



an Open Access Journal by MDPI

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

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)

Message from the Guest Editor

Dear Colleagues,

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.

Dr. Antonio Caballero
Guest Editor



mdpi.com/si/18007

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, Grosspeteranlage 5
4052 Basel, Switzerland

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

mdpi.com/journal/molecules
molecules@mdpi.com
[X@Molecules_MDPI](#)