Special Issue

Environmental Pollutants and Oxidative Stress Chemistry

Message from the Guest Editors

Computational chemistry has emerged as one of the fastest growing and developing branches in chemistry. It has developed from initially treating small molecules with a handful of electrons to accurately modelling large systems with hundreds of atoms and predicting their various chemical and physical properties. The field has received significant recognition, with multiple Nobel prizes, from Kohn and Pople in 1998 to Baker, Hassabis and Jumper in 2024. Indeed, for decades, catalysis has played a crucial role in the development of human civilization. Catalytic technologies have been shown to have huge importance in industrial production, biological systems, environmental protection and green chemistry. The aim of this Special Issue is to provide readers with an overview of applications of computational chemistry in studying various homogeneous and heterogeneous catalytic reactions. Reviews, full papers and short communications covering the theory and application of computational studies of both catalytic and surface reactions are equally welcome. The submission of papers addressing the topics listed below is particularly encouraged.

Guest Editors

Prof. Dr. Leobardo Manuel Gomez-Olivan
Laboratorio de Toxicología Ambiental, Facultad de Química, Universidad Autónoma del Estado de México, Toluca 50120, Mexico

Dr. Gustavo Axel Elizalde-Velázquez
Laboratorio de Toxicología Ambiental, Facultad de Química, Universidad Autónoma del Estado de México, Toluca 50120, Mexico

Deadline for manuscript submissions

28 February 2026

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/255288

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 29th 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 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).

MDPI