

## Special Issue

# From a Molecule to a Drug: Chemical Features Enhancing Pharmacological Potential II

### Message from the Guest Editors

In this Special Issue, we intend to collect contributions (reviews and original research articles) dealing with successful stories of drug improvement or design by classic protocols, by quantum mechanical mechanistic investigation, or by hybrid approaches such as QM/MM or QM/ML (machine learning). Lastly, we also aim to receive works in which the drug design has been performed without computer help but in the lab with the help of chemical intuition and... serendipity! The common aspect that we stress is the recognition of chemical molecular motifs which are the key aspects for the drug potential. Topics of interest include, but are not limited to, the following:

- Antioxidants;
- Natural and semi-synthetic compounds;
- Natural supplements containing bioactive molecules;
- Improved bioactivity of known drugs;
- Drugs and drug-like compounds acting through multiple mechanisms of action.

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### Guest Editors

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### Deadline for manuscript submissions

closed (31 January 2025)



## Molecules

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## About the Journal

### 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.

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### Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

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#### 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 15.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the second half of 2025).