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COMPUTER-AIDED DRUG DISCOVERY

Humana Press **This detailed volume examines computer-aided drug discovery (CADD), a crucial component of modern drug discovery programs that is widely utilized to identity and optimize bioactive compounds for the development of new drugs. With a focus on the methods that are commonly used in the early stage of drug discovery, chapters explore computer simulation, structure prediction, conformational sampling, binding site mapping, docking and scoring, in silico screening, and fragment-based drug design. In addition to the state-of-the-art theoretical concept, this book also includes step-by-step, readily reproducible computational protocols as well as examples of various CADD strategies. The limitations and potential pitfalls of different computational methods are discussed by experts, and tips and advice for their applications are suggested. Practical and thorough, Computer-Aided Drug Discovery serves as an ideal addition to the Methods in Pharmacology and Toxicology series, guiding researchers toward their lab's goals with this exciting and versatile technology.**

COMPUTER AIDED DRUG DESIGN (CADD): FROM LIGAND-BASED METHODS TO STRUCTURE-BASED APPROACHES

Elsevier **Computer-Aided Drug Design (CADD): From Ligand-Based Methods to Structure-Based Approaches outlines the basic theoretical principles, methodologies and applications of different fundamental and advanced CADD approaches and techniques. Including information on current protocols as well as recent developments in the computational methods, tools and techniques used for rational drug design, the book explains the fundamental aspects of CADD, combining this with a practical understanding of the various in silico approaches used in modern drug discovery processes to assess the field in a comprehensive and systematic manner. Providing up-to-date, information and guidance for scientists, researchers, students and teachers, the book helps readers address specific academic and research related problems using illustrative explanations, examples and case studies, which are systematically reviewed. Highlights in silico approaches to drug design and discovery using computational tools and techniques Details ligand-based and structure-based drug design in a comprehensive and systematic approach Summarizes recent developments in computational drug design strategy as novel approaches of rational drug designing**

COMPUTER-AIDED DRUG DESIGN

Springer Nature **This book provides up-to-date information on bioinformatics tools for the discovery and development of new drug molecules. It discusses a range of computational applications, including three-dimensional modeling of protein structures, protein-ligand docking, and molecular dynamics simulation of protein-ligand complexes for identifying desirable drug candidates. It also explores computational approaches for identifying potential drug targets and for pharmacophore modeling. Moreover, it presents structure- and ligand-based drug design tools to optimize known drugs and guide the design of new molecules. The book also describes methods for identifying small-molecule binding pockets in proteins, and summarizes the databases used to explore the essential properties of drugs, drug-like small molecules and their targets. In addition, the book highlights various tools to predict the absorption, distribution, metabolism, excretion (ADME) and toxicity (T) of potential drug candidates. Lastly, it reviews in silico tools that can facilitate vaccine design and discusses their limitations.**

COMPUTER-AIDED DRUG DISCOVERY

This detailed volume examines computer-aided drug discovery (CADD), a crucial component of modern drug discovery programs that is widely utilized to identity and optimize bioactive compounds for the development of new drugs. With a focus on the methods that are commonly used in the early stage of drug discovery, chapters explore computer simulation, structure prediction, conformational sampling, binding site mapping, docking and scoring, in silico screening, and fragment-based drug design. In addition to the state-of-the-art theoretical concept, this book also includes step-by-step, readily reproducible computational protocols as well as examples of various CADD strategies. The limitations and potential pitfalls of different computational methods are discussed by experts, and tips and advice for their applications are suggested. Practical and thorough, Computer-Aided Drug Discovery serves as an ideal addition to the Methods in Pharmacology and Toxicology series, guiding researchers toward their lab{u2019}s goals with this exciting and versatile technology.

IN SILICO METHODS FOR DRUG DESIGN AND DISCOVERY

Frontiers Media SA

CHEMICAL GENOMICS

Cambridge University Press **Advances in chemistry, biology and genomics coupled with laboratory automation and computational technologies have led to the rapid emergence of the multidisciplinary field of chemical genomics. This edited text, with contributions from experts in the field, discusses the new techniques and applications that help further the study of chemical genomics. The beginning chapters provide an overview of the basic principles of chemical biology and chemical genomics. This is followed by a technical section that describes the sources of small-molecule chemicals; the basics of high-throughput screening technologies; and various bioassays for biochemical-, cellular- and organism-based screens. The final chapters connect the chemical genomics field with personalized medicine and the druggable genome for future discovery of new therapeutics. This book will be valuable to researchers, professionals and graduate students in many fields, including biology, biomedicine and chemistry.**

COMPUTER-AIDED DRUG DESIGN AND DELIVERY SYSTEMS

McGraw Hill Professional **THE LATEST BREAKTHROUGHS IN COMPUTER-AIDED DRUG DESIGN AND DELIVERY This definitive text provides in-depth information on computer-assisted techniques for discovering, designing, and optimizing new, effective, and safe drugs. Computer-Aided Drug Design and Delivery Systems offers objective and quantitative data on the use and delivery of drugs in humans. Enabling technologies such as bioinformatics, pharmacokinetics, biosensors, robotics, and bioinstruments are thoroughly discussed in this innovative work. Coverage includes: Computer-aided drug design (CADD) Drug delivery systems Bioinformatics of drug molecules and databases Lipase- and esterase-mediated drugs and drug intermediates Pharmacokinetics and pharmacodynamics of drugs Biomarkers, biosensors, and robotics in medicine Biomedical instrumentation**

BIOMEDICAL SIGNAL PROCESSING FOR HEALTHCARE APPLICATIONS

CRC Press **This book examines the use of biomedical signal processing—EEG, EMG, and ECG—in analyzing and diagnosing various medical conditions, particularly diseases related to the heart and brain. In combination with machine learning tools and other optimization methods, the analysis of biomedical signals greatly benefits the healthcare sector by improving patient outcomes through early, reliable detection. The discussion of these modalities promotes better understanding, analysis, and application of biomedical signal processing for specific diseases. The major highlights of Biomedical Signal Processing for Healthcare Applications include biomedical signals, acquisition of signals, pre-processing and analysis, post-processing and classification of the signals, and application of analysis and classification for the diagnosis of brain- and heart-related diseases. Emphasis is given to brain and heart signals because incomplete interpretations are made by physicians of these aspects in several situations, and these partial interpretations lead to major complications. FEATURES Examines modeling and acquisition of biomedical signals of different disorders Discusses CAD-based analysis of diagnosis useful for healthcare Includes all important modalities of biomedical signals, such as EEG, EMG, MEG, ECG, and PCG Includes case studies and research directions, including novel approaches used in advanced healthcare systems This book can be used by a wide range of users, including students, research scholars, faculty, and practitioners in the field of biomedical engineering and medical image analysis and diagnosis.**

MOLECULAR DOCKING FOR COMPUTER-AIDED DRUG DESIGN

FUNDAMENTALS, TECHNIQUES, RESOURCES AND APPLICATIONS

Academic Press **Molecular Docking for Computer-Aided Drug Design: Fundamentals, Techniques, Resources and Applications offers in-depth coverage on the use of molecular docking for drug design. The book is divided into three main sections that cover basic techniques, tools, web servers and applications. It is an essential reference for students and researchers involved in drug design and discovery. Covers the latest information and state-of-the-art trends in structure-based drug design methodologies Includes case studies that complement learning Consolidates fundamental concepts and current practice of molecular docking into one convenient resource**

APPLIED CASE STUDIES AND SOLUTIONS IN MOLECULAR DOCKING-BASED DRUG DESIGN

IGI Global **As the pharmaceutical industry continues to advance, new techniques in drug design are emerging. In order to deliver optimum care to patients, the development of innovative pharmacological techniques has become a widely studied topic. Applied Case Studies and Solutions in Molecular Docking-Based Drug Design is a pivotal reference source for the latest scholarly research on the progress of pharmaceutical design and computational approaches in the field of molecular docking. Highlighting innovative research perspectives and real-world applications, this book is ideally designed for professionals, researchers, practitioners, and medical chemists actively involved in computational chemistry and pharmaceutical sciences.**

COMPUTER AIDED DRUG DESIGN IN INDUSTRIAL RESEARCH

Springer Science & Business Media **The Ernst Schering Research Foundation sponsored its 15th workshop in Berlin on October 19-21, 1994. Leading scientists from Europe and North America were invited to discuss computer-aided drug**

design in industrial research. Computer-aided drug design is a very exciting field and an intellec tual challenge, like playing chess. But these reasons are no longer suf ficient to justify using this method in industry, if they ever were. Fig. 1. The participants of the workshop VI Preface Therefore, when we, together with Prof. Hoyer, started to think about this workshop, our intentions quickly became clear. We were not so much interested in the very latest developments of methods or in computer-aided drug design itself - enough conferences have dealt with these topics. However, we were very interested in the usefulness and limitations of computer-aided drug design in the indu strial research process. A lot has changed in the pharmaceutical industry recently. These changes are gaining momentum, so it is the right time to think about the role of computer-aided drug design in this changing environment.

COMPUTER APPLICATIONS IN PHARMACEUTICAL RESEARCH AND DEVELOPMENT

John Wiley & Sons **A unique, holistic approach covering all functions and phases of pharmaceutical research and development While there are a number of texts dedicated to individual aspects of pharmaceutical research and development, this unique contributed work takes a holistic and integrative approach to the use of computers in all phases of drug discovery, development, and marketing. It explains how applications are used at various stages, including bioinformatics, data mining, predicting human response to drugs, and high-throughput screening. By providing a comprehensive view, the book offers readers a unique framework and systems perspective from which they can devise strategies to thoroughly exploit the use of computers in their organizations during all phases of the discovery and development process. Chapters are organized into the following sections: * Computers in pharmaceutical research and development: a general overview * Understanding diseases: mining complex systems for knowledge * Scientific information handling and enhancing productivity * Computers in drug discovery * Computers in preclinical development * Computers in development decision making, economics, and market analysis * Computers in clinical development * Future applications and future development Each chapter is written by one or more leading experts in the field and carefully edited to ensure a consistent structure and approach throughout the book. Figures are used extensively to illustrate complex concepts and multifaceted processes. References are provided in each chapter to enable readers to continue investigating a particular topic in depth. Finally, tables of software resources are provided in many of the chapters. This is essential reading for IT professionals and scientists in the pharmaceutical industry as well as researchers involved in informatics and ADMET, drug discovery, and technology development. The book's cross-functional, all-phases approach provides a unique opportunity for a holistic analysis and assessment of computer applications in pharmaceutics.**

COMPUTER-AIDED DRUG DESIGN

CBS Publishers & Distributors Pvt Limited, India **This book is compiled to cover all the topics of computer-aided drug design for pharmacy professionals in industry. Written in easy to understand language, the text is well supplemented by illustrative diagrams, tables, molecular structures of drugs and their synthesis, providing a clear understanding of the subject to the reader.**

DRUG DESIGN AND DISCOVERY

METHODS AND PROTOCOLS

Humana Press **Research in the pharmaceutical sciences and medicinal chemistry has taken an important new direction in the past two decades with a focus on large molecules, especially peptides and proteins, as well as DNA therapeutics. In Drug Design and Discovery: Methods and Protocols, leading experts provide an in-depth view of key protocols that are commonly used in drug discovery laboratories. Covering both classic and cutting-edge techniques, this volume explores computational docking, quantitative structure-activity relationship (QSAR), peptide synthesis, labeling of peptides and proteins with fluorescent labels, DNA-microarray, zebrafish model for drug screening, and other analytical screening and biological assays that are routinely used during the drug discovery process. Written in the highly successful Methods in Molecular BiologyTM series format, chapters include introductions to their respective topics, lists of the necessary materials, step-by-step, readily reproducible laboratory protocols, and tips on troubleshooting and avoiding known pitfalls. Thorough and accessible, Drug Design and Discovery: Methods and Protocols serve as a vital laboratory reference for pharmaceutical chemists, medicinal chemists, and pharmacologists as well as for molecular biologists.**

DRUG DISCOVERY AND DEVELOPMENT

FROM TARGETS AND MOLECULES TO MEDICINES

Springer Nature **This book describes the processes that are involved in the development of new drugs. The authors discuss the history, role of natural products and concept of receptor interactions with regard to the initial stages of drug discovery. In a single, highly readable volume, it outlines the basics of pharmacological screening, drug target identification, and genetics involved in early drug discovery. The final chapters introduce readers to stem therapeutics, pharmacokinetics, pharmacovigilance, and toxicological testing. Given its scope, the book will enable research scholars, professionals and young scientists to understand the key fundamentals of drug discovery, including stereochemistry, pharmacokinetics, clinical trials, statistics and toxicology.**

APPLIED CHEMOINFORMATICS

ACHIEVEMENTS AND FUTURE OPPORTUNITIES

John Wiley & Sons **Edited by world-famous pioneers in chemoinformatics, this is a clearly structured and applications-oriented approach to the topic, providing up-to-date and focused information on the wide range of applications in this exciting field. The authors explain methods and software tools, such that the reader will not only learn the basics but also how to use the different software packages available. Experts describe applications in such different fields as structure-spectra correlations, virtual screening, prediction of active sites, library design, the prediction of the properties of chemicals, the development of new cosmetics products, quality control in food, the design of new materials with improved properties, toxicity modeling, assessment of the risk of chemicals, and the control of chemical processes. The book is aimed at advanced students as well as lectures but also at scientists that want to learn how chemoinformatics could assist them in solving their daily scientific tasks. Together with the corresponding textbook Chemoinformatics - Basic Concepts and Methods (ISBN 9783527331093) on the fundamentals of chemoinformatics readers will have a comprehensive overview of the field.**

BIOPHYSICAL AND COMPUTATIONAL TOOLS IN DRUG DISCOVERY

Springer Nature **This book reviews recent physicochemical and biophysical techniques applied in drug discovery research, and it outlines the latest advances in computational drug design. Divided into 10 chapters, the book discusses about the role of structural biology in drug discovery, and offers useful application cases of several biophysical and computational methods, including time-resolved fluorometry (TRF) with Förster resonance energy transfer (FRET), X-Ray crystallography, nuclear magnetic resonance spectroscopy, mass spectroscopy, generative machine learning for inverse molecular design, quantum mechanics/molecular mechanics (QM/MM,ONIOM) and quantum molecular dynamics (QMT) methods. Particular attention is given to computational search techniques applied to peptide vaccines using novel mathematical descriptors and structure and ligand-based virtual screening techniques in drug discovery research. Given its scope, the book is a valuable resource for students, researchers and professionals from pharmaceutical industry interested in drug design and discovery.**

RECENT ADVANCES IN COMPUTER AIDED DRUG DESIGNING

We are extremely happy to introduce our new book, Recent Advances in Computer Aided Drug Designing. While interacting with many researchers in the field of biotechnology and allied sciences, we felt that there was need for a book that could easily bridge the gap between in silico methods applied in structural bioinformatics for drug designing and wet lab workers. Today, when computational skills in biology and biomedical research are in high demand, this book presents updated content for methods and tools applicable in modern computer-aided drug designing. Researchers are pouring knowledge into databases that are publicly available and laboratories across the globe are accessing this information for analysis and further investigation. There is a battery of data scientists involved in development and maintenance of online databases. Alongside them, there is another class of programmers and scientists involved in development of software tools for analysis of this data. Modern tools based on machine learning are available to provide accuracy and efficiency with speedy analysis of biological and biomedical data. In many cases, analysis of readily available biological data helps to decide future directions for laboratory work. Indications obtained from such analytics save time and resources which could be very crucial in general. Publicly available protein three-dimensional structure and drug databank libraries have facilitated the drug discovery process. Millions of drugs can be screened in a few hours by using virtual screening tools. Molecular viewing tools can be used to visualize macromolecules and their interactions with drugs. Findings from such studies are being used to validate results directly in laboratories.Efforts have been made to cover all areas relevant for computer-aided drug designing to allow this book to serve as a standard reference book and meet the requirements of graduate students and researchers working in drug design and structural bioinformatics. Some chapters are dedicated to basic concepts in computer-aided drug discovery while other chapters present applications of the available tools in the field. Contents from exemplary method-based chapters are easy to follow and will help new researchers in applying contemporary tools for their studies. The book will also stimulate programmers and data scientists interested in developing tools for structural bioinformatics applications to develop new and improved versions of software. Chapters presenting the basic concepts of methods involved in drug design will help new learners in the field to meet the challenges of designing novel therapeutics by using computational tools. Cross-disciplinary research is in trend nowadays and such investigations involving experts of their respective fields are highly promising and fruitful. Drug discovery requires experts from health sciences and medical sciences, molecular biologists, bioinformaticians, biotechnologists, biochemists, statisticians, biophysicists and clinicians. For a complete piece of translated product such as a drug, inputs from specialist researchers are needed. Modern rational drug discovery approaches are truly inter-disciplinary fields which require a systems biology approach for successful ventures. This book covers all steps of drug design, from drug target identification to intermediate steps to successful clinical trials, making it truly essential for modern researchers in the drug discovery and structural bioinformatics fields.

ADVANCES IN ANIMAL BIOTECHNOLOGY

Springer **This book entitled, “Advances in Animal Biotechnology,” is a compilation of state-of-the-art in the field of Animal Biotechnology including fishery, that are not sheltered in depth in earlier publications. It offers an update on avant-garde technologies and advances in key aspects of genetic engineering, metagenomics, assisted reproduction,**

animal genomics, biotechnology in veterinary health, as well as the role of gut and marine microbial ecosystems in livestock and industrial development. The book is divided broadly into five different sections, viz., Gut Microbiome and Nutritional Biotechnology, Assisted Reproduction Biotechnology, Livestock Genomics, Health Biotechnology, and Animal Biotechnology in Global Perspective. The book covers the syllabi of Animal Biotechnology courses in various universities, academia and competitive examinations at various levels. Researchers, Continuing Graduates, and Academicians, Research Institutions, and Biotech Companies will be benefited from this valuable compilation of research. Its broad spectrum makes this work a valuable resource for professionals, researchers, academics and students in the field of veterinary and animal production as well as the biotechnology industry.

PHARMACEUTICAL SCIENCES: BREAKTHROUGHS IN RESEARCH AND PRACTICE

BREAKTHROUGHS IN RESEARCH AND PRACTICE

IGI Global **The delivery of optimal pharmaceutical services to patients is a pivotal concern in the healthcare field. By examining current trends and techniques in the industry, processes can be maintained and improved. Pharmaceutical Sciences: Breakthroughs in Research and Practice provides comprehensive coverage of the latest innovations and advancements for pharmaceutical applications. Focusing on emerging drug development techniques and drug delivery for improved health outcomes, this book is ideally designed for medical professionals, pharmacists, researchers, academics, and upper-level students within the growing pharmaceutical industry.**

COMPUTER APPLICATIONS IN DRUG DISCOVERY AND DEVELOPMENT

IGI Global **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.**

METHODS AND ALGORITHMS FOR MOLECULAR DOCKING-BASED DRUG DESIGN AND DISCOVERY

IGI Global **The role of technology in the medical field has resulted in significant developments within the pharmaceutical industry. Computational approaches have emerged as a crucial method in further advancing drug design and development. Methods and Algorithms for Molecular Docking-Based Drug Design and Discovery presents emerging research on the application of computer-assisted design methods for drugs, emphasizing the benefits and improvements that molecular docking has caused within the pharmaceutical industry. Focusing on validation methods, search algorithms, and scoring functions, this book is a pivotal resource for professionals, researchers, students, and practitioners in the field of theoretical and computational chemistry.**

FRAGMENT-BASED DRUG DISCOVERY

Royal Society of Chemistry **Fragment-based drug discovery is a rapidly evolving area of research, which has recently seen new applications in areas such as epigenetics, GPCRs and the identification of novel allosteric binding pockets. The first fragment-derived drug was recently approved for the treatment of melanoma. It is hoped that this approval is just the beginning of the many drugs yet to be discovered using this fascinating technique. This book is written from a Chemist's perspective and comprehensively assesses the impact of fragment-based drug discovery on a wide variety of areas of medicinal chemistry. It will prove to be an invaluable resource for medicinal chemists working in academia and industry, as well as anyone interested in novel drug discovery techniques.**

DRUG DISCOVERY AND DEVELOPMENT

PRESENT AND FUTURE

BoD – Books on Demand **Drug discovery and development process aims to make available medications that are safe and effective in improving the length and quality of life and relieving pain and suffering. However, the process is very complex, time consuming, resource intensive, requiring multi-disciplinary expertise and innovative approaches. There is a growing urgency to identify and develop more effective, efficient, and expedient ways to bring safe and effective products to the market. The drug discovery and development process relies on the utilization of relevant and robust tools, methods, models, and validated biomarkers that are predictive of clinical effects in terms of diagnosis, prevention, therapy, and prognosis. There is a growing emphasis on translational research, a bidirectional bench to the bedside approach, in an effort to improve the process efficiency and the need for further innovations. The authors in the book discuss the current and evolving state of drug discovery and development.**

CHEMOINFORMATICS APPROACHES TO STRUCTURE- AND LIGAND-BASED DRUG DESIGN

Frontiers Media SA **Chemoinformatics is paramount to current drug discovery. Structure- and ligand-based drug design strategies have been used to uncover hidden patterns in large amounts of data, and to disclose the molecular aspects underlying ligand-receptor interactions. This Research Topic aims to share with a broad audience the most recent trends in the use of chemoinformatics in drug design. To that end, experts in all areas of drug discovery have made their knowledge available through a series of articles that report state-of-the-art approaches. Readers are provided with outstanding contributions focusing on a wide variety of topics which will be of great value to those interested in the many different and exciting facets of drug design.**

FRONTIERS IN COMPUTATIONAL CHEMISTRY

Bentham Science Publishers **Frontiers in Computational Chemistry presents contemporary research on molecular modeling techniques used in drug discovery and the drug development process: computer aided molecular design, drug discovery and development, lead generation, lead optimization, database management, computer and molecular graphics, and the development of new computational methods or efficient algorithms for the simulation of chemical phenomena including analyses of biological activity. The third volume of this series features four chapters covering in silico approaches to computer aided drug design, modeling of platinum and adjuvant anti-cancer drugs, allostery in proteins and studies on the theory of chemical space in electron systems.**

BIOACTIVE NATURAL PRODUCTS

OPPORTUNITIES AND CHALLENGES IN MEDICINAL CHEMISTRY

World Scientific **Bioactive natural products are a rich source of novel therapeutics. Thus, the search for bioactive molecules from nature continues to play an important role in fashioning new medicinal agents. This volume, which comprises sixteen chapters written by active researchers and leading experts in natural products chemistry, brings together an overview of current discoveries in this remarkable field. It also provides information on the industrial application of natural products for medicinal purposes. This book will serve as a valuable resource for researchers to predict promising leads for developing pharmaceuticals to treat various ailments and disease manifestations.**

TEXTBOOK OF MEDICINAL CHEMISTRY

Elsevier Health Sciences **The Textbook of Medicinal Chemistry is a much-awaited masterpiece in its arena. Targeted mainly to B. Pharmacy students, book would also be useful for M. Pharmacy as well as M.Sc. Organic Chemistry/Pharmaceutical Chemistry students. It aims at eliminating the inadequacies in teaching and learning of medicinal chemistry by providing enormous information on all the topics in medicinal chemistry of synthetic drugs. About the Author : - Prof. Dr. V. Alagarsamy, M. Pharm., Ph.D., FIC., D.O.M.H., is Professor and Principal of MNR College of Pharmacy, Gr. Hyderabad, Sangareddy. He has been teaching Medicinal Chemistry and performing research work in Synthetic Medicinal Chemistry on novel heterocyclic bioactive compounds for more than a decade. His research activities are collaborated with various research laboratories/organisations like National Cancer Institute, USA; Rega Institute for Medical Research, Belgium and Southern Research Institute, USA. He is a recipient of Young Scientist award from the Department of Science and Technology, New Delhi. His research publications in journals and presentations in conferences, put together, exceed hundred. His research activities are supported by the funding agencies like CSIR, DST and DSIR. He is a doctoral committee member and recognized Research guide for Ph.D. students in various universities.**

TEXTBOOK OF MEDICINAL CHEMISTRY VOL I - E-BOOK

Elsevier Health Sciences **Dr Alagarsamy's Textbook of Medicinal Chemistry is a much-awaited masterpiece in its arena. Targeted mainly to B. Pharm. students, this book will also be useful for M. Pharm. as well as M. Sc. organic chemistry and pharmaceutical chemistry students. It aims at eliminating the inadequacies in teaching and learning of medicinal chemistry by providing enormous information on all the topics in medicinal chemistry of synthetic drugs. Salient Features Contains clear classification, synthetic schemes, mode of action, metabolism, assay, pharmacological uses with the dose and structure–activity relationship (SAR) of the following classes of drugs: Drugs acting on inflammation Drugs acting on respiratory system Drugs acting on digestive system Drugs acting on blood and blood-forming organs Drugs acting on endocrine system Contains a complete section on chemotherapy and the various classes of chemotherapeutic agents. Also includes recent topics like anti-HIV agents Contains brief introduction about the physiological and pathophysiological conditions of diseases and their treatment under each topic Provides well-illustrated synthetic schemes and alternative synthetic routes for majority of drugs that help in quick and enhanced understanding of the subject Covers the syllabi of majority of Indian universities**

CORONAVIRUS DISEASE-19 (COVID-19): DIFFERENT MODELS AND TREATMENT STRATEGIES

Bentham Science Publishers **In this book volume-2 proposal has been classified into Part IV: Models for SARS-CoV-2 and Part V: Treatment Strategies for SARS-CoV-2. With the emergence of new coronavirus variants, epidemiology, different host tropism permits a thorough analysis of their evolution and acquired adaptability to their host which need different animal models and treatment approaches. No studies are complete without animal models closely related to human physiology to replicate the disease and observe the pathology conditions as in human cases. Such animal models play**

a vital role in virus pathogenesis and prepare a therapeutic immune response. Here describe bio-engineered transgenic mouse model inserting with specific genes, or CRISPR-Case9 gene-editing tool has been used previously for SARS-CoV and MERS-CoV. The chapter will deal with culture techniques or cell lines for COVID-19—also histopathology of COVID-19, essential proteins that up or down-regulate SARS-CoV-2. The last chapter of this part will describe other diseases having similar signs and symptoms and their differentiation. There is no specific treatment available to date, just symptomatic therapy. However, scientists will elucidate effective antiviral drugs in clinical trials, phytochemicals, photomedicine such as ultraviolet A & B, homemade remedies, blood plasma transfusion, stem cell therapy, and computational approaches in vivo and in vitro trials. This book will appear as a baseline for academicians, scientists, and health professionals as still, research is going to overcome this outbreak of COVID-19, the novelty of best animal models, and find an effective treatment. However, just a single book proposal like this wouldn't have flourished without enthusiasm and determined publishers' and investigators' strength to take time from their busy schedule and subsidize on time. We thank the whole investigators who contributed, directly and indirectly, to bring it to reality.

COMPUTATIONAL DRUG DESIGN

A GUIDE FOR COMPUTATIONAL AND MEDICINAL CHEMISTS

John Wiley & Sons **Helps you choose the right computational tools and techniques to meet your drug design goals Computational Drug Design covers all of the major computational drug design techniques in use today, focusing on the process that pharmaceutical chemists employ to design a new drug molecule. The discussions of which computational tools to use and when and how to use them are all based on typical pharmaceutical industry drug design processes. Following an introduction, the book is divided into three parts: Part One, The Drug Design Process, sets forth a variety of design processes suitable for a number of different drug development scenarios and drug targets. The author demonstrates how computational techniques are typically used during the design process, helping readers choose the best computational tools to meet their goals. Part Two, Computational Tools and Techniques, offers a series of chapters, each one dedicated to a single computational technique. Readers discover the strengths and weaknesses of each technique. Moreover, the book tabulates comparative accuracy studies, giving readers an unbiased comparison of all the available techniques. Part Three, Related Topics, addresses new, emerging, and complementary technologies, including bioinformatics, simulations at the cellular and organ level, synthesis route prediction, proteomics, and prodrug approaches. The book's accompanying CD-ROM, a special feature, offers graphics of the molecular structures and dynamic reactions discussed in the book as well as demos from computational drug design software companies. Computational Drug Design is ideal for both students and professionals in drug design, helping them choose and take full advantage of the best computational tools available. Note: CD-ROM/DVD and other supplementary materials are not included as part of eBook file.**

NEXT GENERATION KINASE INHIBITORS

MOVING BEYOND THE ATP BINDING/CATALYTIC SITES

Springer Nature **Protein kinases are fascinating enzymes that maintain the proper function of nearly every task performed by the cells of the human body. By extracting a phosphate from the energy molecule ATP and linking it to another protein, protein kinases alter the structure and ultimate function of other proteins. In this way, protein kinases help monitor the extracellular environment and integrate signaling cues that, for the most part, are beneficial for human health and survival. However, protein kinases are often dysregulated and responsible for the initiation and progression of many types of cancers, inflammatory disorders, and other diseases. Thus, decades of research have revealed much about how protein kinases are regulated and approaches to inhibit these enzymes to treat disease. However, nearly 30 years since the identification of the first clinically beneficial small molecule protein kinase inhibitor, there are only a few examples where these drugs provide sustained and durable patient responses. The goal of this book is to provide biomedical scientists, graduate, and professional degree students insight into different approaches using small molecules to block specific protein kinase functions that promote disease.**

COMPUTER AIDED PHARMACEUTICS AND DRUG DELIVERY

AN APPLICATION GUIDE FOR STUDENTS AND RESEARCHERS OF PHARMACEUTICAL SCIENCES

Springer Nature **This book examines the role of computer-assisted techniques for discovering, designing, optimizing and manufacturing new, effective, and safe pharmaceutical formulations and drug delivery systems. The book discusses computational approaches, statistical modeling and molecular modeling for the development and safe delivery of drugs in humans. The application of concepts of QbD (Quality by Design), DoE (Design of Experiments), artificial intelligence and in silico pharmacokinetic assessment/simulation have been made a lot easier with the help of commercial software and expert systems. This title provides in-depth knowledge of such useful software with illustrations from the latest researches. The book also fills in the gap between pharmaceutics and molecular modeling at micro, meso and maro scale by covering topics such as advancements in computer-aided Drug Design (CADD), drug-polymer interactions in drug delivery systems, molecular modeling of nanoparticles and pharmaceutics/bioinformatics. This book provides abundant applications of computers in formulation designing and characterization are provided as examples, case studies and illustrations. Short reviews of software, databases and expert systems have also been added to culminate the interest of readers for novel applications in formulation development and drug delivery. Computer-aided pharmaceutics and drug delivery is an authoritative reference source for all the latest scholarly**

update on emerging developments in computed assisted techniques for drug designing and development. The book is ideally designed for pharmacists, medical practitioners, students and researchers.

HIGH-PERFORMANCE MODELLING AND SIMULATION FOR BIG DATA APPLICATIONS

SELECTED RESULTS OF THE COST ACTION IC1406 CHIPSET

Springer **This open access book was prepared as a Final Publication of the COST Action IC1406 “High-Performance Modelling and Simulation for Big Data Applications (cHiPSet)“ project. Long considered important pillars of the scientific method, Modelling and Simulation have evolved from traditional discrete numerical methods to complex data-intensive continuous analytical optimisations. Resolution, scale, and accuracy have become essential to predict and analyse natural and complex systems in science and engineering. When their level of abstraction raises to have a better discernment of the domain at hand, their representation gets increasingly demanding for computational and data resources. On the other hand, High Performance Computing typically entails the effective use of parallel and distributed processing units coupled with efficient storage, communication and visualisation systems to underpin complex data-intensive applications in distinct scientific and technical domains. It is then arguably required to have a seamless interaction of High Performance Computing with Modelling and Simulation in order to store, compute, analyse, and visualise large data sets in science and engineering. Funded by the European Commission, cHiPSet has provided a dynamic trans-European forum for their members and distinguished guests to openly discuss novel perspectives and topics of interests for these two communities. This cHiPSet compendium presents a set of selected case studies related to healthcare, biological data, computational advertising, multimedia, finance, bioinformatics, and telecommunications.**

QUALITY IN PHARMACEUTICAL EDUCATION, RESEARCH AND PRACTICE (VISION 2020)

- PUBLISHED BY MANIPAL UNIVERSAL PRESS

Manipal Universal Press **The book discusses the topics related to quality in education and research. It begins with a topic on Good Science, Education, and Teaching. Next chapter on Total Quality Management in pharmacy education highlights the importance of quality pharmacy education. There are focused chapters emphasizing the importance of quality education in pharmaceutics, medicinal chemistry, pharmaceutical biotechnology, pharmaceutical services, and pharmacognosy. The book includes a brief note on scope and potential in pharmacovigilance and quality of pharmaceutical sciences journals.**

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MODELING OF PROTEIN FLEXIBILITY AND INTER-MOLECULAR INTERACTIONS

APPLICATIONS TO COMPUTER-AIDED DRUG DESIGN AND DISCOVERY

COMPUTATIONAL APPROACHES IN DRUG DISCOVERY AND PRECISION MEDICINE

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