



Computational Toxicology: Chapter 3. Multiple Chemical Exposures and Risk Assessment

John C. Lipscomb, Nikki Maples-Reynolds, Moiz Mumtaz

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Humans are exposed to chemicals through voluntary and involuntary actions; to natural and synthetic chemicals all day, every day. Single chemical risk assessments are complex in and of themselves, and the assessment of chemical mixtures exponentially increases the complexity for toxicologists, regulators, and the public. Chemicals produce effects in biological systems which may or may not be related to their toxicity; some effects may be adaptive or may not be a direct part of their mode or mechanism of toxic action. These terms are commonly used and may be distinguished based on the level of detail implied. Mode of action usually describes the effect of a toxicant at the cellular or organ level, while mechanism of action implies an understanding of the interaction of the toxicant at the molecular level. Chemicals can have the same mode of action, but act via different mechanisms. Components in a chemical mixture are characterized by mode and/or mechanism for the purpose of grouping, described later.

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