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 depurate the lead/hit finding with high efficieny/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 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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