

## Special Issue

# Halogen Bonds: Combining Experiment and Theory

### Message from the Guest Editor

In order to constructively contribute to these debates, particularly helpful is the combination of experimental and theoretical data, which can offer a unified and multi-faceted view of halogen bonding interactions. In this way, it is possible to provide a solid framework to interpret the present results and to plan future works. This Special Issue aims to present new interconnections between experimental and theoretical techniques, with the possibility to explore all fields of chemistry: halogen bond-catalyzed reactions, structure–property correlations, solution and solid-state spectroscopy, functional materials engineering. Therefore, original manuscripts (either full-length articles or short communications) reporting on the combination of experimental and theoretical data, and theoretical works strongly based on published experimental studies (and vice-versa), are welcome, together with perspective and review articles.

### Guest Editor

Prof. Dr. Gianluca Ciancaleoni

Dipartimento di Chimica e Chimica Industriale (DCCI) Università di Pisa,  
Via Giuseppe Moruzzi, 13, 56124 Pisa, Italy

### Deadline for manuscript submissions

closed (30 November 2019)



## Molecules

an Open Access Journal  
by MDPI

Impact Factor 4.6  
CiteScore 8.6  
Indexed in PubMed



[mdpi.com/si/21489](https://mdpi.com/si/21489)

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

---

### 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).