Special Issue

Selectivity and Theoretical Studies of Cycloaddition Reactions

Message from the Guest Editors

Cycloaddition reactions represent a cornerstone in synthetic organic chemistry, enabling the efficient construction of cyclic frameworks with full atomic economy. This Special Issue focuses on the selectivity (chemo-, regio-, and stereoselectivity) and theoretical studies of cycloaddition reactions, highlighting recent advances in mechanistic insights, computational modeling, and predictive design. Contributions will explore the interplay between electronic, steric, and catalytic control in governing reaction pathways, as well as the application of modern quantum chemical methods (e.g., DFT, MD, and machine learning) to elucidate pseudocyclic processes. Topics include [2+1], [2+2], [3+2], [4+2], [4+3], and higher-order cycloadditions, asymmetric variants, and emerging catalytic systems. By integrating experimental and theoretical perspectives, this Special Issue provides a comprehensive resource for researchers pursuing precision in carbo- and heterocyclic molecule synthesis.

Guest Editors

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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.

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