

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

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# Minimum Steric Difference The Mtd Method For Qsar Studies

**Corwin Hansch, Albert Leo**



## **Minimum Steric Difference The Mtd Method For Qsar Studies:**

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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

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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.

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*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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