



Chemometrics in Analytical Chemistry

Guest Editor:

Prof. Dr. Lukasz Komsta

Faculty of Pharmacy, Medical
University of Lublin,
Jaczewskiego 4, 20-090 Lublin,
Poland

Deadline for manuscript
submissions:

closed (31 December 2022)

Message from the Guest Editor

Dear Colleagues,

Due to the enormous development of computer technology during the last decades, chemometrics has become the leading and preferred methodology for the experimental data analysis, especially in analytical chemistry. A significant interest in chemometric methods is also connected with the availability of open-source software, removing the financial barriers of expensive software packages. Today, chemometric methods are available for every interested researcher equipped with an average computer.

Therefore, chemometrics can be present everywhere—from simple experimental designs, through multivariate analysis of collected data, up to huge datasets containing millions of samples or variables.

This Special Issue focuses on all aspects of chemometrics in analytical chemistry—experimental design, instrumental data analysis, signal processing, image processing, multivariate data mining, neural networks, genetic algorithms, multi-way methods, and multivariate curve resolution—both in context of new methods and algorithms, as well as novel applications of known approaches. Reviews are also welcome.

Prof. Dr. Lukasz Komsta
Guest Editor





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](#)