QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIPS IN ENVIRONMENTAL SCIENCES-VII

Edited by Fei Chen Gerrit Schüürmann

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Quantitative Structureactivity Relationships In Environmental Sciences Vii Setac Special Publications Series: Quantitative Structure-activity Relationships in Environmental Sciences, VII Fei Chen, Gerrit

Schüürmann, 1997-01-01 The 30 papers cover molecular modeling and computerized techniques physicochemical properties acute toxicity and mutagenicity and statistical validation and risk assessment They were peer reviewed and revised between presentation and publication and both report new information and review and synthesize the current state of the science Among the topics are a new approach to estimating three dimensional similarity that incorporates molecular flexibility calculating molar crystalline and liquid volumes and their temperature dependence identifying mechanisms of the toxic action of phenols to Tetrahymena pyriformis from molecular descriptors and discriminating statistically equivalent variables in quantitative structure activity relationships Annotation copyrighted by Book News Inc Portland OR 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 Advances in OSAR Modeling Kunal Roy, 2017-05-22 The book covers theoretical background and methodology as well as all current applications of Quantitative Structure Activity Relationships QSAR Written by an international group of recognized researchers this edited volume discusses applications of QSAR in multiple disciplines such as chemistry pharmacy environmental and agricultural sciences addressing data gaps and modern regulatory requirements Additionally the applications of QSAR in food science and nanoscience have been included two areas which have only recently been able to exploit this versatile tool This timely addition to the series is aimed at graduate students academics and industrial scientists interested in the latest advances and applications of QSAR Environmental Contamination and Toxicology George W. Ware, 1999-06-04 International concern in scientific industrial and governmental communities over traces of xenobiotics in foods and in both abiotic and biotic environments has justified the present triumvirate of specialized publications in this field comprehensive reviews rapidly published research papers and progress reports and archival documentations These three international publications are integrated and scheduled to provide the coherency essential for nonduplicative and current progress in a field as dynamic and complex as environmental contamination and toxicology This series is reserved exclusively for the diversified literature on toxic chemicals in our food our feeds our homes recreational and working surroundings our domestic animals our wildlife and ourselves Tre mendous efforts worldwide have been mobilized to evaluate the nature pres ence magnitude fate and toxicology of the chemicals

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