

## Special Issue

# DFT Study of the Structure, Spectroscopy and Properties of Biomolecules

### Message from the Guest Editor

DFT methods provide invaluable information, complementary to experimental data, on molecular systems and processes and, therefore, they represent very powerful tools for the interpretation and understanding of the experimental results. These methods, combined with quantum mechanics (QM), Molecular mechanics (MM), molecular docking and others, are very useful for the fundamental understanding of structure–activity relationships in biomolecules and also for applications in drug design and biotechnology. This Special Issue tries to introduce new interesting developments in the field of the molecular structure, vibrational spectroscopy and properties of biomolecules, especially those with chemical, pharmaceutical or biological interest. DFT applications to biomolecules, including molecular optimizations, structure predictions, inter-molecular interactions, spectroscopic calculations, as well as theoretical developments and experiments are welcome.

### Guest Editor

Dr. Mauricio Alcolea Palafox

Departamento de Química-Física, Facultad de Ciencias Químicas,  
Universidad Complutense de Madrid, 28040 Madrid, Spain

### Deadline for manuscript submissions

closed (28 December 2021)



## International Journal of Molecular Sciences

an Open Access Journal  
by MDPI

Impact Factor 4.9  
CiteScore 9.0  
Indexed in PubMed



[mdpi.com/si/88575](https://mdpi.com/si/88575)

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