



## Theoretical Investigations of Reaction Mechanisms

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)**

### 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 Previously unpublished manuscripts that report mechanistic studies of organic, inorganic or organometallic reactions with help of computational methods or deal with understanding of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.





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 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

## Contact Us

*Molecules* Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
[www.mdpi.com](http://www.mdpi.com)

[mdpi.com/journal/molecules](http://mdpi.com/journal/molecules)  
[molecules@mdpi.com](mailto:molecules@mdpi.com)  
[X@Molecules\\_MDPI](https://twitter.com/Molecules_MDPI)