

Special Issue

Computational Toxicology for Environmental Criteria/Benchmarks of Emerging Contaminants

Message from the Guest Editors

The rapid development of computational toxicology is bridging the data gap and providing effective solutions for the comprehensive assessment of hazards. This Special Issue invites contributions from diverse computational toxicological modeling studies pertaining to environmental criteria/benchmarks and risk assessments. We strongly encourage submissions on all relevant topics including the virtual screening of preferential controlled pollutants, quantitative structure–activity relationships (QSARs), simulations of toxicological mechanisms, the modeling of internal and external exposure, interspecies differences, and environmental impacts on the bioavailability of emerging pollutants, as well as their environmental geochemical behaviors. The scope of research also includes new approaches for environmental criterion development, uncertainty analysis in risk assessments, and life cycle risk assessments. Further, contributions originating from meta-analyses based on the present datasets are also embraced for inclusion in this Special Issue.

Guest Editors

Dr. Yunsong Mu

Dr. Jing Liu

Dr. Huiming Cao

Deadline for manuscript submissions

closed (31 December 2024)



Toxics

an Open Access Journal
by MDPI

Impact Factor 4.1
CiteScore 6.4
Indexed in PubMed



mdpi.com/si/200032

Toxics
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
toxics@mdpi.com

[mdpi.com/journal/
toxics](https://mdpi.com/journal/toxics)





Toxics

an Open Access Journal
by MDPI

Impact Factor 4.1
CiteScore 6.4
Indexed in PubMed



[mdpi.com/journal/
toxics](https://mdpi.com/journal/toxics)



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

Dr. Demetrio Raldúa
Department Environmental Chemistry, IDAEA-CSIC, Jordi Girona 18,
08034 Barcelona, Spain

Author Benefits

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, PMC, Embase, CAPlus / SciFinder, AGRIS, and other databases.

Journal Rank:

JCR - Q1 (Toxicology) / CiteScore - Q1 (Chemical Health and Safety)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 17.8 days after submission; acceptance to publication is undertaken in 2.4 days (median values for papers published in this journal in the second half of 2025).