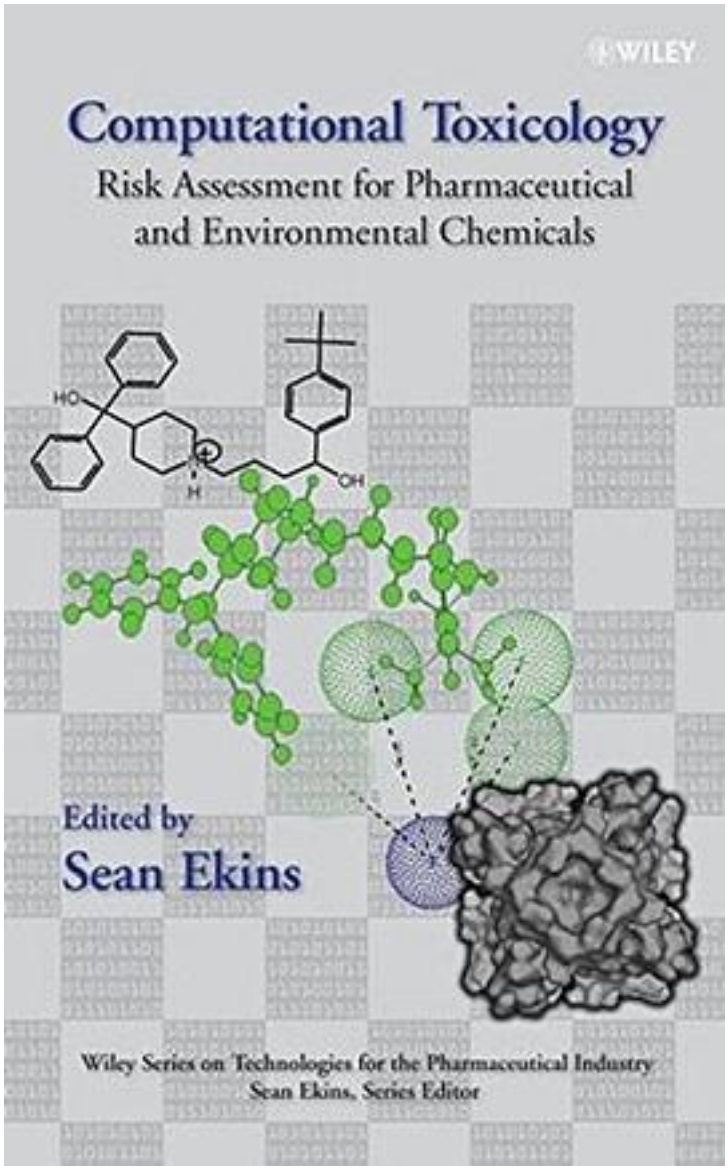
Computational Toxicology



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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 the interaction of molecules with toxicologically relevant targets can be predicted using computer-based tools utilizing X-ray crystal structures or homology, receptor, pharmacophore, and quantitative structure activity relationship (QSAR) models of human proteins. It covers the in vitro models used, newer technologies, and regulatory aspects. The book offers a complete systems perspective to risk assessment prediction, discussing experimental and computational approaches in detail, with:

*An introduction to toxicology methods and an explanation of computational methods

*In-depth reviews of QSAR methods applied to enzymes, transporters, nuclear receptors, and ion channels

*Sections on applying computers to toxicology assessment in the pharmaceutical industry and in the environmental arena

*Chapters written by leading international experts

*Figures that illustrate computational models and references for further information

This is a key resource for toxicologists and scientists in the pharmaceutical industry and environmental sciences as well as researchers involved in ADMET, drug discovery, and technology and software development.

作者介绍:

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