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Molecular Descriptors for Chemoinformatics - Roberto Todeschini 2009-10-30
The number-one reference on the topic now contains a wealth of new data: The entire relevant literature over the past six years has been painstakingly surveyed, resulting in hundreds of new descriptors being added to the list, and some 3,000 new references in the bibliography section. Volume 1 contains an alphabetical listing of more than 3300 descriptors and related terms for chemoinformatic analysis of chemical compound properties, while the second volume lists over 6,000 references selected from 450 journals. To make the data even more accessible, the introductory section has been completely re-written and now contains several "walk-through" reading lists of selected keywords for novice users.
Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences - Navneet Sharma 2021-05-21
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
Quantum Nanochemistry, Volume Five - Mihai V. Putz 2016-04-27
Volume 5 of the 5-volume Quantum Nanochemistry focuses on modeling and predicting of the enzyme kinetics and quantitative structure-activity relationships. It reveals the quantum implications to bio-organic and bio-inorganic systems, to enzyme kinetics, and to pharmacophore binding sites of chemical-biological interaction of molecules through cell

membranes in targeting specific bindings modeled by celebrated QSARs (Quantitative Structure-Activity Relationships) here reshaped as Qu-SAR (Quantum Structure-Activity Relationships).

De novo Molecular Design - Gisbert Schneider 2013-10-10

Systematically examining current methods and strategies, this ready reference covers a wide range of molecular structures, from organic-chemical drugs to peptides, Proteins and nucleic acids, in line with emerging new drug classes derived from biomacromolecules. A leader in the field and one of the pioneers of this young discipline has assembled here the most prominent experts from across the world to provide first-hand knowledge. While most of their methods and examples come from the area of pharmaceutical discovery and development, the approaches are equally applicable for chemical probes and diagnostics, pesticides, and any other molecule designed to interact with a biological system. Numerous images and screenshots illustrate the many examples and method descriptions. With its broad and balanced coverage, this will be the firststop resource not only for medicinal chemists, biochemists and biotechnologists, but equally for bioinformaticians and molecular designers for many years to come. From the content: * Reaction-driven de novo design * Adaptive methods in molecular design * Design of ligands against multitarget profiles * Free energy methods in ligand design * Fragment-based de novo design * Automated design of focused and target family-oriented compound libraries * Molecular de novo design by nature-inspired computing * 3D QSAR approaches to de novo drug design * Bioisosteres in de novo design * De novo design of peptides, proteins and nucleic acid structures, including RNA aptamers and many more.

Risk Assessment of Chemicals: An Introduction - C.J. van Leeuwen 2012-12-06

In recent years many developments have taken place in promote co-operation between governments and other the field of risk assessment of chemicals. Many reports parties involved in chemical safety and to provide policy have been published by national authorities, industries guidance with emphasis on regional and subregional co and scientific researchers as well as by international bod operation. The Inter-Organization Programme for the ies such as the European Union, the Organization of Sound Management of Chemicals (IOMC) was estab Economic Cooperation and Development (OECD) and lished in 1995 and provides a mechanism for the six par the joint International Programme on Chemical Safety ticipating organizations (UNEP, ILO, FAO, UNIDO,WHO (IPCS) of the World Health Organization (WHO), the and OECD) to better co-ordinate policies and activities in International Labour Organization (lLO), and the United the field of chemical risk management. Nations Environment Programme (UNEP). The present book is an introduction to risk assessment of The development and international harmonization of risk chemicals. It contains basic background information on assessment methods is an important challenge. In sources, emissions, distribution and fate processes for Agenda 21 of the United Nations Conference on exposure estimation. It includes dose-effects estimation Environment and Development (UNCED), chapter 19 is for both human health related toxicology and ecotoxicol entirely devoted to the management of chemicals. For ogy as well as information on estimation methodologies. one of its recommendations, i. e.

New Frontiers in Nanochemistry: Concepts, Theories, and Trends - Mihai V. Putz 2020-05-11

The final volume of this new innovative and informative three-volume set explains and explores the essential basic and advanced concepts from various areas within the nanosciences. This volume primarily focuses on increasing awareness of sustainable nanochemistry, meaning the social and economic impact of nanochemistry, in order to mitigate ecological resource depletion and to promote the exploration of nature as a resource for future benefits. This volume adopts a pharmacological lens, examining the multitude of ways in which nano-research can contribute to the development of pharmaceutical drugs and paying particular attention to toxicology and renewable energy within nanochemistry. Under the vast expertise of the editor, the volume contains 34 entries contributed by renowned

international scientists and scholars. The content in this volume covers topics such as anti-HIV agents, ecotoxicology, solar cells and photovoltaic phenomena, spectral-SAR, and more—alphabetically organized and accompanied by equations, figures, and brief letters in order to emphasize the potential applications of the concepts discussed.

QSAR, Rational Approaches to the Design of Bioactive Compounds - C. Silipo 1991

Quantitative structure-activity relationships constitute a subject which has seen enormous growth in the past decade. Techniques which have been developed and used widely outside of medicinal chemistry are now used by those working with QSAR. These techniques employ powerful computers, molecular graphics systems and sophisticated software. Although QSAR techniques have been developed to optimize activities of known sets of analogs, recent methodologies suggest that these techniques can be useful in the modeling of new chemical entities. The contributions in this state-of-the-art volume cover a wide range of disciplines, tools and ideas which will be of interest to medicinal chemists, pharmacologists and biologists. The book gives an update of progress in the science of the quantitative approaches of the interface between chemistry, physical chemistry and biology-pharmacology. The use of molecular graphics, computational and conformational methods in drug research is extensively covered.

Concepts and Experimental Protocols of Modelling and Informatics in Drug Design - Om Silakari 2020-11-05

Concepts and Experimental Protocols of Modelling and Informatics in Drug Design discusses each experimental protocol utilized in the field of bioinformatics, focusing especially on computer modeling for drug development. It helps the user in understanding the field of computer-aided molecular modeling (CAMM) by presenting solved exercises and examples. The book discusses topics such as fundamentals of molecular modeling, QSAR model generation, protein databases and how to use them to select and analyze protein structure, and pharmacophore modeling for drug targets. Additionally, it discusses data retrieval system, molecular surfaces, and freeware and online servers. The book is a valuable source for graduate students and researchers on bioinformatics, molecular modeling, biotechnology and several members of biomedical field who need to understand more about computer-aided molecular modeling. Presents exercises with solutions to aid readers in validating their own protocol Brings a thorough interpretation of results of each exercise to help readers compare them to their own study Explains each parameter utilized in the algorithms to help readers understand and manipulate various features of molecules and target protein to design their study

Mass Spectrometry in Medicinal Chemistry - Klaus Wanner 2007-06-27

This first overview of mass spectrometry-based pharmaceutical analysis is the key to improved high-throughput drug screening, rational drug design and analysis of multiple ligand-target interactions. The ready reference opens with a general introduction to the use of mass spectrometry in pharmaceutical screening, followed by a detailed description of recently developed analytical systems for use in the pharmaceutical laboratory. Applications range from simple binding assays to complex screens of biological activity and systems containing multiple targets or ligands -- all highly relevant techniques in the early stages in drug discovery, from target characterization to hit and lead finding.

QSAR and Strategies in the Design of Bioactive Compounds - Joachim Karl Seydel 1985

QSAR - Hugo Kubinyi 2008-07-11

Finding the new remedy for a certain disease: an inspired goal. QSAR, an invaluable tool in drug design, aids scientists to attain this aim. This book is a long-awaited comprehensive text to QSAR and related approaches. It provides a practice-oriented introduction to the theory, methods and analyses for QSAR relationships, including modelling-based and 3D approaches. Hugo Kubinyi is a leading expert in QSAR. Readers will benefit from the author's 20 years of practical experience, from his careful calculations and recalculations of thousands of QSAR equations. Among the topics covered are: - physiocochemical parameters - quantitative models - statistical methods - Hansch analysis - Free Wilson analysis - 3D-QSAR approaches The

book can readily be used as a textbook due to its high didactic value and numerous examples (over 200 equations and 1100 references).

Quantitative Modeling in Toxicology - Kannan Krishnan 2010-04-01

Governments around the world are passing laws requiring industry to assess the toxicity of the chemicals and products they produce, but to do so while reducing, refining, or even replacing testing on animals. To meet these requirements, experimental toxicologists and risk assessors are adopting quantitative approaches and computer simulations to study the biological fate and effects of chemicals and drugs. In Quantitative Modeling in Toxicology leading experts outline the current state of knowledge on the modeling of dose, tissue interactions and tissue responses. Each chapter describes the mathematical foundation, parameter estimation, challenges and perspectives for development, along with the presentation of a modeling template. Additionally, tools and approaches for conducting uncertainty, sensitivity and variability analyses in these models are described. Topics covered include: the quantitative models of pharmacokinetics of individual chemicals and mixtures models for toxicant-target tissue interaction. models for cellular, organ, and organism responses. approaches, tools and challenges for model application and evaluation A website containing computer codes accompanies the book to help the reader reconstruct the models described and discussed in the various chapters. Quantitative Modeling in Toxicology serves as an essential reference source and tool box for risk assessors and researchers and students in toxicology, public health, pharmacology, and human toxicology interested in developing quantitative models for a better understanding of dose-response relationships.

Drug Design Strategies - Lee Banting 2012-01-04

This book documents the latest research into the theory and application of force-fields, semi-empirical molecular orbital, density functional and ab initio calculations, Quantum Mechanical (QM) based modelling, Atoms in Molecules (AIM) approach, and biomolecular dynamics. It also covers theory and application of 2D cheminformatics, QSAR/QSPR, ADME properties of drugs, drug docking/scoring protocols and approaches, topological methodology, and modelling accurate inhibition constants of enzymes. Finally, the book gives the theory and applications of multiscale modelling of proteins and biomolecular systems. The information need for a book in this area is due to the continuing rapid advance of firstly theoretical approaches, secondly software/hardware and lastly the successful application of the technology and this book fills a gap in the literature. The co-editors have extensive experience of teaching and researching in the field and the book includes contributions from cutting-edge academic and industrial researchers in their respective fields. It is essential reading for medicinal chemists, computational chemists and those in the pharmaceutical industry.

Chemometric Methods in Molecular Design - Han van de Waterbeemd 2008-07-11

The statistical analysis of experimental and theoretical data lies at the heart of modern drug design. This practice-oriented handbook is a comprehensive account of modern chemometric methods in molecular design. It presents strategies for making more rational choices in the planning of syntheses, and describes techniques for analyzing biological and chemical data. Written by the world's experts, it provides in-depth information on * molecular concepts * experimental design in the planning of syntheses * multivariate analysis of chemical and biological data * statistical validation of QSAR results An additional benefit: the book contains a critical survey of commercially available software packages both for statistical analysis as well as for special applications. Industrial and academic researches in medicinal chemistry and organic chemistry will value this book as a useful source of information for their daily work. Also available: Advanced Computer-Assisted Techniques in Drug Discovery, edited by H. van de Waterbeemd

Molecular Interaction Fields - Gabriele Cruciani 2006-05-12

This unique reference source, edited by the world's most respected expert on molecular interaction field software, covers all relevant principles of the GRID force field and its applications in medicinal chemistry. Entire chapters on 3D-QSAR, pharmacophore searches,

docking studies, metabolism predictions and protein selectivity studies, among others, offer a concise overview of this emerging field. As an added bonus, this handbook includes a CD-ROM with the latest commercial versions of the GRID program and related software.

Modelling the Toxicity of Nanoparticles - Lang Tran 2017-02-06

In today's nanotechnology and pharmaceutical research, alternative toxicology testing methods are crucial for ethically and commercially sound practice. This book provides practical guidelines on how to develop and validate quantitative nanostructure-toxicity relationship (QNTR) models, which are ideal for rapidly exploring the effects of a large number of variables in complex scenarios. Through contributions by academic, industrial, and governmental experts, Modelling the Toxicity of Nanoparticles delivers clear instruction on these methods and their integration and use in risk assessment. Specific topics include the physico-chemical characteristics of engineered nanoparticles, nanoparticle interactions, in vivo nanoparticle processing, and more. A much-needed practical guide, Modelling the Toxicity of Nanoparticles is a key text for researchers as well as government and industry regulators.

Rational Approaches to Structure, Activity, and Ecotoxicology of Agrochemicals - Wilfried Draber 1992-07-14

This book presents discussions of the most important aspects in the development of agrochemicals. The book covers such broad areas as structure activity and ecotoxicological analyses in comprehensive reviews for general methods and chronicles for individual examples. Topics in structure-activity relationships include how to combine submolecular structures of pharmacological interests and modify them according to chemorational models with computer-aided procedures such as the traditional Hansch-type QSAR, the sequential, simplex optimization, and molecular modeling. Topics in the ecotoxicology of organo phosphorus compounds are discussed in terms of the quantitative structure-toxicity relationship (QSTR). Chronicles of molecular orbital methodology in predicting environmental fates of agrochemicals are also provided. This volume will be invaluable for researchers in the agrochemical and pharmaceutical industries.

Innovations and Implementations of Computer Aided Drug Discovery Strategies in Rational Drug Design - Sanjeev Kumar Singh 2021-02-02

This book presents various computer-aided drug discovery methods for the design and development of ligand and structure-based drug molecules. A wide variety of computational approaches are now being used in various stages of drug discovery and development, as well as in clinical studies. Yet, despite the rapid advances in computer software and hardware, combined with the exponential growth in the available biological information, there are many challenges that still need to be addressed, as this book shows. In turn, it shares valuable insights into receptor-ligand interactions in connection with various biological functions and human diseases. The book discusses a wide range of phylogenetic methods and highlights the applications of Molecular Dynamics Simulation in the drug discovery process. It also explores the application of quantum mechanics in order to provide better accuracy when calculating protein-ligand binding interactions and predicting binding affinities. In closing, the book provides illustrative descriptions of major challenges associated with computer-aided drug discovery for the development of therapeutic drugs. Given its scope, it offers a valuable asset for life sciences researchers, medicinal chemists and bioinformaticians looking for the latest information on computer-aided methodologies for drug development, together with their applications in drug discovery.

Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment - Roy, Kunal 2015-02-28

Quantitative structure-activity relationships (QSARs) represent predictive models derived from the application of statistical tools correlating biological activity or other properties of chemicals with descriptors representative of molecular structure and/or property. Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment discusses recent advancements in the field of QSARs with special reference to their application in drug development, predictive

toxicology, and chemical risk analysis. Focusing on emerging research in the field, this book is an ideal reference source for industry professionals, students, and academicians in the fields of medicinal chemistry and toxicology.

Applied Case Studies and Solutions in Molecular Docking-Based Drug Design - Dastmalchi, Siavoush 2016-05-11

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.

Medicinal Chemistry and Drug Design - Deniz Ekinci 2012-05-16

Over the recent years, medicinal chemistry has become responsible for explaining interactions of chemical molecules processes such that many scientists in the life sciences from agronomy to medicine are engaged in medicinal research. This book contains an overview focusing on the research area of enzyme inhibitors, molecular aspects of drug metabolism, organic synthesis, prodrug synthesis, in silico studies and chemical compounds used in relevant approaches. The book deals with basic issues and some of the recent developments in medicinal chemistry and drug design. Particular emphasis is devoted to both theoretical and experimental aspect of modern drug design. The primary target audience for the book includes students, researchers, biologists, chemists, chemical engineers and professionals who are interested in associated areas. The textbook is written by international scientists with expertise in chemistry, protein biochemistry, enzymology, molecular biology and genetics many of which are active in biochemical and biomedical research. We hope that the textbook will enhance the knowledge of scientists in the complexities of some medicinal approaches; it will stimulate both professionals and students to dedicate part of their future research in understanding relevant mechanisms and applications of medicinal chemistry and drug design.

Drug Design Strategies - Lee Banting 2012

This book, aimed at academics, industrialists and post-graduates, documents the latest research into computer aided drug design.

Drug Design Strategies - David J. Livingstone 2011

Shows how different parts of the drug discovery process have developed, with particular emphasis on quantitative aspects and possible future progress.

Computational Drug Design - D. C. Young 2009-01-28

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.

Catalyst Design for Tailor-Made Polyolefins - M. Terano 1994-11-01

Recent development of olefin polymerization catalysts has caused marked changes in both industrial and academic research. Industrial use of homogeneous metallocene catalysts has already begun in the fields of high density polyethylene and syndiotactic polypropylene. Moreover, important data have been obtained from academic investigations which have proved useful for understanding conventional heterogeneous Ziegler-Natta catalysts. From the industrial viewpoint, however, heterogeneous high-yield catalysts seem to be more important. The present volume contains invited lectures and contributed papers. The following topics are covered: (1) Heterogeneous Catalysts, (2) Metallocene Catalysts and (3) New Trends in the Polyolefin Industry.

Computational Toxicology - Sean Ekins 2007-06-30

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.

Reviews in Computational Chemistry - Kenny B. Lipkowitz 2003-05-08

Computational chemistry is increasingly used in most areas ofmolecular science including organic, inorganic, medicinal,biological, physical, and analytical chemistry. Researchers inthese fields who do molecular modelling need to understand and staycurrent with recent developments. This volume, like those prior toit, features chapters by experts in various fields of computationalchemistry. Two chapters focus on molecular docking, one of whichrelates to drug discovery and cheminformatics and the other toproteomics. In addition, this volume contains tutorials onspin-orbit coupling and cellular automata modeling, as well as anextensive bibliography of computational chemistry books. FROM REVIEWS OF THE SERIES "Reviews in Computational Chemistryremains the most valuable reference to methods and techniques incomputational chemistry."—JOURNAL OF MOLECULAR GRAPHICS ANDMODELLING "One cannot generally do better than to try to find anappropriate article in the highly successful Reviews inComputational Chemistry. The basic philosophy of the editors seemsto be to help the authors produce chapters that are complete,accurate, clear, and accessible to experimentalists (in particular)and other nonspecialists (in general)."—JOURNAL OF THEAMERICAN CHEMICAL SOCIETY

Combinatorial Library Design and Evaluation - Arup Ghose 2001-06-26

This text traces developments in rational drug discovery and combinatorial library design with contributions from 50 leading scientists in academia and industry who offer coverage of basic principles, design strategies, methodologies, software tools and algorithms, and applications. It outlines the fundamentals of pharmacophore modelling and 3D Quantitative

Structure-Activity Relationships (QSAR), classical QSAR, and target protein structure-based design methods.

Chemoinformatics in Drug Discovery - Tudor I. Oprea 2006-03-06

This handbook provides the first-ever inside view of today's integrated approach to rational drug design. Chemoinformatics experts from large pharmaceutical companies, as well as from chemoinformatics service providers and from academia demonstrate what can be achieved today by harnessing the power of computational methods for the drug discovery process. With the user rather than the developer of chemoinformatics software in mind, this book describes the successful application of computational tools to real-life problems and presents solution strategies to commonly encountered problems. It shows how almost every step of the drug discovery pipeline can be optimized and accelerated by using chemoinformatics tools -- from the management of compound databases to targeted combinatorial synthesis, virtual screening and efficient hit-to-lead transition. An invaluable resource for drug developers and medicinal chemists in academia and industry.

Reviews in Computational Chemistry - Kenny B. Lipkowitz 2009-09-22

This book is an account of current developments in computational chemistry, a new multidisciplinary area of research. Experts in computational chemistry, the editors use and develop techniques for computer-assisted molecular design. The core of the text itself deals with techniques for computer-assisted molecular design. The book is suitable for both beginners and experts. In addition, protocols and software for molecular recognition and the relationship between structure and biological activity of drug molecules are discussed in detail. Each chapter includes a mini-tutorial, as well as discussion of advanced topics. Special Feature: The appendix to this book contains an extensive list of available software for molecular modeling.

Reviews in Computational Chemistry - Kenny B. Lipkowitz 2009-09-22

From reviews of the series: 'Many of the articles are indeed accessible to any interested nonspecialist, even without theoretical background.' Journal of the American Chemical Society '...an invaluable resource for the serious molecular modeler.' Chemical Design Automation News

Fundamentals Of Aquatic Toxicology - Gary M. Rand 1995-10-05

This text is divided into three parts. The first part describes basic toxicological concepts and methodologies used in aquatic toxicity testing, including the philosophies underlying testing strategies now required to meet and support regulatory standards. The second part of the book discusses various factors that affect transport, transformation, ultimate distribution, and accumulation of chemicals in the aquatic environment, along with the use of modelling to predict fate.; The final section of the book reviews types of effects or endpoints evaluated in field studies and the use of structure-activity relationships in aquatic toxicology to predict biological activity and physio-chemical properties of a chemical. This section also contains an extensive background of environmental legislation in the USA and within the European Community, and an introduction to hazard/risk assessment with case studies.

Recent Advances in QSAR Studies - Tomasz Puzyn 2010-01-19

This book presents an interdisciplinary overview on the most recent advances in QSAR studies. The first part consists of a comprehensive review of QSAR methodology. The second part highlights the interdisciplinary aspects and new areas of QSAR modelling.

3D QSAR in Drug Design - Hugo Kubinyi 2006-04-11

Significant progress has been made in the study of three-dimensional quantitative structure-activity relationships (3D QSAR) since the first publication by Richard Cramer in 1988 and the first volume in the series. 3D QSAR in Drug Design. Theory, Methods and Applications, published in 1993. The aim of that early book was to contribute to the understanding and the further application of CoMFA and related approaches and to facilitate the appropriate use of these methods. Since then, hundreds of papers have appeared using the quickly developing techniques of both 3D QSAR and computational sciences to study a broad variety of biological problems. Again the editor(s) felt

that the time had come to solicit reviews on published and new viewpoints to document the state of the art of 3D QSAR in its broadest definition and to provide visions of where new techniques will emerge or new appli- tions may be found. The intention is not only to highlight new ideas but also to show the shortcomings, inaccuracies, and abuses of the methods. We hope this book will enable others to separate trivial from visionary approaches and me-too methodology from in- vative techniques. These concerns guided our choice of contributors. To our delight, our call for papers elicited a great many manuscripts.

Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment - Kunal Roy 2015-03-03

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

Multi-Target Drug Design Using Chem-Bioinformatic Approaches - Kunal Roy 2019-02-04

This detailed book showcases recent advances in computational design of multi-target drug candidates involving various ligand and structure-based strategies. Different chem-bioinformatic modeling strategies that can be applied for design of multi-target drugs as well as important databases and web servers in connection with multi-target drug design are also featured in this collection. Written for the Methods in Pharmacology and Toxicology series, chapters include the kind of key implementation advice that will aid researchers greatly in their laboratory pursuits. Authoritative and practical, Multi-Target Drug Design Using Chem-Bioinformatic Approaches seeks to aid all scientists working in the field of drug discovery research.

Structure—Activity Relationships in Environmental Sciences - M. Nendza 2012-12-06

Structure-Activity Relationships in Environmental Science is the first book of its kind that brings together information from a variety of sources into one document. It provides a comprehensive overview of the entire field of quantitative structure-activity relationships (QSARs) as well as being a reference for SAR experts. The book comprises three parts. Part One covers the theoretical background of structure-activity studies and Part Two deals with the practical applications of such methods in the environmental sciences. Part Three critically discusses SAR models with respect to their reliability and their aptness in environmental hazard and risk assessment. Recommendations are made as to which model to use and the case is presented for using QSARs in hazard assessment. The use of QSARs is becoming increasingly important since there is little experimental data available on environmentally relevant chemicals. Structure-Activity Relationships in Environmental Sciences will thus serve as an invaluable guide to both postgraduate and research scientists as well as professional ecologists.

Smith and Williams' Introduction to the Principles of Drug Design and Action - H. Jphn Smith 2005-10-10

Advances in knowledge and technology have revolutionized the process of drug development, making it possible to design drugs for a given target or disease. Building on the foundation laid by the previous three editions, Smith and Williams Introduction to the Principles of Drug Design and Action, Fourth Edition includes the latest informatio

Handbook of Ecotoxicology, Second Edition - David J. Hoffman 2002-11-13

Handbook of Ecotoxicology, Second Edition focuses on toxic substances and how they affect ecosystems worldwide. It presents methods for quantifying and measuring ecotoxicological effects in the field and in the lab, as well as methods for estimating, predicting, and modeling in ecotoxicology studies. Completely revised and updated with 18 new chapters, this second edition includes contributions from over 75 international experts. Also, a Technical Review Board reviewed all manuscripts for accuracy and currency. This authoritative work is the definitive reference for students, researchers, consultants, and other professionals in the environmental sciences, toxicology, chemistry, biology, and ecology - in academia, industry, and government.

Oncology: Breakthroughs in Research and Practice - Management Association, Information Resources 2016-06-29

Advancements in cancer diagnosis and treatment have extended the lives of many patients facing numerous types of cancer over the years. Research on best practices, new drug development, early identification, and treatment continues to advance with the ultimate goal of uncovering a cure for cancer in all its forms. Oncology: Breakthroughs in Research and Practice features international perspectives on cancer identification, treatment, and management methodologies in addition to patient considerations and outlooks for the future. This collection of emerging research provides valuable insight for researchers, graduate-level students, and professionals in the medical field.