Fast acquisition of high-resolution MRS in inhomogeneous fields via intermolecular single-quantum coherences

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Introduction

Since the line-widths of conventional liquid NMR signals are proportional to the overall magnetic field homogeneity of the sample, NMR experimental techniques based on intermolecular zero-quantum coherences such as HOMOGENIZED [1] were developed to obtain high-resolution spectra in inhomogeneous fields. Recently, we proposed three pulse sequences: SEL-HOMOGENIZED [2], IDEAL [3], and IDEAL-II and IDEAL-III [4]. Although the latter two sequences give higher resolution and signal-to-noise ratio than the former one, they magnify the scalar coupling constants and will aggravate the coupling pattern of strong coupling systems. To solve this problem, the IDEAL-IV sequence based on intermolecular single-quantum coherences (SQCs) was designed.

Methods

Fig.1 shows the pulse sequence of IDEAL-IV. To understand how it works, we consider a spin system consisting of different molecules of *I* (solvent) and *S* (solute), with subscripts of flip angles denoting the spin selectively excited. If $\Delta B(x, y, z)$ is the width of the spatially dependent field inhomogeneity, both the resonance frequencies for the S spins in the F2 and F1 dimensions range between $\Delta\omega_{SQC}(x, y, z) = \omega_S \pm (1/2)\gamma\Delta\omega(x, y, z)$. Therefore, the separate streaks in IDEAL-IV spectra are along the specific direction $\phi = \text{arctg}(1) = \pi/4$, where ϕ is the angle with respect to the F2 axis. Different from IDEAL and IDEAL-II methods, the spins of the solute evolve under *J* coupling only in F2 dimensions, so that the scaling factor of the multiplet splitting is 1, the same as conventional high-resolution ^{1}H spectra. Therefore, the sequence maintains the multiplet pattern in the strongly coupled system. Since the spatial correlation via dipolar field of the solvent affects all the spins of the solutes equally, the relative areas and chemical shifts from intermolecular SQCs are the same for all resonances as those in routine 1D NMR spectrum. To test the IDEAL-IV pulse sequence, a sample of brain phantom solution in an inhomogeneous field (~60Hz in line-width) was measured with a Varian Unity+ 500 spectrometer. An 8-step phase cycling was used, and the coherence selection gradients with strength $G \approx 0.08$ T/m and the duration $\delta = 1.2$ ms were applied.

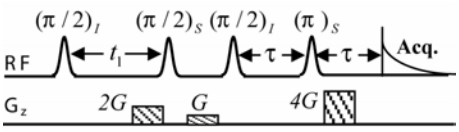

Fig. 1. IDEAL-IV pulse sequence

Results and Discussion

The experimental results of the brain phantom sample are presented in Fig. 2. To obtain a projection spectrum similar to a conventional 1D one, an anticlockwise rotation of $\pi/4$ was performed to the IDEAL-IV spectra. After this shearing operation, a projection along the F1 direction maintains chemical shifts, relative areas, coupling constants, and multiplet patterns while inhomogeneous broadening is suppressed (Fig. 3(b)). The projection of the 2D spectrum (Fig. 3(b)) has much higher resolution than the original 1D spectrum shown in Fig. 3(a). The line-width is reduced from 60 to 3 Hz, remarkably similar to the conventional high-resolution 1H spectrum (Fig. 3(c)). Similar to IDEAL-II method, all rows of data streaks are located in the center of F1 dimension and occupied a narrow range of frequency in F1. This enables a large decrease in experimental time and data space.

Based on long-range dipolar interactions between spins of solvent and solute molecules, a modified pulse sequence, IDEAL-IV, was proposed to obtain high-resolution spectra in inhomogeneous fields maintaining all conventional chemical shifts, coupling constants, patterns of multiplicity, and relative areas. Compared to the IDEAL and IDEAL-II methods, the IDEAL-IV method possesses the following advantages: (1) same scale factor of *J* coupling constants as conventional spectra; (2) high suppression of solvent peak such as water; and (3) slow relaxation decay during the evolution period. Potential applications of the method include in vivo NMR spectroscopy, where the field homogeneity is always degraded and the transverse relaxation time is always shorten by the widely distributed magnetic susceptibilities among various tissues and cellular structures. Potentials of the IDEAL-alike sequences have been demonstrated but intrinsic low SNR remains an issue. Improvement of pulse sequences and optimization of experimental parameters are still needed for practical applications.

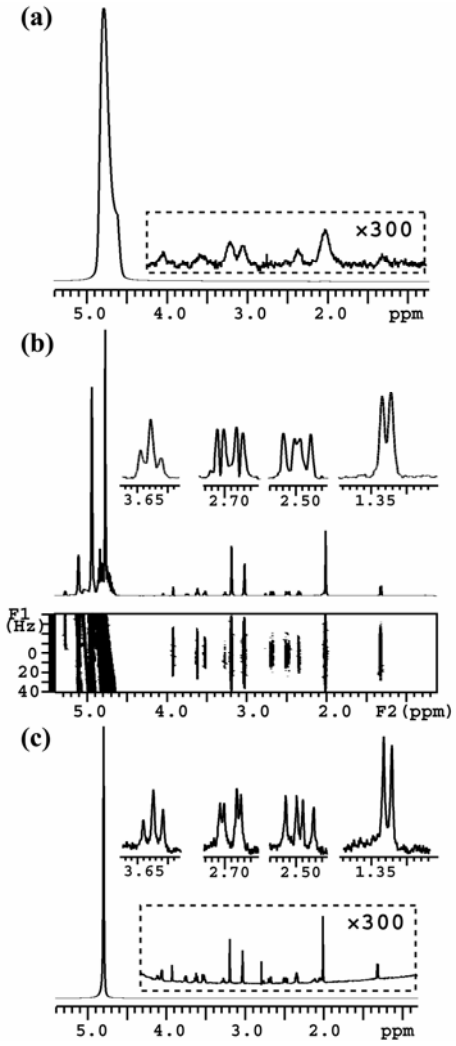

Fig. 2. ^{1}H NMR spectra of brain phantom solution. (a) Conventional 1D spectrum acquiring in an inhomogeneous field, (b) IDEAL-IV spectrum and its projection, and (c) conventional 1D high-resolution spectrum.

Acknowledgments

This work was partially supported by the NNSF of China under Grants 20573084 and 10575085, and NIH under Grant NS41048.

Reference

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