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Applications of NMR Spectroscopy in Structure-Based Drug Discovery

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Message from the Guest Editors

NMR is a supremely versatile experimental technique whose unique strengths have been widely exploited to enable the discovery, characterization and optimization of bioactive molecules with the potential to become new drugs. In this Special Issue, we chart the evolution and application of NMR spectroscopy to structure-based drug discovery, both within industry and in academic labs. From its origins as a largely analytical technique for small-molecule characterization, through the ‘boom years’ of the 1990s and X-ray vs. NMR ‘structure wars’, the emergence of NMR-driven fragment-based drug discovery, and the maturation of NMR as a ‘gold-standard’ method for verification, characterization and annotation of lead–target interactions, NMR has continued to adapt and evolve as the demands and priorities of modern drug discovery have shifted.



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