Special Issue

Computational Studies of Ionic Liquids and Their Analogues

Message from the Guest Editors

Dear colleagues, This Special Issue will explore the latest advances in the computational modelling of ILs and DESs, aiming to deepen our understanding of their complex behaviour. The methods include, but are not limited to, classic and ab initio molecular dynamics simulations, density functional theory, Monte Carlo methods, Cosmo-RS, and machine learning approaches. Through this collection, we aim to showcase the potential of computational chemistry to revolutionize the development and application of these next-generation solvents. Dr. Iuliia V. Voroshylova

Guest Editors

Dr. Iuliia Voroshylova
REQUIMTE-LAQV, Departamento of Chemistry and Biochemistry, Universidade do Porto, Porto, Portugal

Dr. Elisabete Ferreira
REQUIMTE-LAQV, Departamento of Chemistry and Biochemistry, Universidade do Porto, Porto, Portugal

Deadline for manuscript submissions

30 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/217927

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*, 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)