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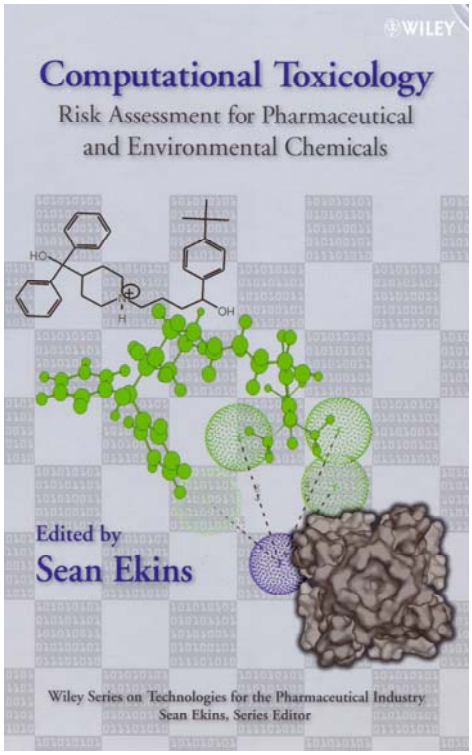
COMPUTATIONAL TOXICOLOGY RISK ASSESSMENT FOR PHARMACEUTICAL AND ENVIRONMENTAL CHEMICALS



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Currently, many companies and organizations have or are evaluating new predictive tools to improve human hazard assessment, (e.g. drug toxicity, P450 metabolism) for applications in both pharmaceutical development and environmental analysis. For example, the interaction of molecules can be predicted through computer-based tools using X-ray crystal structures, homology, receptor, pharmacophore, and QSAR models of human enzymes as well as transporters, nuclear receptors, and ion channels. In silico modeling for toxicology may therefore provide effective pre-screening for chemicals in pharmaceutical discovery and the environment.

This book discusses the validation of such models for regulatory purposes, the validation criteria, and other requirements for regulatory acceptance. The book begins with an introduction to toxicology, risk assessment, and relevant technologies like high throughput and chemical screening and systems biology. Then the book covers the most advanced currently available molecular-modeling software and its role in testing strategies for different types of toxicity. Chapters include in-depth views of QSAR models, physicochemical drug properties, structure-based drug targeting, chemical mixture assessments, and environmental modeling.

A comprehensive analysis of state-of-the-art molecular modeling approaches and strategies applied to risk assessment for pharmaceutical and environmental chemicals.

This unique volume describes how computer–based tools utilizing X–ray crystal structures or homology, receptor, pharmacophore, and QSAR models of human proteins can help in predicting the interaction of molecules with toxicologically relevant targets.

The book covers the in vitro models used, newer technologies, and regulatory aspects. It offers a complete systems perspective to risk assessment prediction, discussing experimental and computational approaches in detail. It provides an introduction to toxicology methods and an explanation of computational methods. The QSAR methods applied to enzymes, transporters, nuclear receptors and ion channels are reviewed in detail. The matter of applying computers to toxicology assessment in the pharmaceutical industry and in the environmental arena is presented in specialized sections. The chapters were written by leading international experts. The book also provides figures to illustrate computational models and lists references for further information.

This book appears as a key resource for toxicologists and scientists in the pharmaceutical industry and environmental sciences. It could also be helpful for researchers involved in ADMET, drug discovery, and technology and software development.

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