

Special Issue

Artificial Intelligence for Drug Design and Discovery

Message from the Guest Editor

Given the growing implication of Artificial Intelligence methods in drug design (note the sharp increase in the number of publications devoted to this technique in PubMed), it seems necessary to review the status, opportunities, developments, challenges, and prospects in these methods and in their role to establish more efficient research strategies. Thus, the goal of this Special Issue would be to allow the drug designers involved in competitive research to measure the real interest in new algorithms for discovering innovative and more effective drugs. It is also important to point out the present limitations of the new methods in order to allow the readers to have an honest idea about the real contribution of AI for them.

Guest Editor

Dr. Bernard Maigret

LORIA Institute (Laboratoire Lorrain de Recherches en Informatique et Applications), Université de Lorraine, CNRS, INRIA, Vandoeuvre les Nancy, France

Deadline for manuscript submissions

closed (30 November 2020)



Molecules

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed



mdpi.com/si/42133

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 29th 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 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).