

## Special Issue

# From Detection to Risk: Data-Driven Advances in Analytical Chemistry and Toxicology

### Message from the Guest Editor

Rapid advances in analytical technologies and data-driven methods are transforming how we assess environmental and human health risks. This Special Issue aims to bridge the gap between identifying chemical contaminants and understanding their real-world impacts. It focuses on recent advances that move beyond traditional monitoring, leveraging advanced analytical methods, computational modelling, machine learning, and FAIR data principles to support integrated and predictive frameworks for exposure and toxicity assessment. This Special Issue will include contributions on the following:

- Advanced analytical methods and chemical identification strategies;
- Machine learning applications in analytical chemistry and toxicology;
- Integration of multi-omics and exposomics data in environmental risk assessment;
- Chemical prioritization methods and exposure modelling;
- Mixture toxicity and risk-based assessment frameworks;
- Integration of bioassay data and mechanistic toxicology endpoints;
- Data curation, standardization, and metadata enrichment for environmental and toxicological datasets;
- Decision support tools for regulatory science and early warning systems.

---

### Guest Editor

Dr. Nikiforos Alygizakis

1. Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece
2. Environmental Institute, Koš, Slovakia

---

### Deadline for manuscript submissions

closed (30 November 2025)



## Toxics

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.1  
CiteScore 6.4  
Indexed in PubMed



[mdpi.com/si/242475](https://mdpi.com/si/242475)

*Toxics*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[toxics@mdpi.com](mailto: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).