

Computer Handling of Chemical Structure Information

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Cambridge, MA

Cambridge University Press

32 Avenue of the Americas, New York, NY

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Miloň Tichý



Computer Handling Of Chemical Structure Information:

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Molecular Databases for Protein Sequences and Structure Studies John A.A. Sillince, Maria Sillince, 2012-12-06

The amount of molecular information is too vast to be acquired without the use of computer bases systems The authors introduce students entering research in molecular biology and related fields into the efficient use of the numerous databases available They show the broad scientific context of these databases and their latest developments They also put the biological chemical and computational aspects of structural information on biomolecules into perspective The book is required reading for researchers and students who plan to use modern computer environment in their research *Data for Science and*

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Journal of Research of the National Bureau of Standards United States. National Bureau of Standards, 1966 **Computer Software Applications in Chemistry** Peter C. Jurs, 1996-02-02 Intended specifically for practicing professionals and advanced students in chemistry and biochemistry this invaluable book covers the full range of the computer applications in these fields including numerical nonnumerical and graphics applications New material includes multiple linear regression using MREG principal components analysis Monte Carlo integration parameterization of the force field and molecular modeling software Major areas covered include Error Statistics and the Floating Point Number System Curve Fitting Multiple Linear Regression Analysis Numerical Integration Numerical Solution of Differential Equations Matrix Methods and Linear Equation Systems Random Numbers and Monte Carlo Simulation Simplex Optimization Chemical Structure Information Handling Mathematical Graph Theory Substructure Searching Molecular Mechanics and Molecular Dynamics Pattern Recognition Artificial Intelligence and Expert Systems Spectroscopic Library Searching and Structure Elucidation Graphical Display of Data and of Molecules Whatever your area of research this comprehensive lucidly written book offers an indispensable resource of computer applications that will facilitate your work **Chemical Structure Information Handling** National Research Council (U.S.). Committee on Chemical Information, 1969 *BASIC Programming for Chemists* Peter C. Jurs, Thomas L.

Isenhour, Charles L. Wilkins, 1987-10-02 Teaches the fundamentals of the BASIC programming language by description and example and presents over 50 chemically oriented BASIC programs that can both teach about the language and be useful in their own right The first part of the book introduces the reader to programming in the BASIC language The second part of the book consists of 52 example problems divided into 44 topics concerning chemical problems These problems progress in difficulty in terms of the chemical concepts mathematical models and programming operations involved The reader can work the problems then copy and run the programs and compare the results The given programs can be modified to suit the reader's needs or new ones be written using the techniques presented in the text

Graphics for Chemical Structures

Wendy A. Warr, American Chemical Society. Division of Chemical Information, 1987 Technical News Bulletin of the National Bureau of Standards, 1967 Quantitative Structure-Activity Relationships Miloň Tichý, 1976 The conference on Chemical Structure Biological Activity Quantitative Approaches was held in Prague Czechoslovakia on June 27-29 1973 It took place under the auspices of the J E Purkyně Czechoslovak Medical Society the Czechoslovak Chemical Society and the International Society of Quantitative Biology Organizing Committee A David Chairman M Tichý Secretary General K Boček J Kopecký R Zahradník This volume contains the lectures and communications presented at the conference There has been an ever increasing interest especially during the last eight years in the study of the quantitative relationships between the chemical structure of substances and their biological activity QSAR quantitative structure activity relationships One of the reasons for this increasing interest has been the desire to find ways of estimating the quantitative characteristics of a given biological activity as well as to shorten time and reduce the costs of research into optimally active compounds In contrast to qualitative studies seeking the critical biologically active group the QSAR approach involves the search for that property or those properties which determine the magnitude of the biological effect Methods of physical chemistry and quantum chemistry appear to be suitable for estimating the quantitative characteristics of the biological activity of different compounds Forecasting the specific activity of a certain substance by means of theoretical methods is still a matter of future development One of the basic ideas of QSAR studies is to work with a series of chemical compounds thereby enabling the collection and classification of experimental data

Technical News Bulletin United States. National Bureau of Standards, 1966 **Dimensions**, 1967 **U.S. Government Research and Development Reports**, 1965 **Whitaker's Cumulative Book List**, 1983 **Computer Applications in Chemical Research and Education** Josef Brandt, Ivar Ugi, 1989 Library & Information Science Abstracts, 2005 **Information Processing Journal**, 1962 **Books in Series**, 1985 Vols for 1980 issued in three parts Series Authors and Titles

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