High-resolution 2D MR spectroscopy via intermolecular multiple-quantum coherences

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Introduction

Intermolecular multiple-quantum coherences (iMQCs) have been utilized to achieve high-resolution 1D spectrum under inhomogeneous fields. The high-resolution iMQC spectroscopy uses two-dimensional approach to average out inhomogeneous broadenings by correlating the iMQC transition and the conventional single-quantum coherence (SQC) one. After the shearing processes, the high-resolution 1D spectrum free of line broadening can be extracted from the projection along one dimension of the processed 2D spectrum; the information along the other dimension, however, will be discarded since it contains only inhomogeneous broadenings. The high-resolution iMQC spectroscopy have been applied to the MRS of the field-distorted voxel, where the spectral linewidths are broadened by the magnetic field gradients caused by susceptibility differences between tissues, bones and air.

2D MRS such as J-resolved spectroscopy (J-RES) and COSY have been explored to obtain better signal separations in the 2D spectra. However, line broadenings still occur in these 2D spectra and lead to overlapping of adjacent resonances. In this abstract, we extend the 1D high-resolution iMQC spectroscopy to 2D, using a three-dimensional approach to achieve a 2D MRS free of inhomogeneous broadening.

Methods

Similar to 1D high-resolution spectroscopy via two-dimensional iMQCs, the directly-acquired dimension (t₁) of the proposed three dimensional approach is conventional SQCs and is subject to inhomogeneous broadenings. On the other hand, the other two dimensions (t₁ and t₂) are either refocused iMQCs or spin echoes, both of which are insensitive to inhomogeneous fields. Normally, the acquisition time of the 3D spectrum would be unbearable for in vivo measurements. Therefore, fast acquisition schemes such as delay acquisition and foldover correction (FOC), can be used to reduce one of the indirect spectral width, and thus the scanning time.

The sequences of high-resolution COSY and J-RES are presented in Fig. 1a and 1b, respectively. In the COSY sequence, the t₁ and t₂ periods are i2QC and iDQC evolutions, respectively. The t₂ period utilizes the delay-acquisition scheme to reduce the scanning time, thus the apparent J coupling constant is scaled up by 3 times. In the J-RES sequence, the t₁ period is iZQCs and the t₂ period is spin echo. The t₁ period utilizes the FOC scheme to speed up the scanning.

All experiments were performed using a Varian NMR System 11.7 T with a 5 mm indirect detection probe. The parameters of coherence selective gradients are \( G' = 0.07 \text{ T m}^{-1} \times 1.2 \text{ ms} \) and \( G = 0.16 \text{ T m}^{-1} \times 1.2 \text{ ms} \) respectively. A 2-step phase cycling was applied: \( \phi = (x, y) \) and receiver = (x, −x). A solution of butanone in cyclohexane (molar ratio = 1:1000) was for the COSY measurements. 192 × 16 × 300 points were acquired with spectral widths of 1200 × 100 × 1200 Hz (F1 × F2 × F3) in 2 h. TR / TE = 1/0.1 s. A water solution containing 10 mM histidine and 10 mM lactate was used for the J-RES experiments. 12 × 10 × 256 points were acquired with spectral widths of 100 × 40 × 4000 Hz (F1 × F2 × F3) in 20 min. The average number was 4 and TR = 2 s.

Results and discussion

A conventional COSY spectrum is presented in Fig. 2a. Broadened lines stretch at the diagonal direction. The projections of both dimensions are subject to line broadenings. The high-resolution COSY spectrum is presented in Fig. 2b. Both dimensions are free of line broadening. The J coupling constants in the F2 dimension are scaled up by 3 times. The conventional and high-resolution J-RES spectra are presented in Fig. 3a and 3b, respectively. The broadened lines stretch along the F2 dimension in Fig. 3a and cause overlapping of strongly-coupled resonances of histidine. In Fig. 3b, these two resonances are well separated and the strongly-coupled artifact can be observed.

The above results primarily present the feasibility of the proposed 2D MRS sequences. For the SNR consideration, the iMQC based high-resolution sequences are more applicable on animal studies with high-field scanning systems. The scanning time of the 3D sequences can be further reduced by using multi-acquisition scheme proposed by Warren's group. Further in vivo experiments are under work.

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Reference