

Topical Collection

Artificial Intelligence and Data Mining for Toxicological Sciences

Message from the Collection Editors

The needs of our society to cope with safety issues when exposed to a wide range of toxics are enormous. As more data are available on two fronts, namely, toxicity of more compounds and real-time/high frequency data, Artificial Intelligence (AI) can improve our understanding of how toxic compounds create harm and improve ways to provide solutions. Although more data are available today, the complex properties and the dispersion of toxics make it very difficult to deal and address them without suitable computer tools. AI and Data Mining (DM) represent not only a methodological approach, but also a way to define new strategies to address toxicology and safety. While experimental studies proceed in sequential steps, also following parsimony criteria, DM and AI tools are able to elucidate a better vision of the complex, toxicological problem in an unprecedented way. We solicit manuscripts addressing the use of AI and DM dealing with toxicity and safety within the Special Issue on this topic. Human toxicology, ecotoxicology and environmental aspects are within the target of this Special Issue. Both manuscripts on the methodological aspects and on specific applications are welcome.

Collection Editors

Dr. Emilio Benfenati

Laboratory of Environmental Chemistry and Toxicology, Istituto di Ricerche Farmacologiche "Mario Negri", 19 Via La Masa, I-20156 Milan, Italy

Dr. Noel Aquilina

Faculty of Science, University of Malta, 2080 Msida, Malta



Toxics

an Open Access Journal
by MDPI

Impact Factor 4.1
CiteScore 6.4
Indexed in PubMed



mdpi.com/si/144686

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).