Computer Applications In Pharmaceutical Research And Development

The evidence of cancer in humans, animals and plant species suggests that it is as old as multicellular life on Earth. Why is it so difficult to understand and fight? Because cancer begins from the organism's own mutated single cell focused on its own survival. It would be naive to expect that cancer could be ever entirely eliminated, but there is still hope for finding effective treatments. The book is to give a view of selected aspects of cancer like its spread in nature, novel anticancer drugs based on Chinese herbs or birch bark, novel promising targets of annexins and kinases and progress in immunotherapy. It is our hope that you will find in this book interesting, inspiring and stimulating information concerning cancer research.

This comprehensive reference text discusses the fundamental concepts of artificial intelligence and its applications in a single volume. Artificial Intelligence: Fundamentals and Applications presents a detailed discussion of basic aspects and ethics in the field of artificial intelligence and its applications in areas, including electronic devices and systems, consumer electronics, automobile engineering, manufacturing, robotics and automation, agriculture, banking, and predictive analysis. Aimed at senior undergraduate

and graduate students in the field of electrical engineering, electronics engineering, manufacturing engineering, pharmacy, and healthcare, this text: Discusses advances in artificial intelligence and its applications. Presents the predictive analysis and data analysis using artificial intelligence. Covers the algorithms and pseudo-codes for different domains. Discusses the latest development of artificial intelligence in the field of practical speech recognition, machine translation, autonomous vehicles, and household robotics. Covers the applications of artificial intelligence in fields, including pharmacy and healthcare, electronic devices and systems, manufacturing, consumer electronics, and robotics.

The combination of Biostatistics and Computer Applications are very much useful for bio-sciences and bioinformatic fields. The book provides both concepts in synoptic view. The first part of the book includes chapters on basic concepts and sampling methods, probability and distributions, correlation and regression, Chi-Square test, analysis of variance, experimental designs and statistical quality control. The second part of the book provides a detailed, yet easy to understand description of the computer fundamentals. Each and every aspect is presented very clearly and logically. This part of book includes chapters on computer and its application history of computer, type of computers, number system, system concept fundamental of operating system, computer languages, networking concept, database management, and C programming. Salient Features All the

chapters are written in a lucid manner A chapter on application of computers in pharmaceutical and clinical studies is added.

Consumer health websites have garnered considerable media attention, but only begin to scratch the surface of the more pervasive transformations the Internet could bring to health and health care. Networking Health examines ways in which the Internet may become a routine part of health care delivery and payment, public health, health education, and biomedical research. Building upon a series of site visits, this book: Weighs the role of the Internet versus private networks in uses ranging from the transfer of medical images to providing video-based medical consultations at a distance. Reviews technical challenges in the areas of quality of service, security, reliability, and access, and looks at the potential utility of the next generation of online technologies. Discusses ways health care organizations can use the Internet to support their strategic interests and explores barriers to a broader deployment of the Internet. Recommends steps that private and public sector entities can take to enhance the capabilities of the Internet for health purposes and to prepare health care organizations to adopt new Internet-based applications.

Fundamentals and Applications

2021 International Conference on Cyber Security Intelligence and Analytics (CSIA2021), Volume 1

Risk Assessment for Pharmaceutical and Environmental Chemicals
Molecular Docking for Computer-Aided Drug Design
Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences

Process Systems Engineering for Pharmaceutical Manufacturing: From Product Design to Enterprise-Wide Decisions, Volume 41, covers the following process systems engineering methods and tools for the modernization of the pharmaceutical industry: computer-aided pharmaceutical product design and pharmaceutical production processes design/synthesis; modeling and simulation of the pharmaceutical processing unit operation, integrated flowsheets and applications for design, analysis, risk assessment, sensitivity analysis, optimization, design space identification and control system design; optimal operation, control and monitoring of pharmaceutical production processes; enterprise-wide optimization and supply chain management for pharmaceutical manufacturing processes. Currently, pharmaceutical companies are going through a paradigm shift, from traditional manufacturing mode to modernized mode, built on cutting edge technology and computer-aided methods and tools. Such shifts can benefit tremendously from the

application of methods and tools of process systems engineering. Introduces Process System Engineering (PSE) methods and tools for discovering, developing and deploying greener, safer, cost-effective and efficient pharmaceutical production processes Includes a wide spectrum of case studies where different PSE tools and methods are used to improve various pharmaceutical production processes with distinct final products Examines the future benefits and challenges for applying PSE methods and tools to pharmaceutical manufacturing

This book presents the outcomes of the 2021 International Conference on Cyber Security Intelligence and Analytics (CSIA 2021), an international conference dedicated to promoting novel theoretical and applied research advances in the interdisciplinary field of cyber security, particularly focusing on threat intelligence, analytics, and countering cybercrime. The conference provides a forum for presenting and discussing innovative ideas, cutting-edge research findings and novel techniques, methods and applications on all aspects of cyber security intelligence and analytics. Due to COVID-19, Authors, Keynote Speakers and PC committees will attend the conference online.

The molecular modeling perspective in drug design. (N. Calude Cohen).

Molecular graphics and modeling: tools of the trade. (Roderick E. Hubbard). Molecular modeling of small molecules. (Tamara Gund). Computer assisted new lead design. (Akiko Itai, Miho Yamada Mizutani, Yoshihiko Nishibata, and Nubuo Tomioka). Experimental techniques and data banks. (John P. Priestle and C. Gregory Paris). Computer-assisted drug discovery. (Peter Gund, Gerald Maggiora, and James P. Snyder). Modeling drug-receptor interactions. (Konrad F. Koehler, Shashidhar N. Rao, and James P. Snyder). Glossary of terminology. (J. P. Tollenaere).

Useful Statistical Approaches for Addressing Multiplicity IssuesIncludes practical examples from recent trials Bringing together leading statisticians, scientists, and clinicians from the pharmaceutical industry, academia, and regulatory agencies, Multiple Testing Problems in Pharmaceutical Statistics explores the rapidly growing area of multiple c

Occupational Outlook Handbook

Bayesian Methods in Pharmaceutical Research

Dosage Form Design Parameters

Process Systems Engineering for Pharmaceutical Manufacturing

Practical and Clinical Applications

Computer-Aided Drug Design

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

Computer Applications in Pharmaceutical Research and DevelopmentJohn Wiley & Sons

Research and development in the pharmaceutical industry is a time-consuming and expensive process, making it difficult for newly developed drugs to be formulated into commercially available products. Both formulation and process development can be optimized by means of statistically organized experiments, artificial intelligence and other computational methods. Simultaneous development and investigation of pharmaceutical products and processes enables application of quality by design concept that is being promoted by the regulatory authorities worldwide. Computer-aided applications in pharmaceutical technology covers the fundamentals of experimental design application and

interpretation in pharmaceutical technology, chemometric methods with emphasis of their application in process control, neural computing (artificial neural networks, fuzzy logic and decision trees, evolutionary computing and genetic algorithms, self-organizing maps), computer-aided biopharmaceutical characterization as well as application of computational fluid dynamics in pharmaceutical technology. All of these techniques are essential tools for successful building of quality into pharmaceutical products and processes from the early stage of their development to selection of the optimal ones. In addition to theoretical aspects of various methods, the book provides numerous examples of their application in the field of pharmaceutical technology. A comprehensive review of the current state of the art on various computer aided applications in pharmaceutical technology Case studies are presented in order to facilitate understanding of various concepts in computer-aided applications

The implementation of cloud technologies in healthcare is paving the way to more effective patient care and management for medical professionals around the world. As more facilities start to integrate cloud computing into their healthcare systems, it is imperative to examine the emergent trends and innovations in the field. Cloud Computing Systems and Applications in Healthcare features innovative research on the impact that cloud technology has on patient care, disease management, and the

efficiency of various medical systems. Highlighting the challenges and difficulties in implementing cloud technology into the healthcare field, this publication is a critical reference source for academicians, technology designers, engineers, professionals, analysts, and graduate students.

A Global Perspective

Artificial Intelligence for Drug Development, Precision Medicine, and Healthcare

An Industrial IoT Approach for Pharmaceutical Industry Growth

Theory, Methods, Challenges, and Applications

Biostatistics and Computer Applications

An Overview of System Manufacturers' Hardware and Software

Research and development in the pharmaceutical industry is a time-consuming and expensive process, making it difficult for newly developed drugs to be formulated into commercially available products. Both formulation and process development can be optimized by means of statistically organized experiments, artificial intelligence and other computational methods. Simultaneous development and investigation of pharmaceutical products and processes enables application of quality by design concept that is being promoted by the regulatory authorities

worldwide. Computer-aided applications in pharmaceutical technology covers the fundamentals of experimental design application and interpretation in pharmaceutical technology, chemometric methods with emphasis of their application in process control, neural computing. It explains how applications are used at various stages. 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. This is essential reading for IT professionals and scientists in the pharmaceutical industry as well as researchers involved in informatics. The book's cross-functional, all-phases approach provides a unique opportunity for a holistic analysis and assessment of computer applications in pharmaceutics. Artificial Neural Network for Drug Design, Delivery and Disposition provides an in-depth look at the use of artificial neural networks (ANN) in pharmaceutical research. With its ability to learn and self-correct in a highly complex environment, this predictive tool has tremendous potential to help researchers more effectively design, develop, and deliver

successful drugs. This book illustrates how to use ANN methodologies and models with the intent to treat diseases like breast cancer, cardiac disease, and more. It contains the latest cutting-edge research, an analysis of the benefits of ANN, and relevant industry examples. As such, this book is an essential resource for academic and industry researchers across the pharmaceutical and biomedical sciences. Written by leading academic and industry scientists who have contributed significantly to the field and are at the forefront of artificial neural network (ANN) research Focuses on ANN in drug design, discovery and delivery, as well as adopted methodologies and their applications to the treatment of various diseases and disorders Chapters cover important topics across the pharmaceutical process, such as ANN in structure-based drug design and the application of ANN in modern drug discovery Presents the future potential of ANN-based strategies in biomedical image analysis and much more

Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences brings together two very important fields in pharmaceutical sciences that have been mostly seen as diverging

from each other: chemoinformatics and bioinformatics. As developing drugs is an expensive and lengthy process, technology can improve the cost, efficiency and speed at which new drugs can be discovered and tested. This book presents some of the growing advancements of technology in the field of drug development and how the computational approaches explained here can reduce the financial and experimental burden of the drug discovery process. This book will be useful to pharmaceutical science researchers and students who need basic knowledge of computational techniques relevant to their projects. Bioscientists, bioinformaticians, computational scientists, and other stakeholders from industry and academia will also find this book helpful. Provides practical information on how to choose and use appropriate computational tools Presents the wide, intersecting fields of chemo-bio-informatics in an easily-accessible format Explores the fundamentals of the emerging field of chemoinformatics and bioinformatics

This book provides comprehensive information of the nanotechnology-based pharmaceutical product development including a diverse range of arenas such as liposomes,

nanoparticles, fullerenes, hydrogels, thermally responsive externally activated theranostics (TREAT), hydrogels, microspheres, micro- and nanoemulsions and carbon nanomaterials. It covers the micro- and nanotechnological aspects for pharmaceutical product development with the product development point of view and also covers the industrial aspects, novel technologies, stability studies, validation, safety and toxicity profiles, regulatory perspectives, scale-up technologies and fundamental concept in the development of products. Salient Features: Covers micro- and nanotechnology approaches with current trends with safety and efficacy in product development. Presents an overview of the recent progress of stability testing, reverse engineering, validation and regulatory perspectives as per regulatory requirements. Provides a comprehensive overview of the latest research related to micro- and nanotechnologies including designing, optimisation, validation and scale-up of micro- and nanotechnologies. Is edited by two well-known researchers by contribution of vivid chapters from renowned scientists across the globe in the field of pharmaceutical sciences. Dr. Neelesh Kumar Mehra is working

as an Assistant Professor of Pharmaceutics & Biopharmaceutics at the Department of Pharmaceutics, National Institute of Pharmaceutical Education & Research (NIPER), Hyderabad, India. He received 'TEAM AWARD' for successful commercialisation of an ophthalmic suspension product. He has authored more than 60 peer-reviewed publications in highly reputed international journals and more than 10 book chapter contributions. He has filed patents on manufacturing process and composition to improved therapeutic efficacy for topical delivery. He guided PhD and MS students for their dissertations/research projects. He has received numerous outstanding awards including Young Scientist Award and Team Award for his research output. He recently published one edited book, 'Dendrimers in Nanomedicine: Concept, Theory and Regulatory Perspectives', in CRC Press. Currently, he is editing books on nano drug delivery-based products with Elsevier Pvt Ltd. He has rich research and teaching experience in the formulation and development of complex, innovative ophthalmic and injectable biopharmaceutical products including micro- and nanotechnologies for regulated market. Dr. Arvind Gulbake is working as an Assistant Professor at the Faculty of

Pharmacy, School of Pharmaceutical & Population Health Informatics, at DIT University, Dehradun, India. He has authored more than 40 peer-reviewed publications in highly reputed international journals, four book chapters and a patent contribution. He has received outstanding awards including Young Scientist Award and BRG Travel Award for his research. He is an assistant editor for IJAP. He guided PhD and MS students for their dissertations/research projects. He has successfully completed extramural project funded by SERB, New Delhi, Government of India. He has more than 12 years of research and teaching experience in the formulation and development of nanopharmaceuticals.

Cyber Security Intelligence and Analytics

Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment

Fundamentals, Techniques, Resources and Applications

Computer Applications in Pharmaceutical Science

Regulatory Aspects of Gene Therapy and Cell Therapy Products

Drug Repurposing

In Silico Drug Discovery and Design: Theory, Methods,

Challenges, and Applications provides a comprehensive, unified, and in-depth overview of the current methodological strategies in computer-aided drug discovery and design. Its main aims are to introduce the theoretical framework and algorithms, discuss the range of validity, strengths and limita

Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment describes the historical evolution of quantitative structure-activity relationship (QSAR) approaches and their fundamental principles. This book includes clear, introductory coverage of the statistical methods applied in QSAR and new QSAR techniques, such as HQSAR and G-QSAR. Containing real-world examples that illustrate important methodologies, this book identifies QSAR as a valuable tool for many different applications, including drug discovery, predictive toxicology and risk assessment. Written in a straightforward and engaging manner, this is the ideal resource for all those looking for general and practical knowledge of QSAR

methods. Includes numerous practical examples related to QSAR methods and applications Follows the Organization for Economic Co-operation and Development principles for QSAR model development Discusses related techniques such as structure-based design and the combination of structure- and ligand-based design tools

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.

The highly experienced authors here present readers with step-wise, detail-conscious information to develop quality pharmaceuticals. The book is made up of carefully crafted sections introducing key concepts and advances in the areas of dissolution, BA/BE, BCS, IVIC, and product quality. It provides a specific focus on the integration of regulatory considerations and includes case histories highlighting the biopharmaceutics strategies adopted in development of successful drugs.

Volume 2

Hypothesis, Molecular Aspects and Therapeutic Applications

Multiple Testing Problems in Pharmaceutical Statistics

Pharmaceutical Data Mining

Biopharmaceutics Applications in Drug Development

Cloud Computing Systems and Applications in Healthcare

Pharmaceutical product development is a multidisciplinary activity involving extensive efforts in systematic product development and optimization in compliance with regulatory authorities to ensure the quality, efficacy and safety of resulting products. Pharmaceutical Product Development equips the pharmaceutical formulation scientist with extensive and up-to-date knowledge of drug product development and covers all steps from the beginning of product conception to the final packaged form that enters the market and lifecycle management thereof. Applications of core scientific principles for product development are also thoroughly discussed in conjunction with the latest approaches involving design of experiment and quality by design with comprehensive illustrations based on practical case studies of several dosage forms. The book presents pharmaceutical product development information in an easy-to-read mode with simplified theories, case studies and guidelines for students, academicians and professionals in the pharmaceutical industry. It is an invaluable resource and hands-on guide covering managerial, regulatory and practical aspects of pharmaceutical product lifecycle management.

Leading experts illustrate how sophisticated computational data mining techniques can impact contemporary drug discovery and development In the era

of post-genomic drug development, extracting and applying knowledge from chemical, biological, and clinical data is one of the greatest challenges facing the pharmaceutical industry. Pharmaceutical Data Mining brings together contributions from leading academic and industrial scientists, who address both the implementation of new data mining technologies and application issues in the industry. This accessible, comprehensive collection discusses important theoretical and practical aspects of pharmaceutical data mining, focusing on diverse approaches for drug discovery–including chemogenomics, toxicogenomics, and individual drug response prediction. The five main sections of this volume cover: A general overview of the discipline, from its foundations to contemporary industrial applications Chemoinformatics-based applications Bioinformatics-based applications Data mining methods in clinical development Data mining algorithms, technologies, and software tools, with emphasis on advanced algorithms and software that are currently used in the industry or represent promising approaches In one concentrated reference, Pharmaceutical Data Mining reveals the role and possibilities of these sophisticated techniques in contemporary drug discovery and development. It is ideal for graduate-level courses covering pharmaceutical science, computational chemistry, and bioinformatics. In addition, it provides insight to pharmaceutical scientists,

principal investigators, principal scientists, research directors, and all scientists working in the field of drug discovery and development and associated industries. A comprehensive analysis of state-of-the-art molecular modeling approaches and strategies applied to risk assessment for pharmaceutical and environmental chemicals This unique volume describes how the interaction of molecules with toxicologically relevant targets can be predicted using computer-based tools utilizing X-ray crystal structures or homology, receptor, pharmacophore, and quantitative structure activity relationship (QSAR) models of human proteins. It covers the in vitro models used, newer technologies, and regulatory aspects. The book offers a complete systems perspective to risk assessment prediction, discussing experimental and computational approaches in detail, with: * An introduction to toxicology methods and an explanation of computational methods * In-depth reviews of QSAR methods applied to enzymes, transporters, nuclear receptors, and ion channels * Sections on applying computers to toxicology assessment in the pharmaceutical industry and in the environmental arena * Chapters written by leading international experts * Figures that illustrate computational models and references for further information This is a key resource for toxicologists and scientists in the pharmaceutical industry and environmental sciences as well as researchers involved in ADMET, drug

discovery, and technology and software development.

This book discusses the different regulatory pathways for gene therapy (GT) and cell therapy (CT) medicinal products implemented by national and international bodies throughout the world (e.g. North and South America, Europe, and Asia). Each chapter, authored by experts from various regulatory bodies throughout the international community, walks the reader through the applications of nonclinical research to translational clinical research to licensure for these innovative products. More specifically, each chapter offers insights into fundamental considerations that are essential for developers of CT and GT products, in the areas of product manufacturing, pharmacology and toxicology, and clinical trial design, as well as pertinent "must-know" guidelines and regulations. Regulatory Aspects of Gene Therapy and Cell Therapy Products: A Global Perspective is part of the American Society of Gene and Cell Therapy sub-series of the highly successful Advances in Experimental Medicine and Biology series. It is essential reading for graduate students, clinicians, and researchers interested in gene and cell therapy and the regulation of pharmaceuticals.

Pharmaceutical Product Development

Artificial Intelligence in Drug Discovery

Artificial Intelligence

Computer Applications in Pharmaceutical Research and Development
Networking Health
Pharmaceutical Statistics

Health Sciences & Professions

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.

Manufacturers of Computerized Equipment for the Pharmaceutical Industry Present Descriptions of Mini- & Microcomputers, Peripheral Hardware, & Software Products

Suitable for Pharmaceutical Research Labs, Production Plants & Office Facilities; Utilization of the Equipment for Process Control, Etc.

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

Computer-Aided Applications in Pharmaceutical Technology

Computer Applications in Pharmaceutical Research and Development. Wiley Series in Drug Discovery and Development

Unique Aspects of Anti-cancer Drug Development

In Silico Drug Discovery and Design

Biochemistry for the Pharmaceutical Sciences

Research and Development in the Pharmaceutical Industry (A CBO Study)

Dosage Form Design Parameters, Volume II, examines the history and current state of the field within the pharmaceutical sciences, presenting key developments. Content includes drug development issues,

the scale up of formulations, regulatory issues, intellectual property, solid state properties and polymorphism. Written by experts in the field, this volume in the Advances in Pharmaceutical Product Development and Research series deepens our understanding of dosage form design parameters. Chapters delve into a particular aspect of this fundamental field, covering principles, methodologies and the technologies employed by pharmaceutical scientists. In addition, the book contains a comprehensive examination suitable for researchers and advanced students working in pharmaceuticals, cosmetics, biotechnology and related industries. Examines the history and recent developments in drug dosage forms for pharmaceutical sciences Focuses on physicochemical aspects, prefomulation solid state properties and polymorphism Contains extensive references for further discovery and learning that are appropriate for advanced undergraduates, graduate students and those interested in drug dosage design

Artificial Intelligence for Drug Development, Precision Medicine, and Healthcare covers exciting developments at the intersection of computer science and statistics. While much of machine-learning is statistics-based, achievements in deep learning for image and language processing rely on computer science's use of big data. Aimed at those with a statistical background who want to use their strengths in pursuing AI research, the book: · Covers broad AI topics in drug

development, precision medicine, and healthcare. · Elaborates on supervised, unsupervised, reinforcement, and evolutionary learning methods. · Introduces the similarity principle and related AI methods for both big and small data problems. · Offers a balance of statistical and algorithm-based approaches to AI. · Provides examples and real-world applications with hands-on R code. · Suggests the path forward for AI in medicine and artificial general intelligence. As well as covering the history of AI and the innovative ideas, methodologies and software implementation of the field, the book offers a comprehensive review of AI applications in medical sciences. In addition, readers will benefit from hands on exercises, with included R code.

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

New Advances

Applications of Computer-aided Drug Discovery in Pharmaceutical Research

Guidebook on Molecular Modeling in Drug Design

Drug Discovery and Development
Approaches and Applications for Drug Discovery
Prescriptions for the Internet

An Industrial IoT Approach for Pharmaceutical Industry Growth, Volume Two uses an innovative approach to explore how the Internet of Things (IoT) and big data can improve approaches and make discoveries. Rapid growth of the IoT has encouraged many companies in the manufacturing sector to make use of this technology to unlock its potential. Using clear language and real-world case studies, this book discusses systems level from both a human-factors point-of-view and the perspective of networking, databases, privacy and anti-spoofing. The wide variety in topics presented offers multiple perspectives on how to integrate the Internet of Things into pharmaceutical manufacturing. This book represents a useful resource for researchers in pharmaceutical sciences, information and communication technologies, and those who specialize in healthcare and pharmacovigilance. Emphasizes efficiency in pharmaceutical manufacturing through an IoT/Big Data approach Explores cutting-edge technologies through sensor enabled environments in the pharmaceutical industry Discusses system levels from both a human-factors point-of-view and the perspective of networking, databases, privacy and anti-spoofing

Since the early 2000s, there has been increasing interest within the pharmaceutical industry in the application of Bayesian methods at various stages of the research, development, manufacturing, and health economic evaluation of new health care interventions. In 2010, the first Applied Bayesian Biostatistics conference was held, with the primary objective to stimulate the practical implementation of Bayesian statistics, and to promote the added-value for accelerating the discovery and the delivery of new cures to patients. This book is a synthesis of the conferences and debates, providing an overview of Bayesian methods applied to nearly all stages of research and development, from early discovery to portfolio management. It highlights the value associated with sharing a vision with the regulatory authorities, academia, and pharmaceutical industry, with a view to setting up a common strategy for the appropriate use of Bayesian statistics for the benefit of patients. The book covers: Theory, methods, applications, and computing Bayesian biostatistics for clinical innovative designs Adding value with Real World Evidence Opportunities for rare, orphan diseases, and pediatric development Applied Bayesian biostatistics in manufacturing Decision making and Portfolio management Regulatory perspective and public health policies Statisticians and data scientists involved in the research, development, and approval of new cures will be inspired by the possible applications of Bayesian methods covered in the book.

The methods, applications, and computational guidance will enable the reader to apply Bayesian methods in their own pharmaceutical research. Emmanuel Lesaffre is Professor of Biostatistics at KU Leuven, Belgium. Gianluca Baio is Professor of Statistics and Health Economics at University College London, UK. Bruno Boulanger is Chief Scientific Officer at PharmaLex, Belgium.

Drug repurposing or drug repositioning is a new approach to presenting new indications for common commercial and clinically approved existing drugs. For example, chloroquine, an old antimalarial drug, showed promising results for treating COVID-19, interfering with MDR in several types of cancer, and chemosensitizing human leukemic cells.This book focuses on the hypothesis, risk/benefits, and economic impacts of drug repurposing on drug discovery in dermatology, infectious diseases, neurological disorders, cancer, and orphan diseases. It brings together up-to-date research to provide readers with an informative, illustrative, and easy-to-read book useful for students, clinicians, and the pharmaceutical industry.

The Aster Guide to Computer Applications in the Pharmaceutical Industry

Insights Into Pharmaceutical Processes, Management and Regulatory Affairs

Artificial Neural Network for Drug Design, Delivery and Disposition

Micro- and Nanotechnologies-Based Product Development

Computer Applications in Drug Discovery and Development
Computational Toxicology