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Advanced Methods and Applications in Chemoinformatics

Research Progress and New Applications



Eduardo A. Castro & A.K. Haghi

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such as data analytics wireless networks mobile clouds and machine learning this publication meets the research needs of data analysts IT professionals researchers graduate students and educators in the areas of data science computer programming and IT development

Pharmaceutical Sciences: Breakthroughs in Research and Practice

Management Association, Information Resources, 2016-12-28 The delivery of optimal pharmaceutical services to patients is a pivotal concern in the healthcare field By examining current trends and techniques in the industry processes can be maintained and improved Pharmaceutical Sciences Breakthroughs in Research and Practice provides comprehensive coverage of the latest innovations and advancements for pharmaceutical applications Focusing on emerging drug development techniques and drug delivery for improved health outcomes this book is ideally designed for medical professionals pharmacists researchers academics and upper level students within the growing pharmaceutical industry

Applications of Density Functional Theory to Biological and Bioinorganic Chemistry Mihai V. Putz, D Michael P Mingos, 2013-02-01 The series Structure and Bonding publishes critical reviews on topics of research concerned with chemical structure and bonding The scope of the series spans the entire Periodic Table and addresses structure and bonding issues associated with all of the elements It also focuses attention on new and developing areas of modern structural and theoretical chemistry such as nanostructures molecular electronics designed molecular solids surfaces metal clusters and supramolecular structures Physical and spectroscopic techniques used to determine examine and model structures fall within the purview of Structure and Bonding to the extent that the focus is on the scientific results obtained and not on specialist information concerning the techniques themselves Issues associated with the development of bonding models and generalizations that illuminate the reactivity pathways and rates of chemical processes are also relevant The individual volumes in the series are thematic. The goal of each volume is to give the reader whether at a university or in industry a comprehensive overview of an area where new insights are emerging that are of interest to a larger scientific audience Thus each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole The most significant developments of the last 5 to 10 years should be presented using selected examples to illustrate the principles discussed A description of the physical basis of the experimental techniques that have been used to provide the primary data may also be appropriate if it has not been covered in detail elsewhere The coverage need not be exhaustive in data but should rather be conceptual concentrating on the new principles being developed that will allow the reader who is not a specialist in the area covered to understand the data presented Discussion of possible future research directions in the area is welcomed Review articles for the individual volumes are invited by the volume editors Readership research scientists at universities or in industry graduate students Special offer For all customers who have a standing order to the print version of Structure and Bonding we offer free access to the electronic volumes of the Series published in the current year via SpringerLink 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 Mathematical Descriptors of Molecules and Biomolecules Subhash C. Basak, 2024-09-02 This book provides an up to date overview of data driven and evidence based empirical approaches in the efficient application of chemodescriptors and biodescriptors Currently there is a steady increase in the use of data analytics and model based decision support systems in basic and applied research in chemoinformatics bioinformatics pharmaceutical drug design predictive toxicology and computational biology Since there are a plethora of modeling methods and a large number of chemodescriptors and biodescriptors available today robust statistical and machine learning methods are applied throughout In addition the development of statistically robust predictive models in rank deficient cases using chemodescrip tors and biodescriptors is discussed Readers are provided with an up to date overview of the theoretical background calculation methods and proper use of chemodescriptors and biodescriptors in model building with special emphasis on computer assisted organic synthesis new drug discovery hazard assessment of chemicals and computational biology of emerging global pathogens The book also discusses the applications of alignment free seguence descriptors AFSDs in vaccine design and the characterization of emerging global pathogens such as the Zika virus and SARS CoV 2 The utility of molecular fragment based descriptors in building useful quantitative structure activity relationship Q SAR models is detailed as is the use of mathematical structural descriptors in chemical synthesis planning

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