Special Issue

Advances in Small Molecule Inhibitor-Based Drug Discovery Through Computational Chemistry

Message from the Guest Editors

The discovery and development of small molecule inhibitors remains a cornerstone of modern pharmacology, offering targeted therapeutic strategies across a wide range of diseases. In recent years, computational chemistry has emerged as a powerful ally in accelerating and refining this process. This Special Issue aims to highlight recent advances in the design, optimization, and validation of small molecule inhibitors using computational methodologies. Its contributions will explore a range of in silico approaches, including molecular docking, structure-based drug design, ligand-based screening, molecular dynamics simulations, quantum mechanics/molecular mechanics (QM/MM) techniques, and machine learning-based models. Emphasis will be placed on integrative strategies that bridge computational predictions with experimental validation, as well as on case studies demonstrating successful translation from virtual hits to biologically active compounds.

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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.

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