

# Special Issue

## Hot Trends in Computational Drug Design

### Message from the Guest Editor

This Special Issue aims to highlight recent progress and novel methodologies in computational drug design. We welcome contributions focusing on novel theoretical frameworks, algorithmic innovations, and practical applications in drug discovery and development. In this Special Issue, original research articles and reviews are welcome. Research areas may include (but are not limited to) the following:

- AI and machine learning in drug discovery;
- Molecular dynamics and docking simulations;
- Structure-based and ligand-based drug design;
- QSAR and cheminformatics;
- Virtual screening and pharmacophore modeling;
- De novo drug design techniques;
- Multi-target drug design and polypharmacology.

We look forward to receiving your contributions.

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### Guest Editor

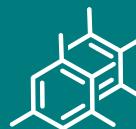
Prof. Dr. Agnieszka A. Kaczor

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### Deadline for manuscript submissions

30 April 2026



# 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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