Special Issue

NMR Spectroscopy in Drug Discovery Research

Message from the Guest Editor

NMR spectroscopy is an ideal technique to study target–ligand interactions that are at the basis of drug discovery research. Due to tremendous improvements, affecting both hardware and methodologies, including the introduction of fast NMR data acquisition, novel NMR screening routes for fragment-based drug discovery and development (FBDD) have been set up to identify small molecules binding to a specific target. This Special Issue will be centered on the above presented topics and looks for contributions (communications, full papers, and reviews) related to the latest trends in NMR-based drug discovery research. In detail, this Special Issue intends to collect studies related to the development of novel NMR methods for screening libraries of compounds and investigating target–ligand interactions and more application-oriented works concerning with NMR-driven identification of compounds targeting specific targets or protein–protein interactions. Works conducted by integrating NMR data with those from other experimental techniques along with computational tools are highly welcome.

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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