

## Special Issue

# Natural Products: Chemical Profiling, Computational Studies and Bioactivities

### Message from the Guest Editors

This Issue presents different studies carried out on natural products isolated or identified from plants or fungal endophytes associated with those plants. Natural products can represent a wide variety of chemical classes, such as flavonoids, terpenoids, essential oils, alkaloids, and many others. Such compounds can be identified via LC-MS, GC-MS, TLC-MS, and different NMR spectroscopic techniques. Metabolomics studies can share in further classification and clustering of these secondary metabolites and the differentiation of closely-related varieties. Moreover, many natural products are well known for promising biological activities such as antioxidant, anti-inflammatory, cytotoxic, hepatoprotective, renoprotective, neuroprotective, etc. The study of such activities can be evaluated through both *in vitro* and *in vivo* studies and can be further supported by various histological and computational studies. *In silico* molecular docking and dynamics can present possible binding interactions with the receptor's active site proteins and binding stability. ADME studies are carried out nowadays for many natural products, such as drug-likeness and *in silico* toxicity profiles.

### Guest Editors

Dr. Nada M. Mostafa

Department of Pharmacognosy, Ain Shams University, Cairo 11566, Egypt

Dr. Wagdy M. Eldehna

1. School of Biotechnology, Badr University in Cairo, Badr City 11829, Cairo, Egypt

2. Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Kafrelsheikh University, Kafrelsheikh 33516, Egypt

### Deadline for manuscript submissions

closed (31 October 2023)



## Metabolites

an Open Access Journal  
by MDPI

Impact Factor 3.7  
CiteScore 8.1  
Indexed in PubMed



[mdpi.com/si/137919](https://mdpi.com/si/137919)

*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 8.1  
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 - Q1 (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).