



an Open Access Journal by MDPI

Advances in the Theoretical and Computational Chemistry

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:

30 September 2024

Message from the Guest Editors

Dear Colleagues,

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.

Dr. Aurora Costales

Dr. Fernando Cortés-Guzmán

Guest Editors



mdpi.com/si/80592

Special Issue



an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical
Biology and Phytochemistry,
University of Münster,
Corrensstrasse 48, D-48149
Münster, Germany

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.

Author Benefits

Open Access: free for readers, with [article processing charges \(APC\)](#) paid by authors or their institutions.

High Visibility: indexed within [Scopus](#), [SCIE \(Web of Science\)](#), [PubMed](#), [MEDLINE](#), [PMC](#), [Reaxys](#), [CaPlus / SciFinder](#), [MarinLit](#), [AGRIS](#), and [other databases](#).

Journal Rank: JCR - Q2 (Chemistry, Multidisciplinary) / CiteScore - Q1 (Chemistry (miscellaneous))

Contact Us

Molecules Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/molecules
molecules@mdpi.com
[X@Molecules_MDPI](https://twitter.com/Molecules_MDPI)