

## Special Issue

# Combining Experimental Reaction Development with Quantum Chemistry and Machine Learning

### Message from the Guest Editor

This Special Issue welcomes synergic approaches containing experimental reaction development with quantum chemistry (QM) and/or machine learning (ML). Relevant examples might include studies in which QM mechanistic studies are employed to understand, improve or expand catalyzed reactions and organic synthesis. Furthermore, ML prediction of more efficient reaction components to improve reactivity and selectivity are similarly encouraged.

---

### Guest Editor

Dr. Juan Vicente Alegre-Requena

Instituto de Síntesis Química y Catálisis Homogénea (ISQCH) CSIC, Universidad de Zaragoza, C/Pedro Cerbuna 12, 50009 Zaragoza, Spain

---

### Deadline for manuscript submissions

closed (30 September 2023)



## International Journal of Molecular Sciences

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.9  
CiteScore 9.0  
Indexed in PubMed



[mdpi.com/si/134036](https://mdpi.com/si/134036)

*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)