Special Issue

Design, Synthesis, and Theoretical Studies of Enzyme Inhibitors

Message from the Guest Editors

The synthesis and evaluation of enzyme inhibitors contribute to the development of therapeutic agents for disease treatment and the production of environmentally safer pesticides, thereby offering significant benefits for both human health and sustainability. The development of enzyme inhibitors requires overcoming challenges of specificity, stability, and bioavailability, necessitating detailed structural analyses and advanced computational modeling to optimize selective binding to disease-associated enzymes. This Special Issue invites high□quality original research and comprehensive reviews on enzyme–inhibitor interactions, with emphasis on synthesis, biological evaluation, molecular modeling, and structure–activity relationship studies that advance innovative strategies in enzyme inhibition. Potential topics include, but are not limited to, the following:

- Innovative strategies in enzyme inhibitor design;
- Computational approaches to enzyme inhibitor discovery;
- In silico strategies for drug design;
- Molecular docking in therapeutic innovation;
- Specific enzyme inhibitors;
- Advancing therapeutics from molecules to medicine;
- Drug discovery and development.

Guest Editors

Dr. Nahit Gençer

1. Biochemistry Division, Faculty of Science & Art, Balikesir University, Balikesir, Türkiye
2. Department of Chemistry, Faculty of Science & Art, Balikesir University, Balikesir, Türkiye

Dr. Muhammed Tilahun Muhammed

Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Suleyman Demirel University, Isparta, Turkey

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Molecules
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
molecules@mdpi.com

mdpi.com/journal/molecules

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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.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt
Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

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