

Special Issue

Advances in Drug Discovery and Synthesis

Message from the Guest Editors

Drug discovery starts with identifying an unsatisfied therapeutic need, including assessing the adequacy of the available therapies and researching a cure for new emerging diseases. Drug discovery and development can be performed using different approaches: serendipity, selective optimization of activity of drugs or natural products, rational drug design, the synthesis of new molecular entities using the information derived from X-ray crystal structures and in silico modeling techniques, etc. In this Special Issue, we focus on all aspects involved in the discovery of new drug candidates, e.g., the design and synthesis of biologically active molecules, new synthetic routes leading to the discovery and optimization of lead compounds, molecular modeling, bioinformatics, structure-based drug design, and crystal structure analysis. Research articles, comprehensive reviews, and short communications are welcome with the aim of collecting the most recent insights and results involving multidisciplinary approaches in the research of biologically active new molecules.

Guest Editors

Dr. Susanna Nencetti

Associate Professor, Department of Pharmacy, University of Pisa, 56126 Pisa, Italy

Dr. Lidia Ciccone

Department of Pharmacy, University of Pisa, Via Bonanno 6, 56126 Pisa, Italy

Deadline for manuscript submissions

closed (20 June 2024)



International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



mdpi.com/si/159222

*International Journal of
Molecular Sciences*
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
ijms@mdpi.com

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





International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



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



About the Journal

Message from the Editor-in-Chief

The *International Journal of Molecular Sciences (IJMS)* is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, and molecular biophysics. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

Editor-in-Chief

Prof. Dr. José L. Quiles
Department of Physiology, Institute of Nutrition and Food Technology
"Jose Mataix", Biomedical Research Center, University of Granada,
Avda. Conocimiento s/n, 18100 Armilla, Granada, Spain

Author Benefits

Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:

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

Journal Rank:

JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)