



an Open Access Journal by MDPI

Machine Learning in Green Chemistry

Guest Editors:

Dr. Tu Le

School of Engineering, RMIT
University, Melbourne, VIC 3001,
Australia

Dr. Haoxin Mai

School of Science, RMIT
University, Melbourne, VIC 3001,
Australia

Message from the Guest Editors

Machine learning has emerged as a powerful tool in green chemistry. It is a data-driven approach harnessing data analysis and computational models to revolutionize the design, optimization, and assessment of sustainable chemical processes. Through predictive modeling, pattern recognition, and informed decision making, machine learning techniques contribute to the development of environmentally friendly and economically viable chemical solutions.

Deadline for manuscript
submissions:

closed (31 December 2024)



mdpi.com/si/181763

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

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