Special Issue

Applications of Computational Chemistry Methods in Viral Diseases Research

Message from the Guest Editors

Computational chemistry has achieved maturity and, nowadays, is one of the central scientific fields in the pharmaceutical industry. It is crucial for planning the early stages of drug design projects, such as designing more efficient and economic synthetic routes for chemical administration, the screening of huge databases, as well as proposing hypotheses for the probable mechanisms of action of drugs in biological systems. Such endeavors are extremely complex and require the usage of modern and sophisticated approaches, such as artificial intelligence, data science, computational molecular simulations through classical mechanics and quantum mechanics, cheminformatics, applied mathematics, and biostatistics. This Special Issue of *Molecules* is dedicated to the application of these methods in medicinal computational chemistry, and we invite our fellow scientists to submit original papers or reviews that will enrich the state of the art in this field.

Guest Editors

Prof. Dr. Osvaldo Andrade Santos-Filho

Center of Health Sciences, Laboratory of Molecular Modeling and Computational Structural Biology, Federal University of Rio de Janeiro, IPPN, Av. Carlos Chagas Filho 373, Bloco H, Rio de Janeiro 21941-599, Brazil

Prof. Dr. Teodorico C. Ramalho

Department of Chemistry, Federal University of Lavras, P.O. Box 3037, Lavras 37200-000, MG, Brazil

Deadline for manuscript submissions

closed (30 June 2023)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/103574

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

About the Journal

Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 30th 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 all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of 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 15.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the second half of 2025).

MDPI