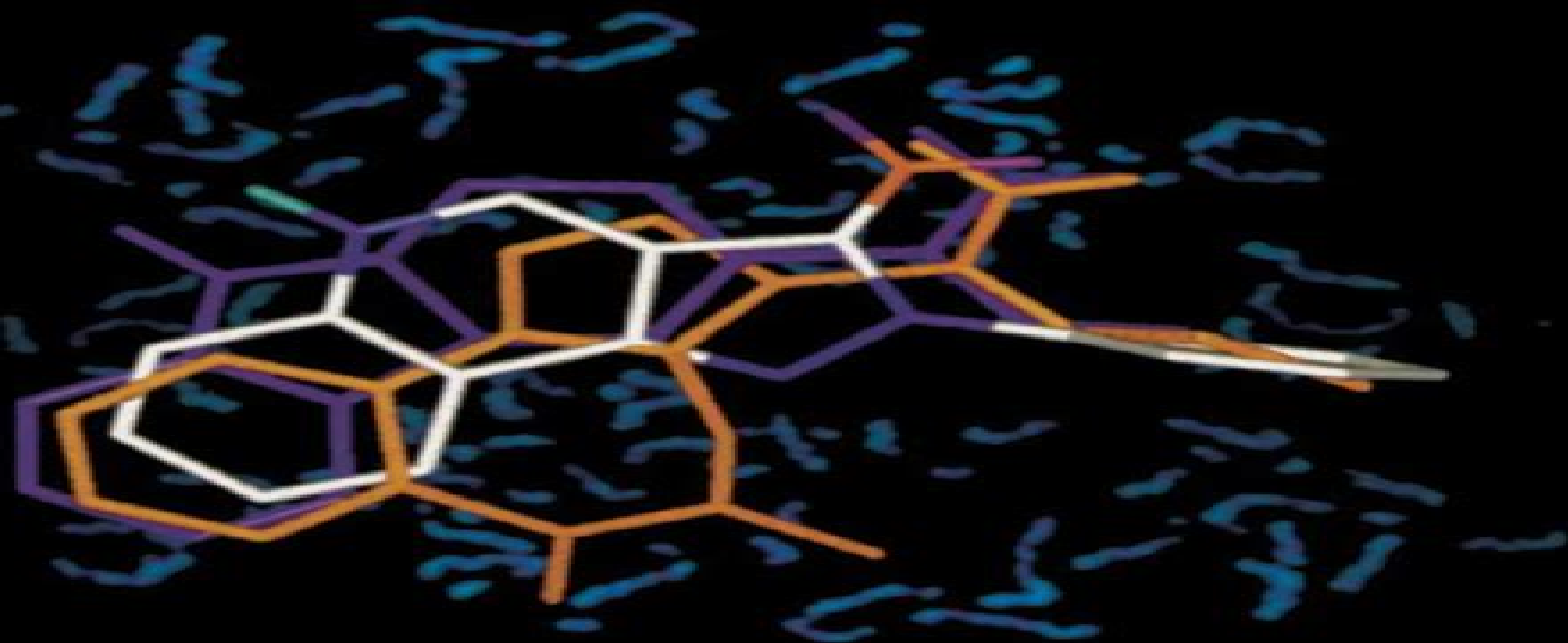


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Genetic Algorithms In Molecular Modeling

Kenny B. Lipkowitz, Donald B. Boyd



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instructional and nonmathematical style these books provide an access to computational methods often outside a researcher's area of expertise Volumes 9 10 represent the next two volumes in the successful series designed to help the chemistry community keep current with the many new developments in computational techniques Many chapters are written as tutorials to introduce the many facets of computational chemistry including molecular modeling computer assisted molecular design CAMD quantum chemistry molecular mechanics and dynamics and quantitative structure activity relationships QSAR The authors provide necessary background and theory strategies for implementing the methods pitfalls to avoid applications and references

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Molecular Modeling of Nucleic Acids Neocles B. Leontis, 1998 Covering numerous topics in modeling nucleic acids this volume looks at the role of various spectroscopic methods simulations of molecular dynamics using particle mesh methods and dynamic and genetic algorithms for predicting RNA secondary structure It also covers the thermodynamics of nucleic acid folding and three dimensional structure prediction based on sequence information

Foundations of Intelligent Systems Ning Zhong, Zbigniew W. Ras, Shusaku Tsumoto, Eino Suzuki, 2003-10-22 This volume contains the papers selected for presentation at the 14th International Symposium on Methodologies for Intelligent Systems ISMIS 2003 held in Maebashi City Japan 28 31 October 2003 The symposium was organized by the Maebashi

Institute of Technology in co operation with the Japanese Society for Artificial Intelligence It was sponsored by the Maebashi Institute of Technology Maebashi Convention Bureau Maebashi City Government Gunma Prefecture Government US AFOSR AOARD the Web Intelligence Consortium Japan Gunma Information Service Industry Association and Ryomo Systems Co Ltd ISMIS is a conference series that was started in 1986 in Knoxville Tennessee Since then it has been held in Charlotte North Carolina Knoxville Tennessee Turin Italy Trondheim Norway Warsaw Poland Zakopane Poland and Lyon France The program committee selected the following major areas for ISMIS 2003 active media human computer interaction autonomic and evolutionary computation intelligent agent technology intelligent information retrieval intelligent information systems knowledge representation and integration knowledge discovery and data mining logic for artificial intelligence soft computing and Web intelligence

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International Journal of Medical and Biological Frontiers, 2001

Handbook of Molecular Descriptors, Volume 11 Roberto Todeschini, Viviana Consonni, 2000-12-07 It will be an invaluable guide for all those dealing with bioactive molecules as well as for those aimed to predict physico chemical or environmental properties by models based on molecular descriptors This book is written in such way to be also a powerful didactic tool for researchers

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Molecular Modeling of Inorganic Compounds, Includes CD-ROM with Tutorial Peter Comba, Trevor W. Hambley, 2001-03-12 In many branches of chemistry Molecular Modeling is a well established and powerful tool for the investigation of complex structures The second completely revised and enlarged edition of this highly recognized book shows how this method can be successfully applied to inorganic and coordination compounds The first part of the book gives a general introduction to Molecular Modeling which will be of use for chemists in all areas The second part discusses numerous carefully selected examples chosen to illustrate the wide range of applicability of molecular modeling to metal complexes and the approaches being taken to dealing with some of the difficulties involved While the general outline is similar to that of the first edition many of the examples chosen for discussion reflect the changes of the past five years In the third part the reader learns how to apply Molecular Modeling to a new system and how to interpret the results The accompanying software features 20 tutorial lessons based on examples from the literature and the book itself The authors take special care to highlight possible pitfalls and offer advice on how to avoid them Therefore this book will be invaluable to everyone working in or entering the field

3D QSAR in Drug Design Hugo Kubinyi, Gerd Folkers, Yvonne Connolly Martin, 1998

Molecular Descriptors for Chemoinformatics Roberto Todeschini, 2009 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 complete

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Materials Design Approaches and Experiences Ji-Cheng Zhao, Michael Fahrman, Tresa M. Pollock, 2001 These papers describe past alloy design experiences and state of the art methodologies and first principle neural network combinational phase field thermodynamic and regression based alloy design

Burger's Medicinal Chemistry and Drug Discovery, Drug Discovery Donald J. Abraham, 2003 This is Volume 1 Drug Discovery of Burger's Medicinal Chemistry and Drug Discovery 6th Edition This new volume contains critical new chapters on Virtual Screening Bioinformatics and Chemical Information Computing Systems in Drug Discovery To purchase the entire 6 volume set please refer to ISBN 0 471 37032 0 For a complete list of articles and contributors as well as FREE sample chapters from this new 6th Edition please visit www.mrw.interscience.wiley.com/bmcdd

Computer-Assisted Lead Finding and Optimization Han van de Waterbeemd, Bernard Testa, Gerd Folkers, 1997-07-14 Computer assisted techniques are well integrated in modern drug discovery and used for the finding of new leads the optimization of receptor or enzyme affinity as well as of pharmacokinetic and physicochemical properties In this book an account is found of current strategies used in computer assisted drug design Important topics include progress in chemometrics molecular modeling and three dimensional QSAR approaches Relatively new mathematical methods such as genetic algorithms or artificial neural networks and fuzzy logic have found their application in rational molecular design As is amply illustrated based on recent developments in these disciplines important progress has been made in lead finding strategies This is of great importance to the pharmaceutical industry Thus all scientists investigating quantitative structure activity relationships in their broadest sense in medicinal agricultural or environmental chemistry will benefit from this book

Technometrics, 2005

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