



an Open Access Journal by MDPI

## 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



[mdpi.com/si/105433](https://mdpi.com/si/105433)

# 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 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.

## 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](#)