Special Issue

Computational Investigation on Molecular Design, Structure, and Solvation

Message from the Guest Editor

Theoretical and computational chemistry as a research field has grown to complement experiments and assumed the mantle of guiding force in predictions and explorations in the fields of chemistry, biology, drug design, and all the interdisciplinary areas encompassed by these three. A rapid development and accessibility of computational hardware, robust code developments, and parallel deployments of codes in these new hardware have helped theoretical and computational chemistry to grow in leaps and bounds. This Special Issue titled “Computational Investigation on Molecular Design, Structure, Reactivity, and Solvation“ aims to bring the latest developments in the research areas covering molecular structure and/or activity prediction, chemical reactivity problems, chemical processes in liquid media, machine learning, and artificial intelligence in (bio)chemical (re)activity predictions.

Guest Editor

Dr. Dipankar Roy

Department of Mechanical Engineering, University of Alberta, 10-203 Donadeo Innovation Centre for Engineering, 9211-116 Street NW, Edmonton, AB T6G 1H9, Canada

Deadline for manuscript submissions

closed (31 July 2023)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/112365

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

mdpi.com/journal/molecules

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/journal/molecules

MDPI

About the Journal

Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt
Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

Author Benefits

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, MEDLINE, PMC, Reaxys, CaPlus / SciFinder, MarinLit, AGRIS, and other databases.

Journal Rank:

JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the first half of 2025).