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Rational Approaches to Structure, Activity, and Ecotoxicology of Agrochemicals

Wilfried Draber, Toshio Fujita

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This book presents discussions of the most important aspects in the development of agrochemicals. The book covers such broad areas as structure activity and ecotoxicological analyses in comprehensive reviews for general methods and chronicles for individual examples. Topics in structure-activity relationships include how to combine submolecular structures of pharmacological interests and modify them according to chemorational models with computer-aided procedures such as the traditional Hansch-type QSAR, the sequential, simplex optimization, and molecular modeling. Topics in the ecotoxicology of organo phosphorus compounds are discussed in terms of the quantitative structure-toxicity relationship (QSTR). Chronicles of molecular orbital methodology in predicting environmental fates of agrochemicals are also provided.

This volume will be invaluable for researchers in the agrochemical and pharmaceutical industries.

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