Special Issue

Design, Synthesis and Biological Evaluation of Medicinal Potential Compounds

Message from the Guest Editors

The design, synthesis, and biological evaluation of new compounds constitute a relevant strategy in modern drug discovery. The discovery and development of new modern drugs require a deep understanding of the biological pathways involved in the disease, as well as the structure of molecules that can act as bioactive compounds. Bioactive compounds are molecules that exert pharmacological and/or toxicological effects on a living organism, tissue, or cell, and can be extracted from natural compounds, mainly secondary metabolites, from plants or other types of living organisms. These compounds can also be obtained using different strategies, such as organic synthesis of new molecules, or via the modification of existing ones, followed by biological screening. In silico-based methods are being increasingly used to support the different steps of this process. This Special Issue aims to collect the most recent developments regarding the design, synthesis, and biological evaluation of bioactive compounds that can lead to an increase in natural or synthetic small active molecules in the search for promising new drugs to prevent and/or treat human diseases.

Guest Editors

Dr. Renato Emanuel Felix Boto

Prof. Dr. Paulo Jorge da Silva Almeida

Dr. Samuel Martins Silvestre

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

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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.

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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