

Minimum Steric Difference:
Minimal Topologic
Difference for Qusar
Studies (Chemometrics
Research Studies Series)

Simon, Z

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Minimum Steric Difference The Mtd Method For Qsar Studies

I. I. Ioffe

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Minimum Steric Difference Zeno Simon,1984 **Molecular Descriptors for Chemoinformatics** Roberto Todeschini, Viviana Consonni, 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 **Minimum Steric Difference** ,1984-07-03 This series of monographs the result of many years of work by the authors offers a different approach to the problem of drug action Starting from a simple concept of the hypermolecule a composite of the molecular structures of a series of compounds the MTD approach elucidates the detailed relationships between the molecular structure of a drug and its biological activity Brings together an impressive array of examples to indicate the utility of the described method *New Frontiers in Nanochemistry: Concepts, Theories, and Trends, 3-Volume Set* Mihai V. Putz, 2022-05-29 New Frontiers in Nanochemistry Concepts Theories and Trends 3 Volume Set explains and explores the important fundamental and advanced modern concepts from various areas of nanochemistry and more broadly the nanosciences This innovative and one of a kind set consists of three volumes that focus on structural nanochemistry topological nanochemistry and sustainable nanochemistry respectively collectively forming an explicative handbook in nanochemistry The compilation provides a rich resource that is both thorough and accessible encompassing the core concepts of multiple areas of nanochemistry It also explores the content through a trans disciplinary lens integrating the basic and advanced modern concepts in nanochemistry with various examples applications issues tools algorithms and even historical notes on the important people from physical quantum theoretical mathematical and even biological chemistry

Alternatives to the Use of Live Vertebrates in Biomedical Research and Testing ,1997 **New Frontiers in Nanochemistry: Concepts, Theories, and Trends** Mihai Putz, 2020-05-06 The final volume of this new innovative and informative three volume set explains and explores the essential basic and advanced concepts from various areas within the nanosciences This volume primarily focuses on increasing awareness of sustainable nanochemistry meaning the social and economic impact of nanochemistry in order to mitigate ecological resource depletion and to promote the exploration of nature as a resource for future benefits This volume adopts a pharmacological lens examining the multitude of ways in which nano research can contribute to the development of pharmaceutical drugs and paying particular attention to toxicology and renewable energy within nanochemistry Under the vast expertise of the editor the volume contains 34 entries contributed by renowned international scientists and scholars The content in this volume covers topics such as anti HIV agents

ecotoxicology solar cells and photovoltaic phenomena spectral SAR and more alphabetically organized and accompanied by equations figures and brief letters in order to emphasize the potential applications of the concepts discussed **Exploring QSAR.: Fundamentals and applications in chemistry and biology** Corwin Hansch,Albert Leo,1995 This two volume set investigates the interaction of organic compounds with various forms of life including macromolecules enzymes and organelles It provides an introduction to the Hammett equation and its applications as well as a discussion of the design of bioactive compounds Volume 2 includes extensive tables of approximately 17 000 partition coefficients from octanol water and a comprehensive listing of electronic and steric parameters in the design and study of bioactive organic compounds

QSAR : Hansch Analysis and Related Approaches Hugo Kubinyi,1993 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 physicochemical 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 Multivariate Chemometrics in QSAR (quantitative Structure-activity Relationships) Peter P. Mager,1988

Application of Pattern Recognition to Catalytic Research I. I. Ioffe,1988-04-28 Addresses the prediction of chemical activity and selectivity of new heterogeneous catalysts based on a pattern recognition approach Written by an internationally recognized and prolific researcher this monograph expands the usefulness of catalysis in synthetic chemistry where study of the mechanisms of catalysis can help answer questions of chemical structure bonding and reactivity Illustrated Distance Geometry and Molecular Conformation G. M. Crippen,Timothy F. Havel,1988

Molecular Connectivity in Structure-activity Analysis Lemont Burwell Kier,Lowell H. Hall,1986 Mathematical and Computational Concepts in Chemistry Nenad Trinajstić,1986 **Three-dimensional Quantitative Structure-activity Relationships Based on Atomic Property Descriptors** Scott Andrew Wildman,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 **BOOK JACKET Potential Pattern Recognition in Chemical and Medical Decision Making** D. Coomans,I. Broeckaert,1986 Annals of West University of Timisoara ,2000 **Comprehensive Medicinal Chemistry II, Volume 4** John Bodenhan Taylor,D. J. Triggle,2007 This e book comprises 8 volumes with all chapter sections available as PDF or HTML and includes bibliographical references and index International Journal of Medical and Biological Frontiers ,2001

Similarity and Clustering in Chemical Information Systems Peter Willett, 1987-05-06 This book describes the latest developments in computational techniques which increase the effectiveness of the storage retrieval and processing of information in computerized chemical information systems. Covers the specifics of searching and clustering methods based upon the calculation of measures of similarity between chemical structures in machine readable files. These techniques are used not only to enhance information retrieval but also as a component of drug development programs. Chapters cover the representation of chemical structures, searching files, quantitative structure activity relationships, similarity and cluster analysis, similarity in chemical information systems, clustering in chemical information systems and nearest neighbor searching algorithms.

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