning models and solution algorithms, including three-dimensional conventional conformal radiation therapy (3DCRT), intensity modulated radiation therapy (IMRT), tomotherapy, and proton therapy. Part two focuses on optimization in biology and discusses computational algorithms for genomic analysis; probe design and selection, properties of probes, and various algorithms and software packages to aid in probe selection and design. Subsequent chapters introduce a new dihedral angle measure for protein secondary prediction, and an optimization approach for tumor virotherapy with recombinant measles viruses. The editors include a short tutorial appendix on Integer Programming (IP). Highlighting the most recent advances in optimization techniques for solving complex problems in medical research, this book facilitates strong collaborative environments among optimization researchers and medical professionals for future medical research.

Optimization in Drug Discovery Jan 10 2021 Thoroughly revised and updated, Optimization in Drug Discovery: In Vitro Methods, Second Edition presents a wide spectrum of in vitro assays including formulation, plasma binding, absorption and permeability, cytochrome P450 (CYP) and UDP-glucuronosyltransferases (UGT) metabolism, CYP inhibition and induction, drug transporters, drug-drug interactions via assessment of reactive metabolites, genotoxicity, and chemical and photo-mutagenicity assays. Written for the Methods in Pharmacology and Toxicology series, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible protocols, and tips on troubleshooting and avoiding known pitfalls. Expert authors have developed and utilized these in vitro assays to achieve “drug-like” characteristics in addition to efficacy properties and good safety profiles of drug candidates. Comprehensive and up-to-date, Optimization in Drug Discovery: In Vitro Methods, Second Edition aims to guide

researchers down the difficult path to successful drug discovery and development.

Optimization in Computational Chemistry and Molecular Biology Oct 26 2019 Optimization in Computational Chemistry and Molecular Biology: Local and Global Approaches covers recent developments in optimization techniques for addressing several computational chemistry and biology problems. A tantalizing problem that cuts across the fields of computational chemistry, biology, medicine, engineering and applied mathematics is how proteins fold. Global and local optimization provide a systematic framework of conformational searches for the prediction of three-dimensional protein structures that represent the global minimum free energy, as well as low-energy biomolecular conformations. Each contribution in the book is essentially expository in nature, but of scholarly treatment. The topics covered include advances in local and global optimization approaches for molecular dynamics and modeling, distance geometry, protein folding, molecular structure refinement, protein and drug design, and molecular and peptide docking. Audience: The book is addressed not only to researchers in mathematical programming, but to all scientists in various disciplines who use optimization methods in solving problems in computational chemistry and biology.

Pharmacokinetic Optimization in Drug Research Jun 26 2022 In this age of combinatorial chemistry and high-throughput technologies, bioactive compounds called hits are discovered by the thousands. However, the road that leads from hits to lead compounds and then to pharmacokinetically optimized clinical and drug candidates is very long indeed. As a result, the screening, design, and optimization of pharmacokinetic properties has become the bottleneck and a major challenge in drug research. To shorten the time-consuming develop-ment and high rate of attrition of active compounds ultimately doomed by hidden pharmacokinetic defects, drug researchers are coming to incorporate structure-permeation, structure-distribution, structure-metabolism, and structure-toxicity relations into drug-design strategies. To this end, powerful biological, physicochemical, and computational approaches are being developed whose objectives are to increase the clinical relevance of drug design, and to eliminate as soon as possible compounds with unfavorable physicochemical properties and pharmacokinetic profiles. Toxicological issues are also of utmost importance in this paradigm. There was, hence, an urgent need for a book covering this field in an authoritative, didactic, comprehensive, factual, and conceptual manner. In this work of unique breadth and depth, international authorities and practicing experts from academia and industry present the most modern biological, physicochemical, and computational strategies to optimize gastrointestinal absorption, protein binding and distribution, brain permeation, and metabolic profile. The biological strategies emphasized in the book include cell cultures and high-throughput screens. The physicochemical strategies focus on the determination and interpretation of solubility, lipophilicity, and related molecular properties as factors and predictors of pharmacokinetic bahavior. Particular attention is paid to the lipophilicity profiles of ionized compounds, to lipophilicity measurements in anisotropic media (liposomes/water, IAM columns), and to permeability across artificial membranes. Computational strategies comprise virtual screening, molecular modelling, lipophilicity, and H-bonding fields and their importance for structure-disposition relations. This book is both about theoretical and technological breakthroughs. Thus, molecular properties are contemplated from a dual perspective, namely a) their interpretation in biological and/or physicochemical terms, and b) their value in screening, lead optimization, and drug-candidate selection. In addition to its 33 chapters, the book includes a CD-ROM containing the invited lectures, oral communications and posters (in full version) presented at the Second LogP Symposium, 'Lipophilicity in Drug Disposition—Practical and Computational Approaches to Molecular Properties Related to Drug Permeation, Disposition and Metabolism', held at the University of Lausanne in March 2000.

Industrialization of Drug Discovery Jan 22 2022 The pharmaceutical industry suffers from an innovation deficit, with clinical attrition and safety-related market-withdrawal rates at the same level as twenty years ago. This book scrutinizes this problem in detail, contrasting the promise of technology and industrialization with the apparent inability of industry to fully realize the tools that ar

Optimization of Pharmaceutical R&D Programs and Portfolios Sep 17 2021 Very little has been published on optimization of pharmaceutical portfolios. Moreover, most of published literature is coming from the commercial side, where probability of technical success (PoS) is treated as fixed, and not as a consequence of development strategy or design. In this book there is a strong focus on impact of study design on PoS and ultimately on the value of portfolio. Design options that are discussed in different chapters are dose-selection strategies, adaptive design and enrichment. Some development strategies that are discussed are indication sequencing, optimal number of programs and optimal decision criteria. This book includes chapters written by authors with very broad backgrounds including financial, clinical, statistical, decision sciences, commercial and regulatory. Many authors have long held executive positions and have been involved with decision making at a product or at a portfolio level. As such, it is expected that this book will attract a very broad audience, including decision makers in pharmaceutical R&D, commercial and financial departments. The intended audience also includes portfolio planners and managers, statisticians, decision scientists and clinicians. Early chapters describe approaches to portfolio optimization from big Pharma and Venture Capital standpoints. They have stronger focus on finances and processes. Later chapters present selected statistical and decision analysis methods for optimizing drug development programs and portfolios. Some methodological chapters are technical; however, with a few exceptions they require a relatively basic knowledge of statistics by a reader.

Transporters in Drug Development Jan 28 2020 Transporters in Drug Development examines how membrane transporters can be dealt with in academic–industrial drug discovery and pharmaceutical development as well as from a regulatory perspective. The book describes methods and examples of in vitro characterization of single transporters in the intestines, liver and kidneys as well as characterization of substrate overlap between various transporters. Furthermore, probes and biomarkers are suggested for studies of the transporters’ impact on the pharmacokinetics of drug substrates/candidates interacting on transporters. The challenges of translating in vitro observed interaction of transporters into in vivo relevance are explored, and the book highlights perspectives of applying targeted proteomics and mechanistic modeling in this process.

Drug Discovery for Leishmaniasis Mar 12 2021 For human health, leishmaniasis is among the most important protozoan diseases, superseded only by malaria. Globally, 10 to 12 million people are infected with 1.5 million new cases every year. The development of cheaper new drugs is urgently needed for this neglected disease that is developing resistance to current treatments. Chemotherapy remains the only treatment option for the bulk of patients. However, this is largely unaffordable for most. In the past three years numerous advances in drug discovery have been made for treating this disease by exploiting diverging metabolic pathways between the Leishmania enzymes and their hosts, using nanotechnology to target the immune cell phagolysosomes where Leishmania resides. Drug Discovery for Leishmaniasis aims to provide a perspective of the current treatments and their challenges, blended with the emerging strategies and methodologies that will drive new target appraisals and drug developments, as well as addressing the molecular basis of resistance in Leishmania. Recent studies have shown that leishmaniasis affects some of the poorest people in the world, with 95% of fatal cases occurring in only 6 countries. With the WHO goal of eliminating this public health problem in the South-east Asia Region by 2020, this book will be important for anyone who is interested in neglected tropical diseases.

Optimization in Drug Discovery Dec 21 2021 Recent analyses of drug attrition rates reveal that a significant number of drug candidates fail in the later stage of clinical development owing to absorption, distribution, metabolism,

elimination (ADME), and toxicity issues. Lead optimization in drug discovery, a process attempting to uncover and correct these defects of drug candidates, is highly beneficial in lowering the cost and time to develop therapeutic drugs by reducing drug candidate failures in development. At present, parallel synthesis combining with high-throughput screening has made it easier to generate highly potent compounds (i. e. , hits). However, to be a potential drug, a hit must have drug-like characteristics in addition to potency, which include optimal physicochemical properties, reasonable ph- macokinetic parameters, and good safety profiles. Therefore, research tools must be available in drug discovery to rapidly screen for compounds with favorable drug-like properties, and thus adequate resources can be directed to projects with high potential. Optimization in Drug Discovery: In Vitro Methods is a compilation of detailed experimental protocols necessary for setting up a variety of assays important in compound evaluation. A total of 25 chapters, contributed by many experts in their research areas, cover a wide spectrum of subjects including physicochemical properties, abso- tion, plasma binding, metabolism, drug interactions, and toxicity. A good pharmacokinetic profile has long been recognized as an imp- tant drug-like characteristic. Pharmacokinetic parameters are affected by many properties of drug molecules such as physicochemical nature, abso- tion, metabolic stability, and so on.

Computer Applications in Drug Discovery and Development Nov 19 2021 With more restrictions upon animal experimentations, pharmaceutical industries are currently focusing on a new generation of experiments and technologies that are considerably more efficient and less controversial. The integration of computational and experimental strategies has led to the identification and development of promising compounds. Computer Applications in Drug Discovery and Development is a pivotal reference source that provides innovative research on the application of computers for discovering and designing new drugs in modern molecular biology and medicinal chemistry. While highlighting topics such as chemical structure databases and dataset utilization, this publication delves into the current panorama of drug discovery, where high drug failure rates are a major concern and properly designed virtual screening strategies can be a time-saving, cost-effective, and productive alternative. This book is ideally designed for chemical engineers, pharmacists, molecular biologists, students, researchers, and academicians seeking current research on the unexplored avenues and future perspectives of drug design.

Inhaled Medicines Jul 24 2019 Inhaled medicines are widely used to treat pulmonary and systemic diseases. The efficacy and safety of these medicines can be influenced by the deposited fraction, the regional deposition pattern within the lungs and by post-depositional events such as drug dissolution, absorption and clearance from the lungs. Optimizing performance of treatments thus requires that we understand and are able to quantify these product and drug attributes. Inhaled Medicines: Optimizing Development through Integration of In Silico, In Vitro and In Vivo Approaches explores the current state of the art with respect to inhalation drug delivery, technologies available to assess product performance, and novel in silico methods now available to link in vitro product performance to clinical performance. Recent developments in the latter field, especially the prospect of integration of three-dimensional Computational Fluid Particle Methods (3D-CFPD) with physiologically based pharmacokinetic (PBPK models), unlocks the potential for in silico population studies that can help inform and optimize treatment and product development strategies. In this highly multidisciplinary field, where progress occurs at the intersection of several disciplines of engineering and science, this work aims to integrate current knowledge and understanding and to articulate a clear vision for future developments. ? Considers the healthcare needs driving the field, and where inhaled drugs could have the maximum impact ? Gives a concise account of the state of the art in key areas and technologies such as device and formulation technologies, clinically relevant in vitro performance assessment, medical imaging, as well as in silico modelling and simulation ? Articulates how the combination of in vitro product performance data, medical imaging and simulations technologies in the framework of large scale in silico pre-clinical trials could revolutionize the field ? Provides systematic and thorough referencing to sources offering a more-in-depth analysis of technical issues

Nanoscale Fabrication, Optimization, Scale-up and Biological Aspects of Pharmaceutical Nanotechnology Nov 07 2020 Nanoscale Fabrication, Optimization, Scale-up and Biological Aspects of Pharmaceutical Nanotechnology focuses on the fabrication, optimization, scale-up and biological aspects of pharmaceutical nanotechnology. In particular, the following aspects of nanoparticle preparation methods are discussed: the need for less toxic reagents, simplification of the procedure to allow economic scale-up, and optimization to improve yield and entrapment efficiency. Written by a diverse range of international researchers, the chapters examine characterization and manufacturing of nanomaterials for pharmaceutical applications. Regulatory and policy aspects are also discussed. This book is a valuable reference resource for researchers in both academia and the pharmaceutical industry who want to learn more about how nanomaterials can best be utilized. Shows how nanomanufacturing techniques can help to create more effective, cheaper pharmaceutical products Explores how nanofabrication techniques developed in the lab have been translated to commercial applications in recent years Explains safety and regulatory aspects of the use of nanomanufacturing processes in the pharmaceutical industry

Physicochemical and Biomimetic Properties in Drug Discovery Jul 04 2020 Demonstrating how and why to measure physicochemical and biomimetic properties in early stages of drug discovery for lead optimization, Physicochemical and Biomimetic Properties in Drug Discovery encourages readers to discover relationships between various measurements and develop a sense of interdisciplinary thinking that will add to new research in drug discovery. This practical guide includes detailed descriptions of state-of-the-art chromatographic techniques and uses real-life examples and models to help medicinal chemists and scientists and advanced graduate students apply measurement data for optimal drug discovery.

Physicochemical and Biomimetic Properties in Drug Discovery Aug 24 2019 Demonstrating how and why to measure physicochemical and biomimetic properties in early stages of drug discovery for lead optimization, Physicochemical and Biomimetic Properties in Drug Discovery encourages readers to discover relationships between various measurements and develop a sense of interdisciplinary thinking that will add to new research in drug discovery. This practical guide includes detailed descriptions of state-of-the-art chromatographic techniques and uses real-life examples and models to help medicinal chemists and scientists and advanced graduate students apply measurement data for optimal drug discovery.

Optimizing the "Drug-Like" Properties of Leads in Drug Discovery Aug 29 2022 This book arises from a workshop organized by the American Association of Pharmaceutical Scientists entitled "Optimizing the Drug-Like Properties of Leads in Drug Discovery," which took place in Parsippany, NJ in September 2004. The workshop focused on the optimization of the drug-like properties of leads in drug discovery. The volume outlines strategies and methodologies designed to guide pharmaceutical and biotechnology companies through the drug discovery and development process.

The Medicinal Chemist's Guide to Solving ADMET Challenges Oct 19 2021 The Medicinal Chemist’s Guide to Solving ADMET Challenges summarizes a series of design strategies and tactics that have been successfully employed across pharmaceutical and academic laboratories to solve common ADMET issues. These are exemplified with a curated collection of concrete examples displayed in a highly visual “table-of-contents” style format, allowing readers to rapidly identify the most promising approaches applicable to their own challenges. Each ADMET parameter is introduced in a concise yet comprehensive manner and includes background, relevance and screening strategies. Medicinal chemistry knowledge of how best to modify molecular structure to solve ADMET issues is challenging to retrieve from the literature, public databases and even corporate data warehouses. The Medicinal Chemist’s Guide to Solving ADMET Challenges addresses this

gap by presenting state-of-the-art design strategies put together by a global group of experienced medicinal chemists and ADMET experts across academia and the pharmaceutical industry.

Static and Dynamic Properties of Liquids Sep 29 2022

Artificial Intelligence in Drug Discovery Nov 27 2019 Following significant advances in deep learning and related areas interest in artificial intelligence (AI) has rapidly grown. In particular, the application of AI in drug discovery provides an opportunity to tackle challenges that previously have been difficult to solve, such as predicting properties, designing molecules and optimising synthetic routes. Artificial Intelligence in Drug Discovery aims to introduce the reader to AI and machine learning tools and techniques, and to outline specific challenges including designing new molecular structures, synthesis planning and simulation. Providing a wealth of information from leading experts in the field this book is ideal for students, postgraduates and established researchers in both industry and academia.

Lead Generation Feb 08 2021 In this comprehensive two-volume resource on the topic senior lead generation medicinal chemists present a coherent view of the current methods and strategies in industrial and academic lead generation. This is the first book to combine both standard and innovative approaches in comparable breadth and depth, including several recent successful lead generation case studies published here for the first time. Beginning with a general discussion of the underlying principles and strategies, individual lead generation approaches are described in detail, highlighting their strengths and weaknesses, along with all relevant bordering disciplines like e.g. target identification and validation, predictive methods, molecular recognition or lead quality matrices. Novel lead generation approaches for challenging targets like DNA-encoded library screening or chemical biology approaches are treated here side by side with established methods as high throughput and affinity screening, knowledge- or fragment-based lead generation, and collaborative approaches. Within the entire book, a very strong focus is given to highlight the application of the presented methods, so that the reader will be able to learn from real life examples. The final part of the book presents several lead generation case studies taken from different therapeutic fields, including diabetes, cardiovascular and respiratory diseases, neuroscience, infection and tropical diseases. The result is a prime knowledge resource for medicinal chemists and for every scientist involved in lead generation.

Computational Methods for GPCR Drug Discovery Feb 29 2020 This volume looks at modern computational strategies and techniques used in GPCR drug discovery including structure and ligand-based approaches and cheminformatics. The chapters in this book describe how these approaches can be applied to address key drug discovery issues, such as receptor structure modelling, function and dynamics, prediction of protein-water-ligand interactions and binding kinetics, free energy of binding, interconversion between agonists and antagonists, deorphanization of GPCRs, and the discovery of biased and allosteric modulators. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary software and tools, step-by-step, readily reproducible modelling protocols, and tips on troubleshooting and avoiding known pitfalls. Cutting-edge and unique,Computational Methods for GPCR Drug Discovery is a valuable resource for structural and molecular biologists, computational and medicinal chemists, pharmacologists, and drug designers.

Recent Highlights in the Discovery and Optimization of Crop Protection Products Jun 22 2019 Recent Highlights in the Discovery and Optimization of Crop Protection Products highlights the most prominent, recent results in the search for safe and effective new crop protection products. With a focus on the design, synthesis, optimization and/or structure-activity relationships of new chemistries targeting insect, disease, weed, nematode, vector and animal parasite control, the book also includes recent developments in crop enhancement chemistries and new approaches to crop protection products. The inclusion of information on testing tools, green chemistry approaches, and the latest discovery tools, like modeling, structure-based design, and testing tools makes this volume complete. Based on key presentations given at the 14th International IUPAC conference on Crop Protection, May 19-24, 2019 in Ghent, Belgium, this book includes the many exciting new discoveries and findings reported. It is designed to inspire additional research and advancement in the field. Based on science presented at the 2019 International Union of Pure and Applied Chemistry Conference on Crop Protection Provides real-world perspectives on pesticide and disease control progress Presents scientific developments from an international array of contributing authors

Dose Optimization in Drug Development Feb 20 2022 This reference provides a concise overview of the key principles in dose selection and optimization and demonstrates applicability to recent successful new drug applications. Compiling key issues and current research of safety, efficacy, and clinical pharmacology, and PK-PD, this volume critically highlights the multidisciplinary nature of drug development and spans the fields of pharmacokinetics, clinical pharmacology, biostatistics, and experimental medicine.

Peptide-based Drug Discovery Mar 24 2022 With potentially high specificity and low toxicity, biologicals offer promising alternatives to small-molecule drugs. Peptide therapeutics have again become the focus of innovative drug development efforts backed up by a resurgence of venture funds and small biotechnology companies. What does it take to develop a peptide-based medicine? What are the key challenges and how are they overcome? What are emerging therapeutics for peptide modalities? This book answers these questions with a holistic story from molecules to medicine, combining the themes of design, synthesis and clinical applications of peptide-based therapeutics and biomarkers. Chapters are written and edited by leaders in the field from industry and academia and they cover the pharmacokinetics of peptide therapeutics, attributes necessary for commercially successful metabolic peptides, medicinal chemistry strategies for the design of peptidase-resistant peptide analogues, disease classes for which peptide therapeutic are most relevant, and regulatory issues and guidelines. The critical themes covered provide essential background information on what it takes to develop peptide-based medicine from a chemistry perspective and views on the future of peptide drugs. This book will be a valuable resource not only as a reference book for the researcher engaged in academic and pharmaceutical setting, from basic research to manufacturing and from organic chemistry to biotechnology, but also a valuable resource to graduate students to understand discovery and development process for peptide-based medicine.

The Agile Approach to Adaptive Research Sep 25 2019 Apply adaptive research to improve results in drug development The pharmaceutical industry today faces a deepening crisis: inefficiency in its core business, the development of new drugs. The Agile Approach to Adaptive Research offers a solution. It outlines how adaptive research, using already-available tools and techniques, can enable the industry to streamline clinical trials and reach decision points faster and more efficiently. With a wealth of real-world cases and examples, author Michael Rosenberg gives readers a practical overview of drug development, the problems inherent in current practices, and the advantages of adaptive research technology and methods. He explains the concepts, principles, and specific techniques of adaptive research, and demonstrates why it is an essential evolutionary step toward improving drug research and development. Chapters explore such subjects as: The adaptive concept Design and operational adaptations Sample-size reestimation Agile clinical development Safety and dose finding Statistics in adaptive research, including frequentist and Bayesian approaches Data management technologies The future of clinical development By combining centuries-old intellectual foundations, recent technological advances, and modern management techniques, adaptive research preserves the integrity and validity of clinical research but dramatically improves efficiency.