

## Special Issue

# Machine Learning Applications in Metabolomics Analysis: 2nd Edition

### Message from the Guest Editors

Metabolomics research is gaining much popularity since it enables the study of biological problems at a biochemical level, and can help us to understand the induction, development and mechanisms of many diseases, complementing information from other 'omics technologies. Similar to other high-throughput biological technologies, metabolomics can produce large volumes of data, and therefore, machine learning strategies can facilitate its application, with the discovery of new biomolecular signatures, which consequently facilitate the diagnosis/prognostic monitoring of diseases, including rare metabolic disorders, etc. This Special Issue aims to attract publications focused on the application of machine learning techniques to the analysis of multidimensional metabolomics data, including the development of methods, data augmentation procedures, preprocessing techniques, the comparisons of different methods, interpretability of results, the identification of new signatures, etc.

---

### Guest Editors

Prof. Dr. Leonardo Franco

Department of Computer Science, Málaga University, 29071 Málaga, Spain

Prof. Dr. Martin Grootveld

Leicester School of Pharmacy, Faculty of Health and Life Sciences, De Montfort University, Leicester LE1 9BH, UK

---

### Deadline for manuscript submissions

31 October 2026



## Metabolites

---

an Open Access Journal  
by MDPI

---

Impact Factor 3.7  
CiteScore 6.9  
Indexed in PubMed



[mdpi.com/si/219860](https://mdpi.com/si/219860)

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

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





# Metabolites

---

an Open Access Journal  
by MDPI

---

Impact Factor 3.7  
CiteScore 6.9  
Indexed in PubMed



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



## 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

Dr. Amedeo Lonardo  
Internal Medicine, Ospedale Civile di Baggiovara, Azienda Ospedaliero-Universitaria, 41126 Modena, Italy

---

### Author Benefits

#### High Visibility:

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

#### Journal Rank:

JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q2 (Endocrinology, Diabetes and Metabolism)

#### Rapid Publication:

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).