Special Issue

From Electronic Structure to Application: Computational Insights into Bioactive and Functional Molecules

Message from the Guest Editor

The search for new compounds with biological potential and the study of existing structures as drug candidates have become some of the most important tasks in modern chemistry. Currently, the fastest screening methods for evaluating the biological potential of molecules are techniques based on computational chemistry. Among these, the most popular and widely used include rule-based filtering, virtual high-throughput screening, similarity searching, molecular docking, and quantitative structure–activity relationships (QSAR).

Therefore, this Special Issue will focus on research concerning the structural properties of molecules based on reactivity descriptors, as well as their potential applications as biological agents and functional materials in various industries. In particular, we invite researchers to submit research and review articles on recent advances in this area.

Guest Editor

Dr. Karolina Kula
Department of Organic Chemistry and Technology, Cracow University of Technology, Warszawska 24, 31-155 Krakow, Poland

Deadline for manuscript submissions

20 August 2026

International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed

mdpi.com/si/248972

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

MDPI

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

MDPI

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, CAPlus / SciFinder, and other databases.

Journal Rank:

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