

## Special Issue

# Solution NMR Spectroscopy in the Early Stage of Target-Based Drug Discovery

### Message from the Guest Editor

Structure-based drug design is a powerful strategy in drug discovery, while knowing the structures of the targets and their complexes with developed compounds is indispensable. Despite some challenges, solution NMR spectroscopy plays important roles in determining the structures and dynamics of a protein and its complexes, meaning that NMR spectroscopy plays an important role in target-based drug discovery. This Special Issue covers the application of solution NMR spectroscopy in the early stage of target-based drug discovery, which usually consists of steps of hit screening, hit conformation, hit to lead, and lead optimization. Papers related to the structural determination of a macromolecule, molecular interactions between a protein and compound, NMR in fragment-based drug discovery, and others related to drug discovery, will be considered for this Special Issue.

### Guest Editor

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### Deadline for manuscript submissions

closed (31 August 2021)



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### Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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