Special Issue

Novel Inhibitors: Design, Synthesis, Biological Activities and Modelling Studies

Message from the Guest Editors

Altering enzyme activity has profound biological and medicinal effects; thus, enzyme inhibitors enable the selective inhibition of essential pathogenic enzymes (acting as antibiotics, antivirals, or antiparasitic agents) or of aberrant human enzymes (correcting for a pathological condition). Enzyme inhibitors may bind irreversibly (through covalent bonding) or reversibly (through non-covalent bonding), but in either case, drawbacks to the inherent mechanism of action must be considered, adding additional barriers to the development of viable inhibitors. This Special Issue pays homage to the drug discovery progress of inhibitors, which requires exceptional dedication, skill, and creativity. For this Special Issue, we welcome papers that highlight the development and biological evaluation of organic compounds (this can be addressed from several sub-disciplines, including medicinal chemistry, total synthesis, natural product chemistry, and computational chemistry).

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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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