Special Issue

Computational and Experimental Insights into Transformation of Environmental Pollutants

Message from the Guest Editors

The environmental fate and impact of pollutants are fundamentally governed by their transformation processes. Understanding these pathways is crucial for assessing environmental persistence and human health risks. While experimental studies provide direct evidence of reaction pathways and products, computational approaches offer powerful tools to elucidate reaction mechanisms and predict kinetics. This Special Issue highlights the synergy between these paradigms. We encourage submissions that not only integrate advanced experimental and computational methods but also showcase the development and application of novel tools—such as the use of kinetic isotope effects (KIE) to elucidate reaction mechanisms, machine-learning models for pathway prediction and QSAR for toxicity assessment—to gain mechanistic insights. Topics include, but are not limited to, the degradation of emerging contaminants; the formation, identity and toxicity of transformation products and the development of integrated frameworks for advancing environmental and human health-risk assessment.

Guest Editors

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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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