

Special Issue

Computational, Structural and Spectroscopic Studies of Macromolecules

Message from the Guest Editor

Understanding the structure and dynamics of macromolecules is essential to clarifying the complex nature of biological systems and promoting progress in fields like molecular and materials science, medicine, and biotechnology. Since macromolecules are so complex and have a variety of functions in life forms, understanding them is a challenge for scientists working in a wide range of fields. Our understanding of macromolecular systems can be improved by combining experimental data from various spectroscopy techniques with computer models. An updated overview of the computational, structural, and spectroscopic studies of macromolecules is intended to be provided by this Special Issue of the *International Journal of Molecular Sciences*, named “Computational, Structural and Spectroscopic Studies of Macromolecules”.

Guest Editor

Dr. Sanja Dolanski Babić

Department of Physics, Biophysics and Medical Physics, School of Medicine, University of Zagreb, 10000 Zagreb, Croatia

Deadline for manuscript submissions

10 September 2025



International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



mdpi.com/si/198294

*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*, ISSN 1422-0067) 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, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *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. Maurizio Battino

Department of Odontostomatologic and Specialized Clinical Sciences,
Sez-Biochimica, Faculty of Medicine, Università Politecnica delle
Marche, Via Ranieri 65, 60100 Ancona, Italy

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)