

Special Issue

Advancement of AI in Natural Product Chemistry

Message from the Guest Editors

The integration of artificial intelligence (AI) into natural product research presents an innovative solution for accelerating the isolation, characterization, and application of natural products in drug development. Leveraging AI algorithms has the potential to enhance the precision and efficiency of discovering novel bioactive compounds and molecular scaffolds. This approach helps to overcome traditional hurdles related to complex data interpretation and advances methodologies for structural elucidation and diverse applications of natural products.

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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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