Computational Toxicology: Chapter 4. Modeling of Sensitive Subpopulations and Interindividual Variability in Pharmacokinetics for Health Risk Assessments

Kannan Krishnan, Brooks McPhail, Weihsueh Chiu, Paul White

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Many health risk assessments develop exposure limits for chemicals, intended to protect the general population, including sensitive subpopulations. Critical toxicokinetic and toxicodynamic determinants of toxicity vary among subgroups of populations, thus making some of them potentially more susceptible than the general population to the health effects of chemicals. This chapter focuses on toxicokinetics and reviews the current computational approaches to address the issue of interindividual variability for health risk assessments. These approaches include individual-based PBPK modeling, P-bounds modeling, Monte Carlo simulation, and Markov Chain Monte Carlo simulation, each of which has different data requirements regarding input parameters. The advantage of these computational approaches is that they allow predictions of variables that cannot be easily accessed or measured in susceptible subpopulations with the available methodologies. Thus, the resulting simulations are useful in characterizing the magnitude of interindividual variability in the human health assessment of chemicals.

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