

Practical Applications of Quantitative Structure-Activity Relationships (QSAR) in Environmental Chemistry and Toxicology

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Practical Applications of Quantitative Structure-Activity Relationships (QSAR) in Environmental Chemistry and Toxicology W. Karcher, J. Devillers, 1990-05-31 Based on the Lectures given during the Eurocourse on Practical Applications of Quantitative Structure Activity QSAR in Environmental Chemistry and Toxicology held at the Joint Research Centre Ispra Italy June 11 15 1990 Chemical and Environmental Science Series, Volume 1; Practical Applications of Quantitative Structure Activity Relationships (QSAR) in Environmental Chemistry and Toxicology W. Karcher, 1990 Einführung in die modellgestützte Bewertung von Umweltchemikalien Rainer Brüggemann, Ute Drescher-Kaden, 2013-03-11 Als roter Faden dient dem Autor hier erstmals der Bewertungsgedanke Die Ausbreitung von Chemikalien wird modelliert um zu sehen wo Akkumulationen denkbar sind Bewertet werden Chemikalien in der Umwelt und die Umwelt in ihren Belastungszuständen Dazu werden Ausbreitungsmodelle Methoden zur Abschätzung von Subanzeigenschaften QSAR Wirkungsmodelle mit kologischem Hintergrund und Bewertungsverfahren vorgestellt Der notwendige mathematische Apparat wird dabei meist Schritt für Schritt erläutert Das Buch eignet sich für alle die sich einen Überblick über weite Bereiche der mathematischen Modellierung von Umweltchemikalien verschaffen wollen sowie für Spezialisten die sich mit Bewertungsverfahren beschäftigen Die begleitende CD ROM beinhaltet kleine Programme Leser können damit in die Modellierung praktisch eingeführt werden und selbst einzelne Schwerpunkte zur Modellierung ausprobieren **Handbook of Ecotoxicology** David J. Hoffman, Barnett A. Rattner, G. Allen Burton Jr., John Cairns Jr., 2002-11-13 Completely revised and updated with 18 new chapters this second edition includes contributions from over 75 international experts Also a Technical Review Board reviewed all manuscripts for accuracy and currency Focusing on toxic substance and how they affect the ecosystems worldwide the book presents methods for quantifying and measuring ecotoxicological effects in the field and in the lab as well as methods for estimating predicting and modeling in ecotoxicology studies This is the definitive reference for students researchers consultants and other professionals in the environmental sciences toxicology chemistry biology and ecology in academia industry and government Ecotoxicology Modeling James Devillers, 2009-08-07 Ecotoxicology Modeling is a comprehensive and well documented text providing a collection of computational methods to the ecotoxicologists primarily interested in the study of the adverse effects of chemicals their mechanisms of action and or their environmental fate and behavior Avoiding mathematical jargon the book presents numerous case studies to enable the reader to understand the interest but also the limitations of linear and nonlinear models in ecotoxicology Written by an international team of scientists Ecotoxicology Modeling is of primary interest to those whose research or professional activity is directly concerned with the development and application of models in ecotoxicology It is also intended to provide the graduate and post graduate students with a clear and accessible text covering the main types of modeling approaches used in environmental sciences

Handbook of Ecotoxicology Peter P. Calow, 2009-06-05 The Handbook of Ecotoxicology provides a readily accessible yet critical collection of information on ecotoxicological testing Now available in a single paperback volume this handbook represents excellent value Part A concentrates on techniques especially those tests used for prediction Thorough descriptions of the main tests are provided followed by critical analyses in terms of ease of handling repeatability and ecological relevance and finally an extensive bibliography citing key documents describing test methods and key papers evaluating them Part B focuses on the toxicants themselves summarising their ecological effects describing ways of predicting effects from physico chemical properties alone and describing and discussing fate models Now available as a single volume in paperback An invaluable reference resource

Predicting Chemical Toxicity and Fate Mark T.D. Cronin, 2004-05-10 Quantitative Structure Activity Relationships QSARs are increasingly used to predict the harmful effects of chemicals to humans and the environment The increased use of these methods in a variety of areas academic industrial regulatory results from a realization that very little toxicological or fate data is available on the vast amount of chemicals to which humans and the environment are exposed Predicting Chemical Toxicity and Fate provides a comprehensive explanation of the state of the art methods that are available to predict the effects of chemicals on humans and the environment It describes the use of predictive methods to estimate the physicochemical properties biological activities and fate of chemicals The methods described may be used to predict the properties of drugs before their development and to predict the environmental effects of chemicals These methods also reduce the cost of product development and the need for animal testing This book fills an obvious need by providing a comprehensive explanation of these prediction methods It is a practical book that illustrates the use of these techniques in real life scenarios This book will demystify QSARs for those students unsure of them and professionals in environmental toxicology and chemistry will find this a useful reference in their everyday working lives

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

QSAR, Rational Approaches to the Design of Bioactive Compounds C. Silipo, A. Vittoria, 1991 Quantitative structure activity relationships constitute a subject which has seen enormous growth in the past decade Techniques which have been developed and used widely outside of medicinal chemistry are now used by those working with QSAR These techniques employ powerful computers molecular

graphics systems and sophisticated software Although QSAR techniques have been developed to optimize activities of known sets of analogs recent methodologies suggest that these techniques can be useful in the modeling of new chemical entities The contributions in this state of the art volume cover a wide range of disciplines tools and ideas which will be of interest to medicinal chemists pharmacologists and biologists The book gives an update of progress in the science of the quantitative approaches of the interface between chemistry physical chemistry and biology pharmacology The use of molecular graphics computational and conformational methods in drug research is extensively covered

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

Forecasting the Environmental Fate and Effects of Chemicals P. S. Rainbow,Steve P. Hopkin,Mark Crane,2001-05-25 The book is the first book to address specifically the issue of forecasting in environmental toxicology and chemistry from a methodological regulatory and practical perspective

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Development of Predictive Capabilities for Intermedia Transfer Factors for Toxic Air Pollutants Yoram Cohen,1997

Classical and Three-dimensional QSAR in Agrochemistry Corwin Hansch,1995 Discusses the applications of classical QSAR and molecular modeling analysis to the discovery of new agrochemicals Examines hydrophobicity parameters derived from various partitioning systems Includes chapters focusing on the use of three dimensional QSAR analyses such as CoMFA and DISCO Presents information on the use of QSAR to study transport and toxicology of agrochemicals

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