Molecular Descriptors For Chemoinformatics Volume I Alphabetical Listing Volume Ii Appendices

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.

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.

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

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 completel.

Computational Methods to Support Drug Design

An Introduction to Chemoinformatics

Complex Computational Methods and Collaborative Techniques
Handbook of Bibliometric Indicators

Prodrugs and Targeted Delivery

This handbook and ready reference presents a combination of statistical, information-theoretic, and data analysis methods to meet the challenge of designing empirical models involving molecular descriptors within bioinformatics. The topics range from investigating information processing in chemical and biological networks to studying statistical and information-theoretic techniques for analyzing chemical structures to employing data analysis and machine learning techniques for QSAR/QSPR. The high-profile international author and editor team ensures excellent coverage of the topic, making this a must-have for everyone working in chemoinformatics and structure-oriented drug design.

"This book is a timely compendium of key elements that are crucial for the study of machine learning in chemoinformatics, giving an overview of current research in machine learning and their applications to chemoinformatics tasks"--Provided by publisher.

This thorough book provides a collection of techniques used in the emerging field of computational chemogenomics, which is an integration of chemoinformatics, bioinformatics, computer science, statistics, automated pattern recognition and

modeling, database usage with data retrieval, and systems integration. Beginning with a section on public chemogenomic data resources, the volume continues by delving into the fundamentals of chemoinformatics, bioinformatics, and chemogenomic data processing. After the reader is comfortable with a core skillset, the volume introduces techniques to analyze specific proteins or compound structures and statistical pattern recognition techniques. Later chapters describe the future of chemogenomics including applications to medical care. Written for the highly successful Methods in Molecular Biology series, chapters include the kind of detailed implementation advice that serves as an ideal guide in the lab. Practical and authoritative, Computational Chemogenomics will greatly aid experimental sciences who are novices to data processing and modeling, as well as those with computationally-oriented backgrounds wishing to engage in this scientific area, which is continually growing and expected to contribute to industry, academic, and government research projects.

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.

Chemoinformatics

Molecular Descriptors for Chemoinformatics, 2 Volume Set

Chemokine Receptors as Drug Targets

Molecular Descriptors for Chemoinformatics: Appendices, references

In Silico Medicinal Chemistry

Achievements and Future Opportunities

This volume focuses on computational modeling of the ecotoxicity of chemicals and presents applications of quantitative structure–activity relationship models (QSARs) in the predictive toxicology field in a regulatory context. The extensive book covers a variety of protocols for descriptor computation, data curation, feature selection, learning algorithms, validation of models, applicability domain assessment, confidence estimation for predictions, and much more, as well as case studies and literature reviews on a number of hot topics. Written for the Methods in Pharmacology and Toxicology series, chapters include the kind of practical advice that is essential for researchers everywhere. Authoritative and comprehensive,

Ecotoxicological QSARs is an ideal source to update readers in the field with current practices and introduce to them new developments and should therefore be very useful for researchers in academia, industries, and regulatory bodies.

This topical reference and handbook addresses the chemistry, pharmacology, toxicology and the patentability of prodrugs, perfectly mirroring the integrated approach prevalent in today's drug design. It summarizes current experiences and strategies for the rational design of prodrugs, beginning at the early stages of the development process, as well as discussing organ- and site-selective prodrugs. Every company employing medicinal chemists will be interested in this practice-oriented overview of a key strategy in modern drug discovery and development.

30 tutorials and more than 100 exercises in chemoinformatics, supported by online software and data sets Chemoinformatics is widely used in both academic and industrial chemical and biochemical research worldwide. Yet, until this unique guide, there were no books offering practical exercises in chemoinformatics methods. Tutorials in Chemoinformatics contains more than 100 exercises in 30 tutorials exploring key topics and methods in the field. It takes an applied approach to the subject with a strong emphasis on problem-solving and computational methodologies. Each tutorial is self-contained and contains exercises for students to work through using a variety of software packages. The majority of the tutorials are

divided into three sections devoted to theoretical background, algorithm description and software applications, respectively, with the latter section providing step-by-step software instructions. Throughout, three types of software tools are used: in-house programs developed by the authors, open-source programs and commercial programs which are available for free or at a modest cost to academics. The in-house software and data sets are available on a dedicated companion website. Key topics and methods covered in Tutorials in Chemoinformatics include: Data curation and standardization Development and use of chemical databases Structure encoding by molecular descriptors, text strings and binary fingerprints The design of diverse and focused libraries Chemical data analysis and visualization Structure-property/activity modeling (QSAR/QSPR) Ensemble modeling approaches, including bagging, boosting, stacking and random subspaces 3D pharmacophores modeling and pharmacological profiling using shape analysis Protein-ligand docking Implementation of algorithms in a high-level programming language Tutorials in Chemoinformatics is an ideal supplementary text for advanced undergraduate and graduate courses in chemoinformatics, bioinformatics, computational chemistry, computational biology, medicinal chemistry and biochemistry. It is also a valuable working resource for medicinal chemists, academic researchers and industrial chemists looking to enhance their

chemoinformatics skills.

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 1 includes chapters on mathematical structural descriptors of molecules and biomolecules, applications of partially ordered sets (posets) in chemistry, optimal characterization of molecular complexity using graph theory, different connectivity matrices and their polynomials, use of 2D fingerprints in similarity-based virtual screening, mathematical approaches to molecular structure generation, comparability graphs, applications of molecular topology in drug design, density functional theory of chemical reactivity, application of mathematical descriptors in the quantification of drug-likeness, utility of pharmacophores in drug design, and much 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 Revised 2015 edition includes a new chapter on the current landscape of hierarchical QSAR modelling 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

Chemoinformatics and Advanced Machine Learning Perspectives: Complex Computational Methods and Collaborative Techniques

Similarity Search and Applications

Structure, Function, Substrates

Advances in Mathematical Chemistry and Applications:

Methods and Protocols

Volume I: Alphabetical Listing / Volume II: Appendices, References

"Advances in Mathematical Chemistry and Applications, Volume 1" highlights the emerging discipline of mathematical chemistry, or, more precisely, discrete mathematical chemistry. This Volume is written by internationally renowned experts in the field. It comprises of a wise

integration of mathematical and chemical concepts and covers numerous applications in the field of drug discovery, bioinformatics, chemoinformatics, computational biology and ecological health. The contents of this book include chapters on mathematical structural descriptors of molecules and biomolecules, topological representation of molecular structure, connectivity matrices, use of weighted 2D Fingerprints in similarity-based virtual screening and much more. This ebook is a valuable resource for MSc and PhD students, academic personnel and researchers seeking updated and critically important information on the fundamental concepts of mathematical chemistry and their applications.

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.
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.
A breakthrough guide employing knowledge that unites cheminformatics

and bioinformatics as innovation for the future Bridging the gap between cheminformatics and bioinformatics for the first time, Computational Approaches in Cheminformatics and Bioinformatics provides insight on how to blend these two sciences for progressive research benefits. It describes the development and evolution of these fields, how chemical information may be used for biological relations and vice versa, the implications of these new connections, and foreseeable developments in the future. Using algorithms and domains as workflow tools, this revolutionary text drives bioinformaticians to consider chemical structure, and similarly, encourages cheminformaticians to consider large biological systems such as protein targets and networks. Computational Approaches in Cheminformatics and Bioinformatics covers: Data sources available for modelling and prediction purposes Developments of conventional Quantitative Structure-Activity Relationships (QSAR) Computational tools for manipulating chemical and biological data Novel ways of probing the interactions between small molecules and proteins Also including insight from public (NIH), academic, and industrial sources (Novartis, Pfizer), this book offers expert knowledge to aid scientists through industry and academic study. The invaluable applications for drug discovery, cellular and molecular biology, enzymology, and metabolism make Computational Approaches in

Cheminformatics and Bioinformatics the essential guidebook for evolving drug discovery research and alleviating the issue of chemical control and manipulation of various systems.

Advances in Mathematical Chemistry and Applications

Computational Chemogenomics

Handbook of Chemoinformatics

Transporters as Drug Carriers

The Data Analysis Handbook

Practical Chemoinformatics

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.

This volume explores techniques that are currently used to understand solid target-specific models in computational toxicology. The chapters are divided into four sections and discuss topics such as molecular descriptors, QSAR and read-across; molecular and data modeling techniques to comply with both scientific and regulatory sides; computational toxicology in drug discovery; and strategies on how to predict various human-health toxicology endpoints. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the methods and software tools used, step-by-step, readily reproducible computational protocols, and tips on troubleshooting and avoiding known pitfalls. Comprehensive and cutting-edge, Computational Toxicology: Methods and Protocols is a valuable resource for researchers who are interested in learning more about this expanding field.

Chemical genomics is a highly interdisciplinary and very exciting field of research both in academics and in the life sciences industry. The Ernst Schering Research Foundation Workshop 58 was organized to bring together scientific leaders in the field to discuss the implications of chemical genomics for drug discovery. Various aspects of the interface between chemistry and biology are covered in this volume, such as chemogenomics efforts in the pharmaceutical industry, diversity-oriented synthesis, chemogenomic approaches to the study of cell function, screening technologies, and natural products as tools in chemical biology.

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.

Chemical Genomics

Methods and Applications

Towards Better ADME Properties

Encyclopedia of Physical Organic Chemistry, 6 Volume Set

Ecotoxicological QSARs

From Data to Knowledge

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

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.

Winner of 2018 PROSE Award for MULTIVOLUME REFERENCE/SCIENCE This encyclopedia offers a comprehensive and easy reference to physical organic chemistry (POC) methodology and techniques. It puts POC, a classical and fundamental discipline of chemistry, into the context of modern and dynamic fields like biochemical processes, materials science, and molecular electronics. Covers basic terms and theories into organic reactions and mechanisms, molecular designs and syntheses, tools and experimental techniques, and applications and future directions Includes coverage of green chemistry and polymerization reactions Reviews different strategies for molecular design and synthesis of functional molecules Discusses computational methods, software packages, and more than 34 kinds of spectroscopies and techniques for studying structures and mechanisms Explores applications in areas from biology to materials science The Encyclopedia of Physical Organic Chemistry has won the 2018 PROSE Award for MULTIVOLUME REFERENCE/SCIENCE. The PROSE Awards recognize the best books, journals and digital content produced by professional and

scholarly publishers. Submissions are reviewed by a panel of 18 judges that includes editors, academics, publishers and research librarians who evaluate each work for its contribution to professional and scholarly publishing. You can find out more at: proseawards.com Also available as an online edition for your library, for more details visit Wiley Online Library

Molecular Descriptors for ChemoinformaticsVolume I: Alphabetical Listing / Volume II: Appendices, ReferencesJohn Wiley & Sons

Computational Approaches in Cheminformatics and Bioinformatics

Molecular Descriptors in QSAR/QSPR

Handbook of Chemoinformatics Algorithms

A Textbook

Chemoinformatics Approaches to Structure- and Ligand-Based Drug Design, Volume II

Quantitative Tools for Studying and Evaluating Research

Molecular descriptors are mathematical values that describe the structure or shape of molecules, helping predict the activity and properties of molecules in complex experiments. This book describes the equations known as QSAR (quantitative structure-activity relationships) and QSPR (quantitative structure-property relationships), showing how they can be used productively in a wide range of industries.

Well-recognized pioneers and investigators from diverse professional environments survey the key concepts in the field, describe cutting-edge methods, and provide exemplary

pharmaceutical applications. The authors explain the theory behind the crucial concepts of molecular similarity and diversity, describe the challenging efforts to use chemoinformatics approaches to virtual and high-throughput screening, and illuminate the latest developments in multidimensional QSAR analysis. Other topics of interest include the use of partitioning algorithms and classification methods for analyzing large compound databases, screening sets, and virtual screening for active molecules; different approaches to target class-specific library design; and the generation of a novel class of molecular surface properties descriptors that can be readily calculated from 2D representations of molecular structures. Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery illuminates the conceptual and methodological diversity of this rapidly evolving field and offers instructive examples of cutting-edge applications in the drug discovery process. Understand the key concepts and novel methods behind chemoinformatics See cutting-edge chemoinformatic methods applied to the drug discovery process Appreciate the conceptual and methodological diversity of chemoinformatics Master the basics of machine learning, library design, and ADME modeling.

This is the first book to focus on the topological index, the Harary index, of a graph, including its mathematical properties, chemical applications and some related and attractive open problems. This book is dedicated to Professor Frank Harary (1921—2005), the grandmaster of graph theory and its applications. It has be written by experts in the field of

graph theory and its applications. For a connected graph G, as an important distance-based topological index, the Harary index H(G) is defined as the sum of the reciprocals of the distance between any two unordered vertices of the graph G. In this book, the authors report on the newest results on the Harary index of a graph. These results mainly concern external graphs with respect to the Harary index; the relations to other topological indices; its properties and applications to pure graph theory and chemical graph theory; and two significant variants, i.e., additively and multiplicatively weighted Harary indices. In the last chapter, we present a number of open problems related to the Harary index. As such, the book will not only be of interest to graph researchers, but to mathematical chemists as well. At last, the first systematic guide to the growing jungle of citation indices and other bibliometric indicators. Written with the aim of providing a complete and unbiased overview of all available statistical measures for scientific productivity, the core of this reference is an alphabetical dictionary of indices and other algorithms used to evaluate the importance and impact of researchers and their institutions. In 150 major articles, the authors describe all indices in strictly mathematical terms without passing judgement on their relative merit. From widely used measures, such as the journal impact factor or the h-index, to highly specialized indices, all indicators currently in use in the sciences and humanities are described, and their application explained. The introductory section and the appendix contain a wealth of valuable supporting information on data sources, tools and techniques for bibliometric and

scientometric analysis - for individual researchers as well as their funders and publishers.
Pharmacokinetics and Metabolism in Drug Design
Handbook of Molecular Descriptors
Chemoinformatics in Drug Discovery
Tutorials in Chemoinformatics
Applied Chemoinformatics
Concepts, Methods, and Tools for Drug Discovery

This book constitutes the refereed proceedings of the 10th International Conference on Similarity Search and Applications, SISAP 2017, held in Munich, Germany, in October 2017. The 23 full papers presented were carefully reviewed and selected from 53 submissions. The papers deal with issues surrounding the theory, design, analysis, practice, and application of content-based and feature-based similarity search. They are organized in the following topical sections: approximate similarity search; improving similarity search methods and applications; distances for complex objects; outlier detection; indexing and applications; and applications and specific domains. The paper 'A New Perspective on the Tree Edit Distance' is published open access under a CC BY 4.0 license at link.springer.com.

Chemokines are hormone-like signaling molecules secreted by cells to signal infection and guide the immune response. Following a decade of basic chemokine research, the pharmaceutical industry has now begun to exploit this crucial signaling pathway for the development of innovative drugs against AIDS, cancer, neural and autoimmune diseases. Here is

the first reference focusing on these novel drug development opportunities. Opening with a general introduction on chemokine function and chemokine receptor biology, the second part covers the known implications of these signaling molecules in human diseases, such as cancer, neural disorders, and viral infection, including AIDS. The third part systematically surveys current drug development efforts at targeting individual chemokine receptors, as well as other chemokine interaction partners, including up-to-date reports from the pharmaceutical industry.
This reference handbook is the first to provide a comprehensive overview, systematically characterizing all known transporters involved in drug elimination and resistance. Combining recent knowledge on all known classes of drug carriers, from microbes to man, it begins with a look at human and mammalian transporters. This is followed by microbial, fungal and parasitic transporters with special attention given to transport across those physiological barriers relevant for drug uptake, distribution and excretion. As a result, this key resource lays the foundations for understanding and investigating the molecular mechanisms for multidrug resistance in cancer cells, microbial resistance to antibiotics and pharmacokinetics in general. For anyone working with antibiotics and cancer chemotherapeutics, as well as being of prime interest to biochemists and biophysicists.
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.

The Harary Index of a Graph

Molecular Descriptors for Chemoinformatics

Chemometrics and Chemoinformatics

Basic Concepts and Methods

10th International Conference, SISAP 2017, Munich, Germany, October 4-6, 2017, Proceedings

Computational Toxicology

"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.

In this new edition of a bestseller, all the contents have been brought upto-date by addressing current standards and best practices in the assessment and prediction of ADMET properties. Although the previous chapter layout has been retained, substantial revisions have been made, with new topics such as pro-drugs, active metabolites and transporters covered in detail in a manner useful to the Drug Discovery scientist. The authors discuss the parameters and processes important for the absorption, distribution and retention of drug compounds in the body, plus the potential problems created by their transformation into toxic byproducts. While aimed at all those dealing professionally with the development and application of pharmaceutical substances, the readily comprehensible style makes this book equally suitable for students of pharmacy and related subjects. Uniquely comprehensive, the book relates physicochemistry and chemical structure to pharmacokinetic properties and ultimately drug efficacy

and safety.

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

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.

Statistical Modelling of Molecular Descriptors in QSAR/QSPR

Small Molecule Probes to Study Cellular Function

Recent Advances in QSAR Studies

Cheminformatics and its Applications