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active compounds for therapeutic development, this book covers rational drug design, high-throughput screening, and genetic approaches to drug discovery. The authors focus on advances in the use of combinatorial chemistry and

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natural products, both of which support the chemical diversity for many drug screening programmes.

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drug design (CADD) tools have
been... 3. ...

*New techniques and strategies in
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Abstract. Great success has been
witnessed in last decades, some
new techniques and strategies

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have been widely used in drug discovery. In this roadmap, several representative techniques and strategies are highlighted to show recent advances in this field. (A) A DOX protocol has been developed for accurate protein-ligand binding structure

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prediction, in which first principle method was used to rank the binding poses.

New techniques and strategies in drug discovery ...

industry and academic research laboratories advances in drug

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discovery techniques covers
rational drug design high
throughput screening and genetic
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guide to techniques for the
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development this book covers
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developing a new drug is over
USD 6 billion. However, it is observed
that the pharmaceutical industry
is gripped by rising failure rates.

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Techniques [PDF]*

Incorporating ADME/Tox data

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earlier in drug discovery
Elimination of unsuccessful
candidates earlier in the drug
discovery process would help to
reduce the resources consumed
and high cost of bringing a drug
to market. Due to the inherent
slow throughput of MS-based

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techniques, ADME/Tox assays are typically pursued late in drug development.

*Recent Technology Advances
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Over the past decade, fragment-based drug discovery (FBDD) has

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garnered increasing interest among drug discovery experts and has established itself as a key approach within the field - acting as an alternative starting point for the discovery of high-quality lead candidates. Despite advances in several screening

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technologies, which have undoubtedly driven FBDD forward, applying a fragment-based approach to more complex biological targets remains a challenge. 1.

Advances in Fragment-based

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Techniques: Harvey, Alan L ...

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rational drug design high
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screening is gaining new

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A guide to techniques for the discovery and evaluation of pharmacologically active compounds for therapeutic development, this book covers rational drug design, high-

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throughput screening, and genetic approaches to drug discovery. The authors focus on advances in the use of combinatorial chemistry and natural products, both of which support the chemical diversity for many drug screening

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programmes. They examine typical screening studies and their link to robotics and informatics in detail and present an overview of current progress within antisense therapeutics. The book explores the rapid changes in drug discovery

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resulting from developments in
molecular biology, robotics, and
informatics.

Small Molecule Drug Discovery:
Methods, Molecules and

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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

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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

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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

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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

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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,

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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

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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

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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

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overview of structural features
and classification of natural
product-derived small molecules,
including carbohydrate
derivatives, peptides and
peptidomimetics, and alkaloid-
inspired small molecules

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The process of drug discovery and development is a complex multistage logistics project spanned over 10-15 years with an average budget exceeding 1 billion USD. Starting with target

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identification and synthesizing
anywhere between 10k to 15k
synthetic compounds to
potentially obtain the final drug
that reaches the market involves
a complicated maze with multiple
inter- and intra-operative fields.
Topics described in this book

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emphasize the progresses in computational applications, pharmacokinetics advances, and molecular modeling developments. In addition the book also contains special topics describing target deorphaning in *Mycobacterium tuberculosis*,

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therapy treatment of some rare diseases, and developments in the pediatric drug discovery process.

Following significant advances in deep learning and related areas interest in artificial intelligence

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(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.

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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.

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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.

Improving and Accelerating

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Therapeutic Development for Nervous System Disorders is the summary of a workshop convened by the IOM Forum on Neuroscience and Nervous System Disorders to examine opportunities to accelerate early phases of drug development for

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nervous system drug discovery. Workshop participants discussed challenges in neuroscience research for enabling faster entry of potential treatments into first-in-human trials, explored how new and emerging tools and technologies may improve the

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efficiency of research, and considered mechanisms to facilitate a more effective and efficient development pipeline. There are several challenges to the current drug development pipeline for nervous system disorders. The fundamental

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etiology and pathophysiology of many nervous system disorders are unknown and the brain is inaccessible to study, making it difficult to develop accurate models. Patient heterogeneity is high, disease pathology can occur years to decades before

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becoming clinically apparent, and diagnostic and treatment biomarkers are lacking. In addition, the lack of validated targets, limitations related to the predictive validity of animal models - the extent to which the model predicts clinical efficacy -

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and regulatory barriers can also impede translation and drug development for nervous system disorders. Improving and Accelerating Therapeutic Development for Nervous System Disorders identifies avenues for moving directly from cellular

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models to human trials, minimizing the need for animal models to test efficacy, and discusses the potential benefits and risks of such an approach. This report is a timely discussion of opportunities to improve early drug development with a focus

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toward preclinical trials.

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

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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,

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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

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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

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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

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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,

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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

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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

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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

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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

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with new case studies includes additional modern examples of drug discovery through high through-put screening, fragment-based drug design, and computational chemistry

A comprehensive guide to cutting-

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edge tools in ADME research The last decade has seen tremendous progress in the development of analytical techniques such as mass spectrometry and molecular biology tools, resulting in important advances in drug discovery, particularly in the area

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of absorption, distribution, metabolism, and excretion (ADME). ADME-Enabling Technologies in Drug Design and Development focuses on the current state of the art in the field, presenting a comprehensive review of the latest tools for

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generating ADME data in drug discovery. It examines the broadest possible range of available technologies, giving readers the information they need to choose the right tool for a given application, a key requisite for obtaining favorable results in a

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Dr. Davide Staedler is CEO of TIBIO Sagl, a consulting company, and chief scientific officer of Scitec Research S.A., a private analytical laboratory. All other Topic Editors declare no competing interests with regards to the Research Topic subject.

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