



# **Computational Toxicology: Chapter 2. Quantitative Structure-Activity Relationship (QSAR) Models, Physiologically Based Pharmacokinetic (PBPK) Models, Biologically ... Computational Tools for Public Health**

*Patricia Ruiz, Xiaoxia Yang, Annie Lumen, Jeff Fisher*

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Human health risk assessment is “the process to estimate the nature and probability of adverse health effects in humans who may be exposed to chemicals in contaminated environmental media, now or in the future.”

Currently, most data required for human risk assessment are derived from toxicological studies conducted in laboratory animals. The “Toxicology in the 21st Century” initiative expands the toxicity testing tools to include the development of alternative toxicity testing methods that examine pathways of toxicity (on a large scale) and the employment of dose-response and extrapolation modeling tools. While the latter methodology is in its infancy, several methodologies for dose-response and extrapolation modeling are more mature. Over the last decade, physiologically based pharmacokinetic (PBPK) modeling has gained acceptance as a computational tool for use in public health assessments. In this chapter, we present examples of quantitative structure-activity relationship (QSAR) models, physiologically based pharmacokinetic (PBPK) models, and biologically based dose response (BBDR) models that have been developed for use in public health assessments and advancing knowledge gained through in silico examinations of biological systems.

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