

Ultrafast 2D high-resolution COSY spectra in inhomogeneous fields

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Introduction

Intermolecular multiple-quantum coherences (iMQCs) originated from distant dipolar field (DDF) possess numerous interesting properties [1]. They have been developed for high-resolution magnetic resonance spectroscopy (MRS) under inhomogeneous fields [2]. These high-resolution iMQC methods mostly based on 1D projection from 2D iMQC spectra [2]. However, 2D high-resolution MRS is often necessary for complex spin systems. Recently, an iMQC method was proposed to obtain high-resolution COSY spectra in inhomogeneous fields [3]. However, this method is very time consuming since it needs routine 3D acquisition, which limits its application. Thus it would be of great value to establish a fast acquisition method. In this abstract, Hadamard method was introduced to speed up the acquisition. The time for a high-resolution COSY spectrum under inhomogeneous fields can be reduced to about ten minutes.

Experiments and results

Experiments were performed at 298 K on a 500 MHz NMR spectrometer (Varian NMR System, USA) using a 5 mm indirect detection probe with three-dimensional gradient coils. The sample is a solution of dichloromethane and aether in acetone. The pulse sequence for high-resolution iMQC COSY was shown in Fig. 1, where $\tau = 20$ ms and TR = 0.8 s were used. The first pulse was a polychromatic pulse. Before the individual soft pulses were combined into a polychromatic pulse, the RF pulses were coded (+ or -) according to the rows of the Hadamard H8 matrix [4]. If the part before the second pulse is deleted, the remnant sequence is a standard IDEAL-II sequence [5]. The experimental results are shown in Figs. 2–4. Fig. 2 was obtained by conventional COSY sequence under a well-shimmed magnetic field, and Fig. 3 was obtained by conventional COSY sequence under an inhomogeneous field created by deliberately detuning the Z1 shim coil to produce a spectral linewidth of 60 Hz. In the same inhomogeneous field, experiment was performed using the pulse sequence shown in Fig. 1. Totally 8 scans were acquired according to the Hadamard H8 matrix. Each scan finished in about one minute and produced a 2D IDEAL-II spectrum. The total acquisition time was less than 10 minutes. After the Hadamard decoding, eight 2D spectra were got. Eight high-resolution 1D spectra can be obtained by projection the 2D spectra along the horizontal axis after a shearing procession. Based on the eight 1D spectra, a high-resolution COSY spectrum can be constructed according to the Hadamard matrix, as shown in Fig. 4.

Discussion

As we can see, the inhomogeneous field leads to line broadening along the diagonal direction of the spectrum (Fig. 3). The J coupling splitting patterns can hardly be resolved in either the 2D spectrum or the projection spectra. Furthermore, the inhomogeneous line broadening may lead to overlap of neighboring diagonal resonances in the 2D spectrum. The COSY spectrum obtained from the new pulse sequence under the inhomogeneous field has comparable high resolution (Fig. 4) to the one obtained under homogeneous field from the conventional COSY method (Fig. 2). Both chemical shift and J scaling information are preserved, and peak overlapping can be avoided. Since the J coupling constants are scaled up by 3 times, this sequence is helpful for the detection of weakly-coupled spin systems.

Acknowledgment

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References

- [1] Galiana G, et al. *Science*, 322 (2008) 421-424.
- [2] Chen Z, et al. *J. Am. Chem. Soc.* 126 (2004) 446-447.
- [3] Chen X, et al. *ISMRM* 17 (2009) 4267.
- [4] Kupce E, et al. *J. Magn. Reson.* 162 (2003) 300-310.
- [5] Chen Z, et al. *J. Chem. Phys.* 130 (2009) 084504.

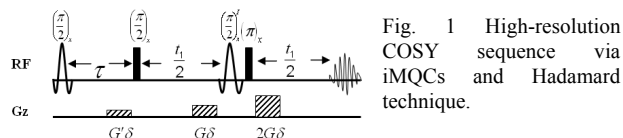


Fig. 1 High-resolution COSY sequence via iMQCs and Hadamard technique.

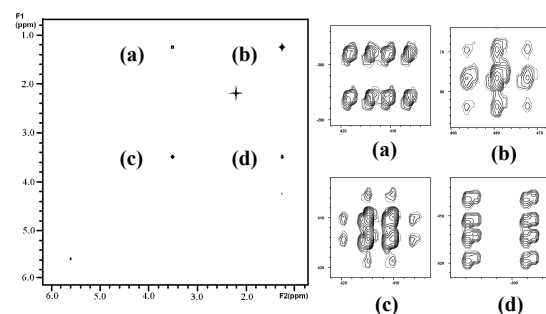


Fig. 2 Conventional COSY spectrum in homogeneous field. The regions labeled as (a), (b), (c) and (d) were expanded for comparison.

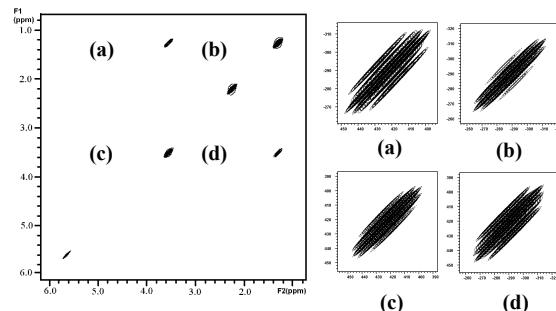


Fig. 3 Conventional COSY spectrum in inhomogeneous field with about 60 Hz linewidth. The regions labeled as (a), (b), (c) and (d) were expanded for comparison.

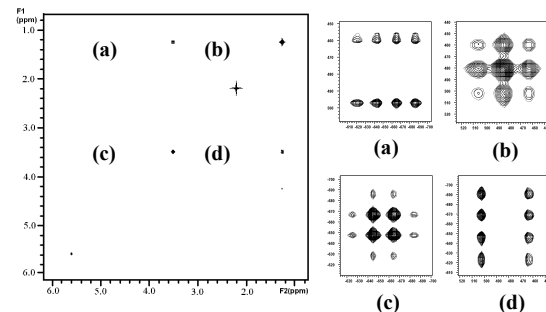


Fig. 4 High resolution COSY spectrum obtained by the pulse sequence shown in Fig. 1 in inhomogeneous with about 60 Hz linewidth. The regions labeled as (a), (b), (c) and (d) were expanded for comparison.