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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.

Covering computational tools in drug design using techniques from chemoinformatics, molecular modelling and computational chemistry, this book explores these methodologies and applications of in silico medicinal chemistry. The first part of the book covers molecular representation methods in computing in terms of chemical structure, together with guides on common structure file formats. The second part examines commonly used classes of molecular descriptors. The third part provides a guide to statistical learning methods using chemical structure data, covering topics such as similarity searching, clustering and diversity selection, virtual library design, ligand docking and de novo design. The final part of the book summarises the application of methods to the different stages of drug discovery, from target ID, through hit finding and hit-to-lead, to lead optimisation. This book is a practical introduction to the subject for researchers new to the fields of chemoinformatics, molecular modelling and computational chemistry.

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 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.

"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.

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.

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.

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.