

Special Issue

Molecular Advance in Cheminformatics and Nanoinformatics: Pioneering Solutions for Modern Challenges

Message from the Guest Editors

This Special Issue, entitled “Molecular Advance in Cheminformatics and Nanoinformatics: Pioneering Solutions for Modern Challenges”, aims to spotlight groundbreaking developments at the nexus of cheminformatics, nanoinformatics, and their broad applications. While the traditional realms of drug discovery remain central, there is a pronounced emphasis on contemporary issues such as precision toxicology, personalized medicine, precision agriculture and, notably, big data’s role in addressing COVID-19 challenges. We ardently seek manuscripts that bridge experimental work with cheminformatics/nanoinformatics, offering insights into computational toxicology and nanosafety. Manuscripts highlighting innovations tailored for the COVID-19 drug discovery are of special interest. This Special Issue also holds space for comprehensive reviews and meta-analyses that aim to consolidate existing knowledge. Contributions revolving around the genesis of novel computational methodologies and concepts are highly encouraged.

Guest Editors

Dr. Georgia Melagraki
Hellenic Military Academy, P.O. Box 16673 Vari, Greece
Dr. Antreas Afantitis
Entelos Institute, Nicosia 2102, Cyprus

Deadline for manuscript submissions

closed (20 October 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/188981

*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)