Molecular Descriptors For Chemoinformatics Volume 41 2 Volume Set Methods And Principles In Medicinal Chemistry

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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.

Innovations in Biomedical Engineering - Ewaryst Tkacz 2019-08-14
This book presents the proceedings of the “Innovations in Biomedical Engineering IBE’2018” Conference held in Katowice, Poland from October 18 to 20, 2018, and discusses recent research on innovations in biomedical engineering. The book covers a broad range of subjects related to biomedical engineering innovations. Divided into four parts, it presents state-of-the-art advances in: Engineering of biomaterials, Modelling and simulations in biomechanics, Informatics in medicine, and Signal analysis. By doing so, it helps bridge the gap between technological and methodological engineering achievements on the one hand and clinical requirements in the three major areas diagnosis, therapy and rehabilitation on the other.

Advances in Chromatography - Nelu Grinberg 2017-08-15
For more than five decades, scientists and researchers have relied on the Advances in Chromatography series for the most up-to-date information on a wide range of developments in chromatographic methods and applications. For Volume 54, the series editors have invited established, well-known chemists to offer cutting-edge reviews of chromatographic methods applied in the life sciences that emphasize the underlying principle of separation science. The clear presentation of topics and vivid illustrations for which this series has become known makes the material accessible and engaging to analytical, biochemical, organic, polymer, and pharmaceutical chemists at all levels of technical skill.

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.

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.

New Developments in Medicinal Chemistry - Carlton Anthony Taft 2014-10-10
This e-book series is recommended for readers who are interested in or work with current theoretical and experimental research in medicinal chemistry, with an emphasis on computer aided-drug design and organic synthesis for therapeutic purposes. The e-book series encompasses the multidisciplinary field of medicinal chemistry which overlaps the knowledge of chemistry, physics, biochemistry, biology and pharmacology. The second volume of the series contains the following topics: -Current State-of-the-Art for Virtual Screening and Docking Methods -Estimating Protein-Ligand Binding Affinity by NMR -ADME/Tox Predictions in Drug Design -Bioisosteric Replacements in Drug Design

Mathematical Chemistry and Chemoinformatics - Adalbert Kerber 2013-12-12
More than 20 years of experience in molecular structure generation, from conceptualization through to applications Innovative, interdisciplinary text demonstrating example queries with software packages such as MOLGEN-online Detailed explanations on establishing QSPRs and QSARs as well as structure elucidation using mass spectrometry and structure generation. Aims and Scope This work provides an introduction to mathematical modeling of molecules and the resulting applications (structure generation,

structure elucidation, QSAR/QSPR etc.). Most chemists have experimented with some software that represents molecules in an electronic form, and such models and applications are of increasing interest in diverse and growing fields such as drug discovery, environmental science and metabolomics. Furthermore, structure generation remains the only way to systematically create molecules that are not (yet) present in a database. This book starts with the mathematical theory behind representing molecules, explaining chemical concepts in mathematical terms and providing exercises that can be completed online. The later chapters cover applications of the theory, with detailed explanations on QSPR and QSAR investigations and finally structure elucidation combining mass spectrometry and structure generation. This book is aimed in particular at the users of structure generation methods and corresponding techniques, but also for those interested in teaching and learning mathematical chemistry, and for software designers in chemoinformatics.

Cheminformatics and its Applications - Amalia Stefaniu 2020-07-15

Cheminformatics has emerged as an applied branch of Chemistry that involves multidisciplinary knowledge, connecting related fields such as chemistry, computer science, biology, pharmacology, physics, and mathematical statistics.The book is organized in two sections, including multiple aspects related to advances in the development of informatic tools and their specific use in compound structure databases with various applications in life sciences, mainly in medicinal chemistry, for identification and development of new therapeutically active molecules. The book covers aspects related to genomic analysis, semantic similarity, chemometrics, pattern recognition techniques, chemical reactivity prediction, drug-likeness assessment, bioavailability, biological target recognition, machine-based drug discovery and design. Results from various computational tools and methods are discussed in the context of new compound design and development, sharing promising opportunities, and perspectives.

Chemoinformatics - Thomas Engel 2018-05-18

This essential guide to the knowledge and tools in the field includes everything from the basic concepts to modern methods, while also forming a bridge to bioinformatics. The textbook offers a very clear and didactical structure, starting from the basics and the theory, before going on to provide an overview of the methods. Learning is now even easier thanks to exercises at the end of each section or chapter. Software tools are explained in detail, so that the students not only learn the necessary theoretical background, but also how to use the different software packages available. The wide range of applications is presented in the corresponding book Applied Chemoinformatics - Achievements and Future Opportunities (ISBN 9783527342013). For Master and PhD students in chemistry, biochemistry and computer science, as well as providing an excellent introduction for other newcomers to the field.

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

Advances in Mathematical Chemistry and Applications: - Subhash C. Basak 2016-02-11

Advances in Mathematical Chemistry and Applications highlights the recent progress in the emerging discipline of discrete mathematical chemistry. Editors Subhash C. Basak, Guillermo Restrepo, and Jose Luis Villaveces have brought together 27 chapters written by 68 internationally renowned experts in these two volumes. Each volume comprises a wise integration of mathematical and chemical concepts and covers numerous applications in the field of drug discovery, bioinformatics, chemoinformatics, computational biology, mathematical proteomics, and ecotoxicology. Volume 2 explores deeper the topics introduced in Volume 1, with numerous additional topics such as topological approaches for classifying fullerene isomers; chemical reaction networks; discrimination of small molecules using topological molecular descriptors; GRANCH methods for the mathematical characterization of DNA, RNA and protein sequences; linear regression methods and Bayesian techniques; in silico toxicity prediction methods; drug design; integration of bioinformatics and systems biology, molecular docking, and molecular dynamics; metalloenzyme models; protein folding models; molecular periodicity; generalized topologies and their applications; and many more. Brings together both the theoretical and practical aspects of the fundamental concepts of mathematical chemistry Covers applications in diverse areas of physics, chemistry, drug discovery, predictive toxicology, systems biology, chemoinformatics, and bioinformatics About half of the book focuses primarily on current work, new applications, and emerging approaches for the mathematical characterization of essential aspects of molecular structure, while the other half describes applications of structural approach to new drug discovery, virtual screening, protein folding, predictive toxicology, DNA structure, and systems biology

Drug Discovery - Varaprasad Bobbarala PhD 2018-09-19

The book "Drug Discovery - Concepts to Market" is a collection of reviewed and relevant research chapters, offering a comprehensive overview of recent developments in the latest drug discovery trends that have been revolutionized with up-to-date technological developments. This book comprises single chapters authored by various researchers and edited by an expert active in the drug development research area. All chapters are independently complete but united under a common research study topic. This publication aims to provide a thorough overview of the latest research efforts in this field from international authors and open new possible research paths for further novel developments.

Chemoinformatics - Thomas Engel 2018-12-10

This essential guide to the knowledge and tools in the field includes everything from the basic concepts to modern methods, while also forming a bridge to bioinformatics. The textbook offers a very clear and didactical structure, starting from the basics and the theory, before going on to provide an overview of the methods. Learning is now even easier thanks to exercises at the end of each section or chapter. Software tools are explained in detail, so that the students not only learn the necessary theoretical background, but also how to use the different software packages available. The

wide range of applications is presented in the corresponding book Applied Chemoinformatics - Achievements and Future Opportunities (ISBN 9783527342013). For Master and PhD students in chemistry, biochemistry and computer science, as well as providing an excellent introduction for other newcomers to the field.

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).

The Practice of Medicinal Chemistry - Camille Georges Wermuth 2011-05-02

The Practice of Medicinal Chemistry fills a gap in the list of available medicinal chemistry literature. It is a single-volume source on the practical aspects of medicinal chemistry. Considered ""the Bible"" by medicinal chemists, the book emphasizes the methods that chemists use to conduct their research and design new drug entities. It serves as a practical handbook about the drug discovery process, from conception of the molecules to drug production. The first part of the book covers the background of the subject matter, which includes the definition and history of medicinal chemistry, the measurement of biological activities, and the main phases of drug activity. The second part of the book presents the road to discovering a new lead compound and creating a working hypothesis. The main parts of the book discuss the optimization of the lead compound in terms of potency, selectivity, and safety. The Practice of Medicinal Chemistry can be considered a ""first-read"" or ""bedside book"" for readers who are embarking on a career in medicinal chemistry. NEW TO THIS EDITION: * Focus on chemoinformatics and drug discovery * Enhanced pedagogical features * New chapters including: - Drug absorption and transport - Multi-target drugs * Updates on hot new areas: NEW! Drug discovery and the latest techniques NEW! How potential drugs can move through the drug discovery/ development phases more quickly NEW! Chemoinformatics

Topological Indices and Related Descriptors in QSAR and QSPR - James Devillers 2000-03-09

Topological Indices and Related Descriptors in QSAR and QSPR reviews the state of the art in this field and highlights the important advances in the generation of descriptors calculated directly from the structure of molecules. This long-awaited comprehensive book provides all the necessary information to calculate and use these descriptors for deriving structure-activity and structure-property relationships. Written by leading experts in the field, this book discusses the physicochemical significance, strengths, and weaknesses of these indices and presents numerous examples of applications. This book will be a valuable reference for anyone involved in the use of QSAR and QSPR in the pharmaceutical, applied chemical, and environmental sciences. It is also suitable for use as a supplementary textbook on related graduate level courses.

The British National Bibliography - British Library. Bibliographic Services Division 1950

Practical Chemoinformatics - Muthukumarasamy Karthikeyan 2014-05-06

Chemoinformatics is equipped to impact our life in a big way mainly in the fields of chemical, medical and material sciences. This book is a product of several years of experience and passion for the subject written in a simple lucid style to attract the interest of the student community who wish to master chemoinformatics as a career. The topics chosen cover the entire spectrum of chemoinformatics activities (methods, data and tools). The algorithms, open source databases, tutorials supporting theory using standard datasets, guidelines, questions and do it yourself exercises will make it valuable to the academic research community. At the same time every chapter devotes a section on development of new software tools relevant for the growing pharmaceutical, fine chemicals and life sciences industry. The book is intended to assist beginners to hone their skills and also constitute an interesting reading for the experts.

Drug Discovery and Development - Vishwanath Gaitonde 2020-03-11

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.

Handbook of Chemoinformatics Algorithms - Jean-Loup Faulon 2010-04-21

Unlike in the related area of bioinformatics, few books currently exist that document the techniques, tools, and algorithms of chemoinformatics. Bringing together worldwide experts in the field, the Handbook of Chemoinformatics Algorithms provides an overview of the most common chemoinformatics algorithms in a single source.After a historical persp

Natural Compounds as Drugs, Volume I - Frank Petersen 2007-12-27

In a real tour de force of pharmacological literature, this edited volume’s chapters highlight the biodiversity-driven approaches which are now of eminent importance in natural products research. It addresses the question why natural products display such complex chemical information, what makes them unique, as they often are, and what their characteristics are. Practical questions such as supply of natural substances and production optimization strategies are also covered.

Medicinal Chemistry - Thomas Nogrady 2005-08-11

Fully updated and rewritten by a basic scientist who is also a practicing physician, the third edition of this popular textbook remains comprehensive, authoritative and readable. Taking a receptor-based, target-centered approach, it presents the concepts central to the study of drug action in a logical, mechanistic way grounded on molecular and principles. Students of pharmacy, chemistry and pharmacology, as well as researchers interested in a better understanding of drug design, will find this book an invaluable resource. Starting with an overview of basic principles, Medicinal Chemistry examines the properties of drug molecules, the characteristics of drug receptors, and the nature of drug-receptor interactions. Then it systematically examines the various families of receptors involved in human disease and drug design. The first three classes of receptors are related to endogenous molecules:

neurotransmitters, hormones and immunomodulators. Next, receptors associated with cellular organelles (mitochondria, cell nucleus), endogenous macromolecules (membrane proteins, cytoplasmic enzymes) and pathogens (viruses, bacteria) are examined. Through this evaluation of receptors, all the main types of human disease and all major categories of drugs are considered. There have been many changes in the third edition, including a new chapter on the immune system. Because of their increasingly prominent role in drug discovery, molecular modeling techniques, high throughput screening, neuropharmacology and genetics/genomics are given much more attention. The chapter on hormonal therapies has been thoroughly updated and re-organized. Emerging enzyme targets in drug design (e.g. kinases, caspases) are discussed, and recent information on voltage-gated and ligand-gated ion channels has been incorporated. The sections on antihypertensive, antiviral, antibacterial, anti-inflammatory, antiarrhythmic, and anticancer drugs, as well as treatments for hyperlipidemia and peptic ulcer, have been substantially expanded. One new feature will enhance the book's appeal to all readers: clinical-molecular interface sections that facilitate understanding of the treatment of human disease at a molecular level.

Chemoinformatics - Johann Gasteiger 2006-12-13

This first work to be devoted entirely to this increasingly important field, the "Textbook" provides both an in-depth and comprehensive overview of this exciting new area. Edited by Johann Gasteiger and Thomas Engel, the book provides an introduction to the representation of molecular structures and reactions, data types and databases/data sources, search methods, methods for data analysis as well as such applications as structure elucidation, reaction simulation, synthesis planning and drug design. A "hands-on" approach with step-by-step tutorials and detailed descriptions of software tools and Internet resources allows easy access for newcomers, advanced users and lecturers alike. For a more detailed presentation, users are referred to the "Handbook of Chemoinformatics", which will be published separately. Johann Gasteiger is the recipient of the 1991 Gmelin-Beilstein Medal of the German Chemical Society for Achievements in Computer Chemistry, and the Herman Skolnik Award of the Division of Chemical Information of the American Chemical Society (ACS) in 1997. Thomas Engel joined the research group headed by Johann Gasteiger at the University of Erlangen-Nuremberg and is a specialist in chemoinformatics.

Solubility in Pharmaceutical Chemistry - Christoph Saal 2019-12-16

This book describes the physicochemical fundamentals and biomedical principles of drug solubility. Methods to study and predict solubility in silico and in vitro are described and the role of solubility in a medicinal chemistry and pharmaceutical industry context are discussed. Approaches to modify and control solubility of a drug during the manufacturing process and of the pharmaceutical product are essential practical aspects of this book.

Encyclopedia of Complexity and Systems Science - 2009-06-26

This encyclopedia provides an authoritative single source for understanding and applying the concepts of complexity theory together with the tools and measures for analyzing complex systems in all fields of science and engineering. It links fundamental concepts of mathematics and computational sciences to applications in the physical sciences, engineering, biomedicine, economics and the social sciences.

Molecular Descriptors for Chemoinformatics, 2 Volume Set - Roberto Todeschini 2009-08-17

Molecular Descriptors for Chemoinformatics As every chemist knows, there is a direct (if complex) relationship between the molecular structure of a compound and its chemical behavior. Predicting such behavior is possible by an abstract representation of its structure in terms of chemical similarity parameters, socalled ‘descriptors’. These are most useful in predicting the pharmacological properties of drug candidates, but are also used in predicting reactivity, toxicity and other important chemical characteristics. The number-one reference on the topic now contains a wealth of new data: The entire relevant literature over the past eight years has been pain-stakingly 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 around 3300 terms for the chemoinformatic analysis of chemical compound properties, while the second volume contains 6343 references selected from 450 journals with about 7000 authors quoted covering the period from the beginning of molecular descriptor research until the year 2008. In this second edition, several sections have been completely rewritten and organized in a more effective way. The greatly expanded introductory section now contains several “walk-through” reading lists of selected keywords to make the data even more accessible for novice users.

Comprehensive Medicinal Chemistry II, Volume 4 - Jonathan S Mason 2007

This e-book comprises 8 volumes, with all chapter sections available as PDF or HTML, and includes bibliographical references and index.

Big Data in Predictive Toxicology - Andrea-Nicole Richarz 2019-12-10

The rate at which toxicological data is generated is continually becoming more rapid and the volume of data generated is growing dramatically. This is due in part to advances in software solutions and cheminformatics approaches which increase the availability of open data from chemical, biological and toxicological and high throughput screening resources. However, the amplified pace and capacity of data generation achieved by these novel techniques presents challenges for organising and analysing data output. Big Data in Predictive Toxicology discusses these challenges as well as the opportunities of new techniques encountered in data science. It addresses the nature of toxicological big data, their storage, analysis and interpretation. It also details how these data can be applied in toxicity prediction, modelling and risk assessment. This title is of particular relevance to researchers and postgraduates working and studying in the fields of computational methods, applied and physical chemistry, cheminformatics, biological sciences, predictive toxicology and safety and hazard assessment.

Chemometrics and Chemoinformatics - Barry K. Lavine 2005-11-24

Chemometrics and Chemoinformatics will provide chemists and other scientists with the fundamental knowledge on chemometrics coupled with chemoinformatics.

Handbook of Computational Chemistry -

Handbook of Chemoinformatics - Johann Gasteiger 2003

"The new discipline of chemoinformatics covers the application of computer-assisted methods to chemical problems such as information storage and retrieval, the prediction of physical, chemical or biological properties of compounds, spectra simulation, structure elucidation, reaction modeling, synthesis planning and drug design. ... this four-volume Handbook contains in-depth contributions from top authors from around the world, with the content organized into chapters dealing with the representation of molecular structures and reactions, data types and databases/data sources, search methods, methods for data analysis as well as applications"--Back cover.

Predictive Toxicology - Christoph Helma 2005-03-17
A comprehensive overview of techniques and systems currently utilized in predictive toxicology, this reference presents an in-depth survey of strategies to characterize chemical structures and biological systems—covering prediction methods and algorithms, sources of high-quality toxicity data, the most important commercial and noncommercial predictive toxicology programs, and advanced technologies in computational chemistry and biology, statistics, and data mining.
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.
Mass Spectrometry in Medicinal Chemistry - Klaus Wanner 2007-04-09
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.
Lead Generation Approaches in Drug Discovery - Zoran Rankovic 2010-04-07
An integrated overview of modern approaches to lead discovery Lead generation is increasingly seen as a distinct and success-determining phase of the drug discovery process. Over recent years, there have been major advances in the understanding of what constitutes a good lead compound and how to improve the chances of finding such a compound. Written by leading scientists and established opinion leaders from industry and academia, this book provides an authoritative overview of the field, as well as the theory, practice, and scope, of the principal Lead Generation Approaches in Drug Discovery, including: The evolution of the lead discovery process, key concepts, current challenges, and future directions Strategies and technologies driving the high-throughput screening (HTS) approach to lead discovery, including the shifting paradigms in the design of compound collections and best practice in the hit confirmation process Knowledge-based in silico or "virtual" screening Theory and practice of the fragment-based approach to lead discovery The opportunities and challenges presented by multi-target drug discovery (MTDD) De novo design of lead compounds and new approaches to estimating the synthetic accessibility of de novo–designed molecules The impact of natural products on drug discovery, and potential of natural product–like compounds for exploring regions of biologically relevant chemical space Using early screening of hits and leads for metabolic, pharmacokinetic, and toxicological liabilities to reduce attrition during the later phases of drug discovery The utility of parallel synthesis and purification in lead discovery With each topic supported by numerous case studies, this is indispensable reading for researchers in industry and academia who wish to keep up to date with the latest strategies and approaches in drug discovery.
An Introduction to Chemoinformatics - Andrew R. Leach 2007-09-04
This book aims to provide an introduction to the major techniques of chemoinformatics. It is the first text written specifically for this field. The first part of the book deals with the representation of 2D and 3D molecular structures, the calculation of molecular descriptors and the construction of mathematical models. The second part describes other important topics including molecular similarity and diversity, the analysis of large data sets, virtual screening, and library design. Simple illustrative examples are used throughout to illustrate key concepts, supplemented with case studies from the literature.
The Data Analysis Handbook - I.E. Frank 1994-09-30
Analyzing observed or measured data is an important step in applied sciences. The recent increase in computer capacity has resulted in a revolution both in data collection and data analysis. An increasing number of scientists, researchers and students are venturing into statistical data analysis; hence the need for more guidance in this field, which was previously dominated mainly by statisticians. This handbook fills the gap in the range of textbooks on data analysis. Written in a dictionary format, it will serve as a comprehensive reference book in a rapidly growing field. However, this book is more structured than an ordinary dictionary, where each entry is a separate, self-contained entity. The authors provide not only definitions and short descriptions, but also offer an overview of the different topics. Therefore, the handbook can also be used as a companion to textbooks for undergraduate or graduate courses. 1700 entries are given in alphabetical order grouped into 20 topics and each topic is organized in a hierarchical fashion. Additional specific entries on a topic can be easily found by following the cross-references in a top-down manner. Several figures and tables are provided to enhance the comprehension of the topics and a list of acronyms helps to locate the full terminologies. The bibliography offers suggestions for further reading.
Handbook of Molecular Descriptors - Roberto Todeschini 2008-07-11
Quantitative studies on structure-activity and structure-property relationships are powerful tools in directed drug research. In recent years, various strategies have been developed to characterize and classify structural patterns by means of molecular descriptors. It has become possible not only to assess diversities or similarities of structure databases, but molecular descriptors also facilitate the identification of potential bioactive molecules from the rapidly increasing number of compound libraries. They even allow for a controlled de-novo design of new lead structures. This is the most comprehensive collection of molecular descriptors and presents a detailed review from the origins of this research field up to present day. This practically oriented reference book gives a thorough overview of the different molecular descriptors representations and their corresponding molecular descriptors. All descriptors are listed with their definition, symbols and labels, formulas, some numerical examples, data and molecular graphs, while numerous figures and tables aid comprehension of the definitions. Cross-references throughout, a list of acronyms and notations allow easy access to the information needed to solve a specific research problem. Examples of descriptor calculations along with tables of descriptor values for a set of selected reference compounds and an up-to-date reference list add to the practical value of the book, making it an invaluable guide for all those dealing with bioactive molecules as well as for researchers.
Chemical Drug Design - Girish Kumar Gupta 2016-10-10
Chemical Drug Design provides a compact overview on recent advances in this rapidly developing field. With contributions on in silico drug design, natural product based compounds, as well as on ligand- and structure-

based approaches, the authors present innovative methods and techniques for identifying and synthetically designing novel drugs.

Artificial Intelligence in Drug Design - Alexander Heifetz 2021-11-04

This volume looks at applications of artificial intelligence (AI), machine learning (ML), and deep learning (DL) in drug design. The chapters in this book describe how AI/ML/DL approaches can be applied to accelerate and revolutionize traditional drug design approaches such as: structure- and ligand-based, augmented and multi-objective de novo drug design, SAR and big data analysis, prediction of binding/activity, ADMET, pharmacokinetics and drug-target residence time, precision medicine and selection of favorable chemical synthetic routes. How broadly are these approaches applied and where do they maximally impact productivity today and potentially in the near future. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary software and tools, step-by-step, readily reproducible modeling protocols, and tips on troubleshooting and avoiding known pitfalls. Cutting-edge and unique, Artificial Intelligence in Drug Design is a valuable resource for structural and molecular biologists, computational and medicinal chemists, pharmacologists and drug designers.