

## Special Issue

# Advances in Chemical Research on Biomarkers, Drugs of Abuse, Medicines, and Computational Approaches

### Message from the Guest Editor

The editorial board of *Molecules* (IF: 4.2, ISSN 1420-3049) invites you to submit an article or review to a Special Issue entitled "Advances in Chemical Research on Biomarkers, Drugs of Abuse, Medicines, and Computational Approaches". This Special Issue seeks contributions on innovative bioanalytical methods for detecting disease biomarkers and drugs of abuse, new therapeutic agents, and molecular mechanisms, especially those elucidating protein structure and function. Research that leverages high-resolution analytical techniques (e.g., time-of-flight, Orbitrap, and mass spectrometry), as well as advanced computational methods such as molecular dynamics simulations, protein-ligand docking, and machine learning models, is particularly encouraged. We also welcome submissions focused on novel sample preparation methods, especially those promoting low-sample, low-cost, and low-solvent usage, as well as the analysis of alternative samples.

### Guest Editor

Dr. Huixiao Hong

National Center for Toxicological Research, U.S. Food and Drug Administration, 3900 NCTR Road, Building 5, Room 5C-109A, Jefferson, AR 72079, USA

### Deadline for manuscript submissions

30 June 2025



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## 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.

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### Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

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