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High-resolution NMR spectroscopy applied for field inhomogeneity and spectral congestion

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NMR spectroscopy presents a non-invasive detection technique for molecular structure elucidation and dynamic effect analyses. In general NMR applications, spectral resolution is the key index determining the availability of resulting spectra. Due to limited chemical shift ranges and appended J coupling splittings, conventional ^1H NMR spectra are subject to spectral congestions in complex samples. In addition, there exist adverse experimental conditions in which magnetic fields suffer from spatial or temporal inhomogeneity, constituting the second factor degrading spectral resolution in ^1H NMR applications. Therefore, an NMR method available for high-resolution NMR measurements under the condition of inhomogeneous fields and complex samples is greatly demanded.

In our previous studies, a series of NMR methods based on intermolecular multiple-quantum coherence (iMQC)[1] is proposed for high-resolution applications in inhomogeneous magnetic field conditions. And other pure-shift based methods are also designed to eliminate J coupling splittings and further enhance spectral resolution.[3] For example, a high-resolution NMR method, named UPSIF, has been proposed to extract high-resolution 1D pure shift or 2D J-resolved spectra, suitable for direct analyses on biological samples. The proposed method is designed based on the combination of constant-time module and iMQC scheme. The constant-time module constitutes a direct decoupling manner for removing J couplings and extracting pure chemical shifts. The iMQC scheme is proved to be immune to field inhomogeneity. The performance of the proposed high-resolution method is demonstrated by experiments on biological samples with intrinsic field inhomogeneities and in situ electrochemical detection under externally adverse field conditions. Our proposed methods can be applied for high-resolution measurements under the condition of field inhomogeneity and spectral congestion.

Reference

[2] Z. Chen, S.H. Cai, Y.Q. Huang, Y.L. Lin, *Prog. Nucl. Magn. Reson. Spectrosc.*, 90-91, 1-31, 2015.

[3] K. Zangger, H. Sterk, *J. Magn. Reson.*, 124, 486-489, 1997.

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