Development Of Chemistry Based Screening Platform

Drug Discovery and Development, Volume 2
Cheminformatics, QSAR and Machine Learning Applications for Novel Drug Development
Contemporary Accounts in Drug Discovery and Development
High Throughput Screening
High-Throughput Screening in Drug Discovery
The Process of New Drug Discovery and Development, Second Edition
Diversity-Oriented Synthesis
Biocatalysis for the Pharmaceutical Industry
Drug Discovery and Development, Volume 1
Development of Paper-based Immunoassay and Reaction Screening Platforms for Direct Mass Spectrometry Detection Under Ambient Condition
Advances in Combinatorial Chemistry & High Throughput Screening
High Throughput Screening Methods
Structure-activity Relationship Studies in Drug Development by NMR Spectroscopy
Handbook of Assay Development in Drug Discovery
High Throughput Screening Methods
Lead Generation Approaches in Drug Discovery
Medicinal Chemistry
Development of Chemistry-Based Screening Platform for Access to Mirror-Image Library of Natural Products
Fundamentals of Early Clinical Drug Development
Structure-based Drug Discovery
Label-Free Technologies For Drug Discovery
Fragment-Based Drug Discovery
A Practical Guide to Assay Development and High-Throughput Screening in Drug Discovery
Burger's Medicinal Chemistry, Drug Discovery and Development, 8 Volume Set
Current Methods In Medicinal Chemistry And Biological Physics
Virtual Screening: An Alternative or Complement to High Throughput Screening?
Platform Technologies in Drug Discovery and Validation
Basic Principles of Drug Discovery and Development
Drug Discovery
High-Throughput Formulation Development of Biopharmaceuticals
A Handbook for DNA-Encoded Chemistry
Fragment-based Approaches in Drug Discovery
Modern Methods of Drug Discovery
Chemoinformatics
New Synthetic Technologies in Medicinal Chemistry
Chemoinformatics Approaches to Virtual Screening
Progress in Medicinal Chemistry
Virtual Screening for Chemists
Drug Discovery and Development

MAREN JERAMIAH

Drug Discovery and Development, Volume 2 Springer Science & Business Media
The development of suitable assays, the integration of appropriate technology, and the effective management of the essential infrastructure are all critical to the success of any high-throughput screening (HTS) endeavor. However, few scientists have the multidisciplinary experience needed to control all aspects of an HTS drug discovery project. A P
Cheminformatics, QSAR and Machine Learning Applications for Novel Drug Development John Wiley & Sons
Chemoinformatics is broadly a scientific discipline encompassing the design, creation, organization, management, retrieval, analysis, dissemination, visualization and use of chemical information. It is distinct from other computational molecular modeling approaches in that it uses unique representations of chemical structures in the form of multiple chemical descriptors; has its own metrics for defining similarity and diversity of chemical compound libraries; and applies a wide array of statistical, data mining and machine learning techniques to very large collections of chemical compounds in order to establish robust relationships between chemical structure and its physical or biological properties. Chemoinformatics addresses a broad range of problems in chemistry and biology; however, the most commonly known applications of chemoinformatics approaches have been arguably in the area of drug discovery where chemoinformatics tools have played a central role in the analysis and interpretation of structure-property data collected by the means of modern high throughput screening. Early stages in modern drug discovery often involved screening small molecules for their effects on a selected protein target or a model of a biological pathway. In the past fifteen years, innovative technologies that enable rapid synthesis and high throughput screening of large libraries of compounds have been adopted in almost all major pharmaceutical and biotech companies. As a result, there has been a huge increase in the number of compounds available on a routine basis to quickly screen for novel drug candidates against new targets/pathways. In contrast, such technologies have rarely become available to the academic

research community, thus limiting its ability to conduct large scale chemical genetics or chemical genomics research. However, the landscape of publicly available experimental data collection methods for chemoinformatics has changed dramatically in very recent years. The term "virtual screening" is commonly associated with methodologies that rely on the explicit knowledge of three-dimensional structure of the target protein to identify potential bioactive compounds. Traditional docking protocols and scoring functions rely on explicitly defined three dimensional coordinates and standard definitions of atom types of both receptors and ligands. Albeit reasonably accurate in many cases, conventional structure based virtual screening approaches are relatively computationally inefficient, which has precluded them from screening really large compound collections. Significant progress has been achieved over many years of research in developing many structure based virtual screening approaches. This book is the first monograph that summarizes innovative applications of efficient chemoinformatics approaches towards the goal of screening large chemical libraries. The focus on virtual screening expands chemoinformatics beyond its traditional boundaries as a synthetic and data-analytical area of research towards its recognition as a predictive and decision support scientific discipline. The approaches discussed by the contributors to the monograph rely on chemoinformatics concepts such as: -representation of molecules using multiple descriptors of chemical structures -advanced chemical similarity calculations in multidimensional descriptor spaces -the use of advanced machine learning and data mining approaches for building quantitative and predictive structure activity models -the use of chemoinformatics methodologies for the analysis of drug-likeness and property prediction -the emerging trend on combining chemoinformatics and bioinformatics concepts in structure based drug discovery The chapters of the book are organized in a logical flow that a typical chemoinformatics project would follow - from structure representation and comparison to data analysis and model building to applications of structure-property relationship models for hit identification and chemical library design. It opens with the overview of modern methods of compounds library design, followed by a chapter devoted to molecular similarity analysis. Four sections describe virtual screening based on the using of molecular fragments, 2D pharmacophores and 3D pharmacophores. Application of fuzzy pharmacophores for libraries design is the subject of the next chapter followed by a chapter dealing with QSAR studies based on local molecular parameters. Probabilistic approaches based on 2D descriptors in assessment of biological activities are also described with an overview of the modern methods and software for ADME prediction. The book ends with a chapter describing the new approach of coding the receptor binding sites and their respective ligands in multidimensional chemical descriptor space that affords an interesting and efficient alternative to traditional docking and screening techniques. Ligand-based approaches, which are in the focus of this work, are more computationally efficient compared to structure-based virtual screening and there are very few books related to modern developments in this field. The focus on extending the experiences accumulated in traditional areas of chemoinformatics research such as Quantitative Structure Activity Relationships (QSAR) or chemical similarity searching towards virtual screening make the theme of this monograph essential reading for researchers in the area of computer-aided drug discovery. However, due to its generic data-analytical focus there will be a growing application of chemoinformatics approaches in multiple areas of chemical and biological research such as synthesis planning, nanotechnology, proteomics, physical and analytical chemistry and chemical genomics.

Contemporary Accounts in Drug Discovery and Development CRC Press

From first principles to real-world applications-here is the first comprehensive guide to drug discovery and development Modern drug discovery and development require the collaborative efforts of specialists in a broadarray of scientific, technical, and business disciplines-from biochemistry to molecular biology, organic chemistry to medicinal chemistry, pharmacology to marketing. Yet surprisingly, until now, there were no authoritative references offering a complete, fully integrated picture of the process. The only comprehensive guide of its kind, this groundbreaking two-volume resource provides an overview of the entire sequence of operations involved in drug discovery and develop-?ment-from initial conceptualization to commercialization to clinicians and medical practitioners. Volume 1: Drug Discovery describes all the steps in the discovery process, including conceptualizing a drug, creating a library of candidates for testing, screening candidates for in vitro and in vivo activity, conducting and analyzing the results of clinical trials, and modifying a drug as necessary. Volume 2: Drug Development delves into the nitty-gritty details of optimizing the synthetic route, drug manufacturing, outsourcing, and marketing-including drug coloring and delivery methods. Featuring contributions from a world-class team of experts, Drug Discovery and Development: Features fascinating case studies, including the discovery and development of erythromycin analogs, Tagamet, and Ultiva (remifentanil) Discusses the discovery of medications for bacterial infections, Parkinson's disease, psoriasis, peptic ulcers, atopic dermatitis, asthma, and cancer Includes chapters on combinatorial chemistry, molecular biology-based drug discovery, genomics, and chemogenomics Drug Discovery and Development is an indispensable working resource for industrial chemists, biologists, biochemists, and executives who work in the pharmaceutical industry.

High Throughput Screening John Wiley & Sons

Medicinal Chemistry begins with the history of the field, starting from the serendipitous use of plant preparations to current practice of design- and target-based screening methods. Written from the perspective of practicing medicinal chemists, the text covers key drug discovery activities such as pharmacokinetics and patenting, as well as the classes and structures of drug targets (receptors, enzymes, nucleic acids, and protein-protein and lipid interactions) with numerous examples of drugs acting at each type. Selected therapeutic areas include drugs to treat cancer, infectious diseases, and central nervous system disorders. Throughout the book, historical and current examples illustrate the progress to market and case studies explore the applications of concepts discussed in the text. Each chapter features a Journal Club, as well as review and application questions to enhance and test comprehension. This textbook is ideal for upper-level undergraduates and graduate students taking a one-semester survey course on medicinal chemistry and/or drug discovery, as well as scientists entering the pharmaceutical industry.

High-Throughput Screening in Drug Discovery Bentham Science Publishers

Basic Principles of Drug Discovery and Development presents the multifaceted process of identifying a new drug in the modern era, which requires a multidisciplinary team approach with input from medicinal chemists, biologists, pharmacologists, drug metabolism experts, toxicologists, clinicians, and a host of experts from numerous additional fields. Enabling technologies such as high throughput screening, structure-based drug design, molecular modeling, pharmaceutical profiling, and translational medicine

are critical to the successful development of marketable therapeutics. Given the wide range of disciplines and techniques that are required for cutting edge drug discovery and development, a scientist must master their own fields as well as have a fundamental understanding of their collaborator's fields. This book bridges the knowledge gaps that invariably lead to communication issues in a new scientist's early career, providing a fundamental understanding of the various techniques and disciplines required for the multifaceted endeavor of drug research and development. It provides students, new industrial scientists, and academics with a basic understanding of the drug discovery and development process. The fully updated text provides an excellent overview of the process and includes chapters on important drug targets by class, in vitro screening methods, medicinal chemistry strategies in drug design, principles of in vivo pharmacokinetics and pharmacodynamics, animal models of disease states, clinical trial basics, and selected business aspects of the drug discovery process. Provides a clear explanation of how the pharmaceutical industry works, as well as the complete drug discovery and development process, from obtaining a lead, to testing the bioactivity, to producing the drug, and protecting the intellectual property Includes a new chapter on the discovery and development of biologics (antibodies proteins, antibody/receptor complexes, antibody drug conjugates), a growing and important area of the pharmaceutical industry landscape Features a new section on formulations, including a discussion of IV formulations suitable for human clinical trials, as well as the application of nanotechnology and the use of transdermal patch technology for drug delivery Updated chapter with new case studies includes additional modern examples of drug discovery through high through-put screening, fragment-based drug design, and computational chemistry

The Process of New Drug Discovery and Development, Second Edition John Wiley & Sons

Mass spectrometry (MS) is a powerful analytical tool that plays crucial roles in many fields, including disease diagnosis, environmental monitoring, drug discovery, and chemical reaction screening and their mechanistic studies. The plethora of applications using MS continue to expand; this, in turn, has enabled continuous explorations that have resulted in the development of innovative ion sources and analyzers. Ambient ionization is a recent innovation that enables direct in-situ complex mixture analysis without having lengthy pretreatment of the sample (e.g., extraction, precipitation, lyophilization). Therefore, direct analysis using ambient ionization reduces analysis time and allows high throughput chemical detection. With such developments in ionization techniques, chemical instrumentation is getting advanced into new applications which were not previously possible. A future outlook on instrumentation is manufacturing portable mass spectrometers. In addition to basic figures of merits of the mass spectrometer, portable mass spectrometer broadens the scope of modern MS due to less power consumption, relatively low cost, and fieldable application. This dissertation describes the development of MS-based applications for clinical diagnosis utilizing ambient ionization and portable mass spectrometer (Chapters 2-4) and reaction screening (Chapter 5). Chapters 2-4 describe the innovations of coupling microfluidic paper-based analytical device (μPAD) to the portable mass spectrometer for ultrasensitive malaria diagnostic. Diagnosis of malaria, which is one of the deadliest infectious diseases, is the primary focus of this dissertation. This disease is encountered in developing countries and other resource-limited settings. Thus, the objective is positioned toward developing an ultrasensitive point-of-care tool so that all people can have equal opportunity to get diagnosed early and accurately. In chapter 2, the use of a portable mass spectrometer became the focus of the work and demonstrated the capability of field study using a mass spectrometer. Less required power consumption, economic burden, and lighter weight of portable mass spectrometer opened another opportunity for chemical detection in low resource settings. In chapter 3, dendrimer-mediated signal amplification technology was developed and applied to the 2D μPAD-MS platform to target asymptomatic diagnosis. The most challenging aspect of eradicating malaria is controlling asymptomatic infection due to no specific symptom and low parasite density. Without control, these asymptomatic infections prompt to generate parasite transmission continuously. Dendrimer contains multiple sites that can link numerous copies of mass tag, enhancing ion signal for MS detection. In chapter 4, next-generation three-dimensional (3D) μPAD was designed and fabricated. Compared to 2D biofluid sampling, a self-sustained and automated 3D μPAD system can serve as a single platform for microsampling, splitting a sample into multiple testing zones, room temperature storage of collected samples and direct MS analysis by paper spray ionization. Lastly, chapter 5 develops a novel nano-atmospheric pressure chemical ionization (APCI) source for monitoring and screening gas-phase chemical reactions. The ionic wind from corona discharge in APCI provides relatively high-energy electrons, which enable numerous collisions at atmospheric pressure. Abundant collisions led to an efficient uncatalyzed N-alkylation reaction for various primary amine compounds (e.g., propyl-, butyl-, hexyl-, and cyclohexylamine). By performing the reactions at atmospheric pressure, not only were we able to monitor reactions in real-time using mass spectrometry, but the following gas-phase reaction products were collected and offered for preparative-scale opportunities.

John Wiley & Sons

A revised and updated edition of Drug Discovery: The Evolution of Modern Medicine, this book provides expanded coverage of pre-twentieth century drugs, including emphasis on setting chapters in a wide historical and social context.

Diversity-Oriented Synthesis John Wiley & Sons

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.

Biocatalysis for the Pharmaceutical Industry Bentham Science Publishers

In the next couple of years the human genome will be fully sequenced. This will provide us with the sequence and overall

function of all human genes as well as the complete genome for many micro-organisms. Subsequently it is hoped, by means of powerful bioinformatic tools, to determine the gene variants that contribute to various multifactorial diseases and genes that exist in certain infectious agents but not humans. As a consequence, this will allow us to define the most appropriate levels for drug intervention. It can be expected that the number of potential drug targets will increase, possibly by a factor of 10 or more. Nevertheless, sequencing the human genome or, for that matter, the genome of other species will only be the starting point for the understanding of their biological function. Structural genomics is a likely follow-up, combined with new techniques to validate the therapeutic relevance of such newly discovered targets. Accordingly, it can be expected that in the near future we will witness a substantial increase in novel putative targets for drugs. To address these new targets effectively, we require new approaches and innovative tools. At present, two alternative, yet complementary, techniques are employed: experimental high-throughput screening (HTS) of large compound libraries, increasingly provided by combinatorial chemistry, and computational methods for virtual screening and de novo design. As kind of status report on the maturity of virtual screening as a technique in drug design, the first workshop on new approaches in drug design and discovery was held in March 1999, at Schloß Rauischholzhausen, near Marburg in Germany. More than 80 scientists gathered and discussed their experience with the different techniques. The speakers were invited to summarize their contributions together with their impressions on the present applicability of their approach. Several of the speakers followed this request which is summarized in this publication.

Drug Discovery and Development, Volume 1 Royal Society of Chemistry

The modern synthetic chemist applies all the tools available to identify the drug-like molecules with the best chances of becoming novel drugs. This book will act as a primer for graduates and postgraduates interested in a career in drug discovery. It covers both synthetic technologies currently impacting medicinal chemistry and emerging areas. The chapters focus on topics including: parallel medicinal chemistry; solid supported reagents; microwave assisted chemistry; flow synthesis, and high throughput reaction screening.

Development of Paper-based Immunoassay and Reaction Screening Platforms for Direct Mass Spectrometry Detection Under Ambient Condition John Wiley & Sons

With unprecedented interest in the power that the modern therapeutic armamentarium has to combat disease, the new edition of Drug Discovery and Development is an essential resource for anyone interested in understanding how drugs and other therapeutic interventions are discovered and developed, through to clinical research, registration, and market access. The text has been thoroughly updated, with new information on biopharmaceuticals and vaccines as well as clinical development and target identification. Drug discovery and development continues to evolve rapidly and this new edition reflects important changes in the landscape. Edited by industry experts Raymond Hill and Duncan Richards, this market-leading text is suitable for undergraduates and graduates undertaking degrees in pharmacy, pharmacology, toxicology, and clinical development through to those embarking on a career in the pharmaceutical industry. Key stages of drug discovery and development Chapters outline the contribution of individual disciplines to the overall process Supplemented by specific chapters on different modalities Includes coverage of Oligonucleotide therapies; cell and gene therapy Now comes with online access on StudentConsult

Advances in Combinatorial Chemistry & High Throughput Screening Woodhead Publishing

The Process of New Drug Discovery and Development, Second Edition presents a practical methodology and up-to-date scientific information for maximizing the ability of a multidisciplinary research team to discover and bring new drugs to the marketplace. This new addition updates the scientific advances in new drug discovery and development for areas such as combinatorial chemistry, screening technologies, metabonomics, biotechnology approaches and preclinical testing. It also greatly expands the focus on the business aspects of bringing new drugs to the market and offers coverage of essential topics for companies involved in drug development, such as the financial aspects of starting up a pharmaceutical enterprise, the regulatory process, liability and litigation, and patent law.

High Throughput Screening Methods Royal Society of Chemistry

In the literature, several terms are used synonymously to name the topic of this book: chem-, chemi-, or chemo-informatics. A widely recognized de- nition of this discipline is the one by Frank Brown from 1998 (1) who defined chemoinformatics as the combination of “all the information resources that a scientist needs to optimize the properties of a ligand to become a drug. ” In Brown’s definition, two aspects play a fundamentally important role: de- sion support by computational means and drug discovery, which distinguishes it from the term “chemical informatics” that was introduced at least ten years earlier and described as the application of information technology to ch- istry (not with a specific focus on drug discovery). In addition, there is of course “chemometrics,” which is generally understood as the application of statistical methods to chemical data and the derivation of relevant statistical models and descriptors (2). The pharmaceutical focus of many developments and efforts in this area—and the current popularity of gene-to-drug or si- lar paradigms—is further reflected by the recent introduction of such terms as “discovery informatics” (3), which takes into account that gaining kno- edge from chemical data alone is not sufficient to be ultimately successful in drug discovery. Such insights are well in accord with other views that the boundaries between bio- and chemoinformatics are fluid and that these d- ciplines should be closely combined or merged to significantly impact b- technology or pharmaceutical research (4).

Structure-activity Relationship Studies in Drug Development by NMR Spectroscopy John Wiley & Sons

"NMR (Nuclear Magnetic Resonance) Spectroscopy has found significant applications in drug discovery based on its capacity to map molecular interactions at the atomic level. Chemical shifts, cross relaxation, and exchange of protons are among the NMR parame"

Handbook of Assay Development in Drug Discovery Development of Chemistry-Based Screening Platform for Access to Mirror-Image Library of Natural Products

An integrated overview of modern approaches to lead discovery Lead generation is increasingly seen as a distinct and success-determining phase of the drug discovery process. Over recent years, there have been major advances in the understanding of what constitutes a good lead compound and how to improve the chances of finding such a compound. Written by leading scientists and established opinion leaders from industry and academia, this book provides an authoritative overview of the field, as well as the theory, practice, and scope, of the principal Lead Generation Approaches in Drug Discovery, including: The evolution of the lead discovery process, key concepts, current challenges, and future directions Strategies and technologies driving the high-throughput screening (HTS) approach to lead discovery, including the shifting paradigms in the design of

compound collections and best practice in the hit confirmation process Knowledge-based in silico or "virtual" screening Theory and practice of the fragment-based approach to lead discovery The opportunities and challenges presented by multi-target drug discovery (MTDD) De novo design of lead compounds and new approaches to estimating the synthetic accessibility of de novo–designed molecules The impact of natural products on drug discovery, and potential of natural product–like compounds for exploring regions of biologically relevant chemical space Using early screening of hits and leads for metabolic, pharmacokinetic, and toxicological liabilities to reduce attrition during the later phases of drug discovery The utility of parallel synthesis and purification in lead discovery With each topic supported by numerous case studies, this is indispensable reading for researchers in industry and academia who wish to keep up to date with the latest strategies and approaches in drug discovery.
High Throughput Screening Methods Academic Press
Development of Chemistry-Based Screening Platform for Access to Mirror-Image Library of Natural ProductsSpringer
Lead Generation Approaches in Drug Discovery Royal Society of Chemistry
Discover an enhanced synthetic approach to developing andscreening chemical compound libraries Diversity-oriented synthesis is a new paradigm for developinglarge collections of structurally diverse small molecules as probesto investigate biological pathways. This book presents the mosteffective methods in diversity-oriented synthesis for creatingsmall molecule collections. It offers tested and proven strategiesfor developing diversity-oriented synthetic libraries and screeningmethods for identifying ligands. Lastly, it explores some promisingnew applications based on diversity-oriented synthesis that havethe potential to dramatically advance studies in drug discovery andchemical biology. Diversity-Oriented Synthesis begins with an introductorychapter that explores the basics, including a discussion of therelationship between diversity-oriented synthesis and classiccombinatorial chemistry. Divided into four parts, the book: Offers key chemical methods for the generation of smallmolecules using diversity-oriented principles, includingpeptidomimetics and macrocycles Expands on the concept of diversity-oriented synthesis bydescribing chemical libraries Provides modern approaches to screening diversity-orientedsynthetic libraries, including high-throughput and high-contentscreening, small molecule microarrays, and smart screeningassays Presents the applications of diversity-oriented syntheticlibraries and small molecules in drug discovery and chemicalbiology, reporting the results of key studies and forecasting therole of diversity-oriented synthesis in future biomedicalresearch This book has been written and edited by leading internationalexperts in organic synthesis and its applications. Theircontributions are based on a thorough review of the currentliterature as well as their own firsthand experience developingsynthetic methods and applications. Clearly written and extensively referenced,Diversity-Oriented Synthesis introduces novices to thishighly promising field of research and serves as a springboard forexperts to advance their own research studies and develop newapplications.
Medicinal Chemistry Academic Press
Cheminformatics, QSAR and Machine Learning Applications for Novel Drug Development aims at showcasing different structure-based, ligand-based, and machine learning tools currently used in drug design. It also highlights special topics of computational drug design together with the available tools and databases. The integrated presentation of chemometrics, cheminformatics, and machine learning methods under is one of the strengths of the book.The first part of the content is devoted to establishing the foundations of the area. Here recent trends in computational modeling of drugs are presented. Other topics present in this part include QSAR in medicinal chemistry, structure-based methods, chemoinformatics and chemometric approaches, and machine learning methods in drug design. The second part focuses on methods and case studies including molecular descriptors, molecular similarity, structure-based based screening, homology modeling in protein structure predictions, molecular docking, stability of drug receptor interactions, deep learning and support vector machine in drug design. The third part of the book is dedicated to special topics, including dedicated chapters on topics ranging from de design of green pharmaceuticals to computational toxicology. The final part is dedicated to present the available tools and databases, including QSAR databases, free tools and databases in ligand and structure-based drug design, and machine learning resources for drug design. The final chapters discuss different web servers used for identification of various drug candidates. Presents chemometrics, cheminformatics and machine learning methods under a single reference Showcases the different structure-based, ligand-based and machine learning tools currently used in drug design Highlights special topics of computational drug design and available tools and databases
Development of Chemistry-Based Screening Platform for Access to Mirror-Image Library of Natural Products John Wiley & Sons
This book comprehensively describes the development and practice of DNA-encoded library synthesis technology. Together, the chapters detail an approach to drug discovery that offers an attractive addition to the portfolio of existing hit generation technologies such as high-throughput screening, structure-based drug discovery and fragment-based screening. The book: Provides a valuable guide for understanding and applying DNA-encoded combinatorial chemistry Helps chemists generate and screen novel chemical libraries of large size and quality Bridges interdisciplinary areas of DNA-encoded combinatorial chemistry – synthetic and analytical chemistry, molecular biology, informatics, and biochemistry Shows medicinal and pharmaceutical chemists how to efficiently broaden available “chemical space” for drug discovery Provides expert and up-to-date summary of reported literature for DNA-encoded and DNA-directed chemistry technology and methods
Fundamentals of Early Clinical Drug Development CRC Press
This book describes some of the most exciting developments for the discovery of new drugs, such as Fragment-based methods. It contains the latest developments in technologies that can be used to obtain the 3-D structures. This book includes experimental approaches using X-ray crystallography and NMR for Fragment-based screening as well as other biophysical methods for studying protein/ligand interactions.