Special Issue

NMR in the Drug Design

Message from the Guest Editor

NMR spectroscopy has been widely applied in the early stages of drug discovery. It is especially suited to the structure-based approach in lead design strategies, as it is the most powerful method for studies of structure, dynamics, and the interaction of molecules in solution. With the development of cryogenic NMR probe technology, it has also become a high-throughput screening method, which is particularly powerful for the identification of the binding of low-affinity, low-molecular-mass fragments in fragment-based drug design. NMR spectroscopy can provide atomic resolution insight with regard to both molecular structure and dynamics. Such combined structure-dynamic insight can improve the efficiency of structure-based design and accelerate the discovery of novel drugs.

The aim of this Special Issue is to attract contributions on all aspects of the application of NMR spectroscopy in the design and discovery of drug candidates, with special emphasis on the NMR studies addressing molecular flexibilities in relation to the biological profile of drug candidates or the druggability of targets.

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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