

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

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Dr. Hideya Nakamura

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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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