

Special Issue

Advances in the Theoretical and Computational Chemistry

Message from the Guest Editors

Reactivity, along with its structure, is at the core of chemistry, and is still a challenge because as the molecular or supra-molecular systems become more realistic and include explicitly more reactive environmental effects, electron transfer or photo-excitation processes, and cooperative interactions, theoretical chemistry needs to develop new approaches and algorithms to model, explain, or predict the reactivity within these systems. This Special Issue aims to provide a forum for the dissemination of the latest information on new computational and theoretical methods to describe and understand chemical reactivity.

Guest Editors

Dr. Aurora Costales

Department of Analytical and Physical Chemistry, University of Oviedo, 33006 Oviedo, Spain

Dr. Fernando Cortés-Guzmán

Instituto de Química, Universidad Nacional Autónoma de México, Ciudad Universitaria, Mexico City 04510, Mexico

Deadline for manuscript submissions

closed (31 August 2025)



Molecules

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed



mdpi.com/si/80592

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

[mdpi.com/journal/
molecules](https://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](https://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).