Special Issue

Natural Product-Inspired Drug Discovery: From Molecular Design to Safety and Translational Pharmacology

Message from the Guest Editors

About 50% of today's pharmaceuticals are natural products (NPs), NPs derivatives, NPs-mimics or synthetics based on NPs pharmacophores or mimics. NP-based drugs have been especially successful in oncology, infectious diseases, and CNS disorders such as neurodegeneration, cognitive decline, and pain. Derived from plants, microbes, or marine organisms, NPs offer regioselective scaffolds due to enzymatic biosynthesis. However, many promising leads fail in clinical development due to poor PK/PD profiles, off-target effects, or metabolic issues. Early molecular design and the use of RNA/DNA sequencing, bioinformatics, AI/ML, and modeling tools are essential to improve safety, selectivity, and clinical success. This Special Issue invites studies focused on NP-based molecular design, safety, pharmacokinetics/dynamics, and translational potential.

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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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