Line broadening interference for high-resolution MRS under inhomogeneous magnetic fields

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Target audience

Those who are engaged or interested in the field of high-resolution magnetic resonance spectroscopy (MRS) under inhomogeneous fields, e. g. in biological tissues or at interfaces among bones and tissues, and expect a method with high signal-to-noise ratio (SNR) are target readers.

Purpose

MRS serves an important tool for analyzing biological metabolites and medical treatments. Unfortunately, *in vivo* study inevitably suffers from magnetic-field inhomogeneity, which may arise due to susceptibility variations etc. As a result, the performance of MRS will degenerate due to the broadening effect induced by inhomogeneous fields. Conventionally, various techniques, including zero-quantum coherence (ZQC) [1], spin-echo correlation spectroscopy (SECSY) [2], magic-angle spinning (MAS) [3] and intermolecular multi-quantum coherence (iMQC) [4], have been proposed to enhance the performance of MRS under these circumstances. However, ZQC and SECSY merely exhibit chemical-shift differences among scalar-coupled resonances; MAS sets strict and special requirements on hardware and may damage samples due to high spin rates; iMQC techniques are associated with intrinsic low SNRs. In this study, a method addressed as line broadening interference (LBI) is proposed for yielding high-resolution information under inhomogeneous fields by taking advantage of the inhomogeneity-induced line broadening.

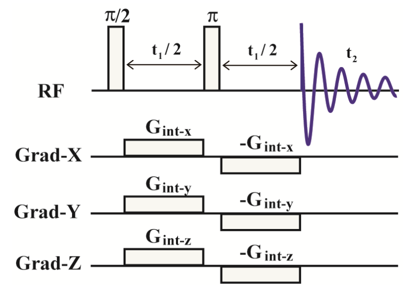

Fig. 1. Schematic diagram of the line broadening interference method; G_{int-x}, G_{int-y}, G_{int-z} denotes interferential gradients along the X, Y and Z axes, respectively.

Method

As the schematic diagram shows, the LBI sequence starts with an hard 90^{o} pulse to excite all longitudinal magnetizations, follows an spin echo module for refocusing the chemical shifts along with dephasing induced by field inhomogeneity, and ends up with the regular acquisition. Note that the spin echo module is implemented in unison with bipolar gradients along three orthogonal axes (denoted as interferential gradients). With the interferential gradients, the line broadening orientations will be interfered, thus avoiding overlapping among adjacent resonances and restoring high-resolution information. Furthermore, an inhomogeneity correction algorithm is developed based on pattern recognition to recover the high-resolution information from LBI spectra [5]. For demonstrating the principle and feasibility of the LBI method, experiments on a phantom solution, which comprises of ethyl 3-bromopropionate and 2-butanone in identical volume, were conducted. The shimming coils of X1, Y1, Z1, and Z2 were detuned to simulate the 3D inhomogeneous field. In practical applications, the LBI can be implemented in two styles: first, when the field inhomogeneity is primarily along one axis, only the interference gradient along the same axis retains and the other two are removed; second, when the field inhomogeneity distribute comparably along three orthogonal axes, the three interference gradients should be set with certain proportions according to pre-acquired field map.

All experiments were carried out at 298 K on a NMR System (Varian 500 MHz, Agilent Technologies, Santa Clara, CA, USA) equipped with a 5-mm indirect detection probe and three-dimensional pulse field gradients. Raw data were all processed with in-house programs developed with MATLAB and all data matrices were zero-filled to ensure digital resolutions in both F1 and F2 dimensions.

Results and discussion

The experimental results under the 3D inhomogeneous field are presented in Fig. 2. The conventional single-pulse sequence merely exhibits broad envelops at every resonance. The spectral resolution is insufficient to provide meaningful information. With the LBI, the spectral lines are recorded in a non-overlapping way, and high-resolution information is thus retained (Fig. 2b). The curved broadened lines can then be corrected with the aid of inhomogeneity correction algorithm, as shown from Fig. 2b to Fig. 2c. The projection onto the F2 dimension offers the high-resolution chemical shift information along with accurate scalar-coupling splitting, as shown in Fig. 2d. The triplets at 1.02, 1.30, 2.98 and 3.69 ppm, singlet at 2.13 ppm, and quartets at 2.50 and 4.19 ppm can all be well-resolved in Fig. 2d. In order to investigate the SNR performance of LBI, we performed LBI on a sample of low concentration (5 mM) under inhomogeneous fields. The experimental results (not provided here) verified the SNR advantage of LBI under inhomogeneous fields.

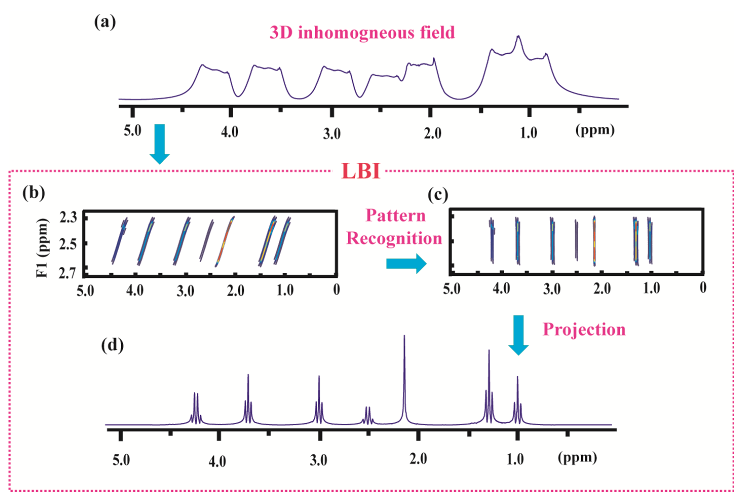

Fig. 2. Spectra of phantom solution under the XYZ inhomogeneous field. (a) denotes the spectrum by single-pulse sequence; (b) original LBI spectrum; (c) high-resolution spectrum after pattern recognition based inhomogeneity correction of (b); (d) the projection spectrum of (c) onto the F2 dimension.

Conclusion

From the experimental results, the LBI method is capable of performing well under 3D inhomogeneous magnetic fields. The high-resolution information, including chemical shifts and scalar coupling splitting, can be recovered with the aid of inhomogeneity correction algorithm. Based on its robustness against magnetic-field inhomogeneity and elegant SNR performance, the LBI may prove helpful in analyzing inhomogeneous systems, including biological tissues etc.

Acknowledgments

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