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Harnessing the Power of NMR in Drug Discovery

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Abstract

Nuclear Magnetic Resonance (NMR) spectroscopy has emerged as a powerful and versatile tool in drug discovery, explores the various applications of NMR spectroscopy in drug discovery, including ligand screening, protein-ligand

advancements in NMR technology, such as high-throughput screening methods and the development of selective power of NMR spectroscopy holds great promise for accelerating the drug discovery process and driving innovation in

pro ling of small molecule metabolites in biological samples [8]. Metabolomic pro ling using NMR can identify biomarkers associated with disease states, drug response, and toxicity, providing valuable insights into disease mechanisms and drug e ects. By integrating metabolomic data with other omics datasets, such as genomics and proteomics [9], NMR enables the identication of novel drug targets and the development of personalized therapeutic strategies.

In vivo imaging and pharmacokinetics: In addition to its applications in vitro, NMR spectroscopy is utilized for in vivo imaging and pharmacokinetic studies in preclinical drug development. Magnetic resonance imaging (MRI) and magnetic resonance spectroscopy (MRS) enable non-invasive visualization and quanti cation of drug distribution, metabolism, and pharmacokinetics in animal models and humans [10]. NMR-based imaging techniques provide valuable pharmacokinetic data for drug candidates, helping to optimize dosing

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Nuclear Ma ace (NMR) spectroscopy has become scovery, providing essential insights an indispensable to into molecular struc ics, and interactions. From target ead optimization and preclinical identi cation and valid able researchers to unravel the development, NMR tec complexities of biological d design novel therapeutics with As NMR technology ensitivity, resolution, overy is poised to grow, driving and automation, its impact of innovation and accelerating lopment of new medicines to address unmet medical need

References

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