Special Issue

Computational Modeling of Ionic Liquids and Solutions for Modern Applications

Message from the Guest Editor

Computational simulations have become an extremely useful tool and complementary partner to experimental techniques for the investigation of myriad systems. The papers in this special issue are focused on the development of methods and application of computational techniques for the investigation of room temperature ionic liquids and related solutions for modern applications including solvation, catalysis, electrochemistry, etc. The purpose of this collection is to highlight the broad applicability of state-of-the-art computational modeling to address open questions in these types of systems.

Guest Editor

Prof. Dr. Jesse McDaniel Georgia Institute of Technology, Atlanta, GA, USA

Deadline for manuscript submissions

closed (30 June 2020)



International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9 CiteScore 9.0 Indexed in PubMed



mdpi.com/si/29519

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





International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9 CiteScore 9.0 Indexed in PubMed





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)