

Special Issue

Artificial Intelligence and Machine Learning in Metabolomics

Message from the Guest Editor

This Special Issue invites contributions that highlight cutting-edge advancements in artificial intelligence (AI) and machine learning (ML) for metabolomics. We welcome original research and reviews covering topics such as the following:

- AI/ML algorithms for metabolomic data analysis;
- Advanced pipelines for raw data processing, feature extraction, and compound identification;
- Integrative approaches for multi-omics data;
- Biomarkers and predictive models;
- Translational applications in clinical and pharmaceutical research.

Guest Editor

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Deadline for manuscript submissions

closed (31 January 2026)



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About the Journal

Message from the Editor-in-Chief

The metabolome is the result of the combined effects of genetic and environmental influences on metabolic processes. Metabolomic studies can provide a global view of metabolism and thereby improve our understanding of the underlying biology. Advances in metabolomic technologies have shown utility for elucidating mechanisms which underlie fundamental biological processes including disease pathology. *Metabolites* is proud to be part of the development of metabolomics and we look forward to working with many of you to publish high quality metabolomic studies.

Editor-in-Chief

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manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.7 days after submission; acceptance to publication is undertaken in 3.6 days (median values for papers published in this journal in the second half of 2025).