



Computational Toxicology: Risk Assessment for Chemicals

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DESCRIPTION

A key resource for toxicologists across a broad spectrum of fields, this book offers a comprehensive analysis of molecular modelling approaches and strategies applied to risk assessment for pharmaceutical and environmental chemicals.

- Provides a perspective of what is currently achievable with computational toxicology and a view to future developments
- Helps readers overcome questions of data sources, curation, treatment, and how to model / interpret critical endpoints that support 21st century hazard assessment
- Assembles cutting-edge concepts and leading authors into a unique and powerful single-source reference
- Includes in-depth looks at QSAR models, physicochemical drug properties, structure-based drug targeting, chemical mixture assessments, and environmental modeling
- Features coverage about consumer product safety assessment and chemical defense along with chapters on open source toxicology and big data

ABOUT THE AUTHOR

Sean Ekins, MSc, PhD, DSc has over 20 years of pharmaceutical and toxicology experience. He is the founder or co-founder of two companies and Adjunct Professor at three universities. He has been awarded 16 NIH grants as Principal Investigator. He has authored or co authored over 285 peer-reviewed papers and book chapters and edited five books with Wiley. His research is focused on collaborations to facilitate rare and neglected disease drug discovery.

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