



an Open Access Journal by MDPI

NMR in the Drug Design

Guest Editor:

**Prof. Dr. Simona Golič
Grdadolnik**

Laboratory for Molecular
Structural Dynamics, National
Institute of Chemistry Hajdrihova
19, SI-1000 Ljubljana, Slovenia

Deadline for manuscript
submissions:

closed (15 December 2020)

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.



mdpi.com/si/29321

Special Issue



an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical
Biology and Phytochemistry,
University of Münster,
Corrensstrasse 48, D-48149
Münster, Germany

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.

Author Benefits

Open Access: free for readers, with [article processing charges \(APC\)](#) paid by authors or their institutions.

High Visibility: indexed within [Scopus](#), [SCIE \(Web of Science\)](#), [PubMed](#), [MEDLINE](#), [PMC](#), [Reaxys](#), [CaPlus / SciFinder](#), [MarinLit](#), [AGRIS](#), and [other databases](#).

Journal Rank: JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

Contact Us

Molecules Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/molecules
molecules@mdpi.com
[X@Molecules_MDPI](#)