



an Open Access Journal by MDPI

## Combining Experimental Reaction Development with Quantum Chemistry and Machine Learning

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)**

### Message from the Guest Editor

Dear Colleagues,

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.

Dr. Juan Vicente Alegre-Requena  
*Guest Editor*



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

# Special Issue



an Open Access Journal by MDPI

## 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

## 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.

## 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 (Inorganic Chemistry)

## Contact Us

---

*International Journal of Molecular  
Sciences* Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
www.mdpi.com

mdpi.com/journal/ijms  
ijms@mdpi.com  
X@IJMS\_MDPI