

Special Issue

Data and Low-Data Tools for Artificial Intelligence in Medicinal Chemistry

Message from the Guest Editors

In the last few years, the scientific community has witnessed the renaissance of so-called “artificial intelligence” (AI) methods in many scientific domains. This unparalleled emergence of AI can also be observed in medicinal chemistry and toxicology, where machine learning is starting to be routinely applied for several tasks.

In this Special Issue, we welcome original research articles and reviews aimed to improve the current status of data and their usage for AI in medicinal chemistry and related fields. The Special Issue will include, but is not limited to, ligand- and structure-based approaches, molecular design, virtual screening, target identification, drug repurposing as well as bioactivity, safety, and ADMET property prediction. We particularly welcome papers focused on the creation and curation of novel datasets or describing the curation and/or usefulness of well-established databases. We also encourage the submission of papers addressing the development/application of AI approaches in low-data regimes. Papers providing accessible code and data are also particularly welcome.

Guest Editors

Dr. Angelica Mazzolari

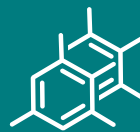
Department of Pharmaceutical Sciences, University of Milan, Via Mangiagalli 25, 20133 Milan, Italy

Dr. Francesca Grisoni

Department of Biomedical Engineering, Institute for Complex Molecular Systems, Eindhoven University of Technology, Groene Loper 3, 5612 AE, Eindhoven, The Netherlands

Deadline for manuscript submissions

closed (15 August 2022)



Molecules

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed



mdpi.com/si/69229

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 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).