Special Issue

Advances in Computational Chemistry for Drug Design, Discovery and Screening

Message from the Guest Editors

New advances in computational biology such as molecular modeling, molecular dynamics, virtual screening, and, more recently, artificial intelligence play more and more important roles. Many tedious and time-consuming steps can be replaced or facilitated by these technologies. This could lead to noticeable savings in the costs of modern drug discovery, in terms of both time and finance. Contributions to this Special Issue may cover all advances related to computational drug discovery, including new target identification, virtual screening, drug design, lead optimization, properties prediction by artificial intelligence, binding energy calculation, WebGL based real-time simulation and data analysis, molecular dynamics simulation, and drug re-purposing.

Guest Editors

Prof. Dr. Shuguang Yuan

Prof. Dr. Sławomir Filipek

Dr. Hideya Nakamura

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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 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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