

Special Issue

σ and π Holes: A New Class of Non-Covalent Interactions

Message from the Guest Editor

For many years, the research field of the non-covalent interactions has been largely dominated by electrostatic interactions and especially hydrogen bonding interactions. Recently, the study of new non-covalent interactions, based on the existence of the denominated sigma or pi hole, has grown enormously from a theoretical and experimental point of view. Without any doubt, halogen bonding interactions have become in the most promising interactions and numerous examples have been reported. Motivated by the relevance of the results obtained for halogen atoms, many researchers have focused their research on the study of other groups: aerogen, chalcogen, pnictogen, tetrel and icosagen atoms. This Special Issue aims to highlight the role of this brand new form of noncovalent interaction that has recently appeared in several research fields, including catalysis, crystal engineering, molecular recognition, materials science, as well as theoretical aspects.

Guest Editor

Dr. Antonio Caballero

Departamento de Química Orgánica, Universidad de Murcia, Campus de Espinardo, E-30100 Murcia, Spain

Deadline for manuscript submissions

closed (30 April 2019)



Molecules

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed



mdpi.com/si/18007

Molecules
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
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 molecular chemistry, now in its 30th 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 15.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the second half of 2025).