# Special Issue

# Computational Toxicology: Expanding Frontiers in Risk Assessment

## Message from the Guest Editors

Emerging technologies and advances in computational toxicology coupled with an improved understanding of mechanistic adverse outcome pathways (AOPs), in a new era of systems-focused thinking, are radically expanding the frontiers for risk assessment. New approach methodologies (NAMs) are increasingly providing biokinetic and mechanistic data from in vitro assays and in silico predictions that can aid evidence integration. In this Special Issue, we explore this new computational capacity across the source-to-outcome spectrum with examples of specific models and informatics approaches in both the environmental and medical arenas, including strategies for systematic review and harnessing big data. Conceptual constructs as well as quantitative examples are highlighted to illustrate impacts. Cross-cutting challenges such as how to foster the FAIR (findable, accessible, interoperable, and reproducible) principles and management of data repositories are also featured.

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## Deadline for manuscript submissions

closed (30 September 2022)


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# About the Journal

## Message from the Editor-in-Chief

*Toxics* (ISSN 2305-6304) is an international, peer-reviewed, open access journal which provides an advanced forum for studies related to all aspects of toxic chemicals and materials. We aim to publish high quality work that furthers our understanding of the exposure, effects, and risks of chemicals and materials in humans and the natural environment as well as approaches to assess and/or manage the toxicological and ecotoxicological risks of chemicals and materials. Please consider publishing in *Toxics* when preparing your next paper.

## Editor-in-Chief

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