

## Special Issue

# NMR Spectroscopy in Structural Biology and Drug Discovery Research

### Message from the Guest Editors

We are glad to announce the launch of this *Molecules* Special Issue, “NMR Spectroscopy in Structural Biology and Drug Discovery Research”. This Special Issue intends to collect communications, full papers, and reviews related to the cutting-edge trends in NMR-based structural biology and drug discovery research. In detail, this Special Issue will focus on both technical studies such as those related to the development of 1-novel NMR screening libraries, 2-original NMR screening strategies that go beyond classical FBDD (fragment-based drug-discovery) approaches, and more application-oriented works concerning the NMR-driven identification of novel ligands of target macromolecules (including, but not limited to, proteins and protein/protein interactions playing crucial functions in cancer onset and progression, as well as neurodegenerative disorders). Research articles reporting on multidisciplinary studies deriving from merging virtual screening outcomes with NMR data, along with those deriving from other experimental techniques, are highly welcome.

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### Guest Editors

Dr. Marilisa Leone  
Dr. Flavia Anna Mercurio  
Dr. Marian Vincenzi

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### Deadline for manuscript submissions

30 June 2026



## Molecules

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## About the Journal

### 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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### Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

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

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