

Special Issue

Combinatorial, Computational and High Throughput Screening for Bioactive/Lead Finding from Nature/Synthesis

Message from the Guest Editor

High throughput screening has been considered since last century as a meaningful strategy for the discovery of bioactives from different sources and to enhance the finding of leads that become clinical candidates as effective therapies in different problems/disorders/diseases. In this sense, combinatorial chemistry was firstly employed in those purposes, due to their remarkable influence on the expansion of the available chemical through generation of a large sets of structurally-related substances from different synthetic procedures. Computer-aided design and in-silico protocols/approaches have been also considered as a high throughput screening and they were rapidly used to improve, filtrate and/or deplete the lead/hit finding with high efficiency/efficacy. This Special Issue aims to collect some of the latest advances, techniques, approaches, methods, outcome and reviews on topics related to finding/identification of bioactives/hits/leads from natural sources and/or through synthetic procedures using combinatorial, computational, chemometrics and/or other high throughput approaches.

Guest Editor

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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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