Special Issue

Theoretical Investigations of Reaction Mechanisms

Message from the Guest Editor

Knowledge of reaction mechanisms and driving forces of chemical processes is crucial for the molecular design, the optimization of reaction conditions, and the planning of a chemical synthesis. Elucidation of reaction mechanisms and key factors controlling chemical reactions may be effectively achieved using computational quantum chemical methods, which represent powerful tools for the interpretation and understanding of experimental results and provide invaluable information, complementary to the experimental data, about molecular systems and processes. Computational methods are indispensable for mechanistic studies of reactions proceeding via formation of short-lived intermediates that cannot be detected experimentally, being the only possibility to obtain information about intimate details of the chemical processes when experimental methods cannot help in the understanding of the reaction mechanisms. Previously unpublished manuscripts that report mechanistic studies of organic, inorganic or organometallic reactions with help of computational methods or deal with understanding of the key factors and driving forces governing chemical processes are welcome for this Special Issue.

Guest Editor

Dr. Maxim L. Kuznetsov

Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Avenue Rovisco Pais, 1049-001 Lisbon, Portugal

Deadline for manuscript submissions

closed (31 May 2019)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/14673

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 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).