Special Issue

Calculations in Solution

Message from the Guest Editor

Many industrial processes, all the processes occurring within living organisms, and the processes occurring in the water bodies in our planet are all processes in which the relevant molecules are in solution. Solute molecules and solvent molecules interact, and these interactions cause changes in many properties of solute molecules, such as their conformational preferences, energetics, separation of the various types of energy levels and, therefore, electronic and IR spectra, NMR signals, the way in which molecules of different solutes interact with each other, etc. This Special Issue of *Computation* is devoted to the theoretical/computational study of molecules and molecular processes in solution. The scope of the Special Issue is broad, extending to all the aspects of these studies, from theoretical modeling to the study of specific molecules, classes of molecules or processes.

Guest Editor

Prof. Dr. Liliana Mammino
Department of Chemistry, University of Venda, Thohoyandou 0950, South Africa

Deadline for manuscript submissions

14 August 2025

Computation

an Open Access Journal by MDPI

Impact Factor 1.9
CiteScore 4.1

mdpi.com/si/108383

Computation
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
computation@mdpi.com

mdpi.com/journal/computation

Computation

an Open Access Journal by MDPI

Impact Factor 1.9
CiteScore 4.1

mdpi.com/journal/computation

About the Journal

Message from the Editor-in-Chief

You are invited to submit the results of your research for consideration and publication in *Computation,* an international open access journal, which is published monthly online by MDPI.
The editorial board and staff of *Computation* are dedicated to establishing a benchmark journal for the world scientific and engineering communities for original research articles, reviews, conference proceedings (i.e., peer reviewed full articles), and communications, in the cutting-edge areas of computational biology, computational chemistry, computational social science and computational engineering.

Editor-in-Chief

Prof. Dr. Ali Cemal Benim
Center of Flow Simulation (CFS), Department of Mechanical and Process Engineering, Duesseldorf University of Applied Sciences, D-40476 Duesseldorf, Germany

Author Benefits

High Visibility:

indexed within Scopus, ESCI (Web of Science), CAPlus / SciFinder, Inspec, dblp, and other databases.

Journal Rank:

JCR - Q2 (Mathematics, Interdisciplinary Applications) / CiteScore - Q1 (Applied Mathematics)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.7 days after submission; acceptance to publication is undertaken in 5.6 days (median values for papers published in this journal in the first half of 2025).

MDPI