High-resolution localized 2D J-resolved spectroscopy via intermolecular single-quantum coherences

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Target audience

The target audience of present paper is basic scientists and clinical scientists who are interested in two-dimensional magnetic resonance spectroscopy.

Purpose

Magnetic resonance spectroscopy (MRS) has been widely used as a reliable noninvasive tool for the detection of metabolites in biological tissues. Compared to the one-dimensional MRS, localized two-dimensional (2D) *J*-resolved spectroscopy, *J*PRESS, separates chemical shifts and *J* couplings into two different dimensions,[1] which is helpful for alleviating the signal overlap and quantifying the sample concentration. However, due to the intrinsic magnetic susceptibility in biological tissues, *J*PRESS is usually suffered from field inhomogeneities, especially when it is applied to large voxel. It is well known that intermolecular multiple-quantum coherences provide a feasible way to obtain high-resolution spectra in inhomogeneous fields.[2] In this report, a pulse sequence based on intermolecular single-quantum coherences (iSQCs) is proposed to obtain high-resolution localized 2D *J*-resolved spectrum in inhomogeneous fields.

Methods

The iSQC 2D *J*-resolved sequence is shown in Fig. 1. In two indirect detection periods t_1 and t_2 are iSQC and spin echo evolution. A PRESS-like module with three refocusing π RF pulses along orthogonal directions is used for spatial localization.[3] An excitation sculpting scheme before acquisition is used for water suppression. After three-dimensional (3D) acquisition, the location of the observable signal is $(\Omega_1, \Omega_2, \Omega_3) = (\omega_I + \gamma\Delta B, \pm\pi J, \omega_S + \gamma\Delta B \pm \pi J)$. To obtain a high-resolution spectrum, a shearing processing of F1-F3 plane along F2 axis and then F2-F3 plane along F1 axis is required. The location of the 3D signal then becomes $(\Omega_1, \Omega_2, \Omega_3) = (\omega_I + \gamma\Delta B, \omega_S, \pm\pi J)$. A high-resolution 2D *J*-resolved spectrum can be extracted by projecting the processed 3D data onto the F2-F3 plane. Although 3D acquisition is required for this sequence, the spectral widths of F1 and F2 dimensions only need to cover the inhomogeneous broadening and *J* coupling splitting respectively, thus the acquisition efficiency is improved greatly.

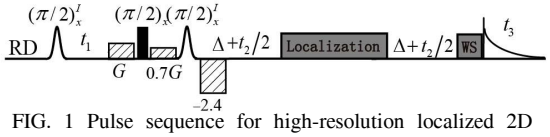

FIG. 1 Pulse sequence for high-resolution localized 2D *J*-resolved spectroscopy from inhomogeneous fields.

Results

Experiments were performed on a 7 T small animal MR scanner with a 160 mm inner bore diameter and a 63/95 mm quad birdcage coil. A solution of butyl methacrylate in DMSO filled in a cylindrical plastic bottle was studied in an intentionally deshimmed inhomogeneous field (80 Hz line-width). The voxel size was set to 10 × 10 × 10 mm^3. For the iSQC 2D *J*-resolved sequence, the repetition delay RD was 1 s and 60 × 30 × 4000 points were acquired with spectral widths of 100 Hz × 50 Hz × 2500 Hz (F1 × F2 × F3) in 30 minutes. The 3D data was processed with Matlab software. A *J*PRESS experiment was also performed under the same condition for comparison. The experimental results are shown in Fig. 2.

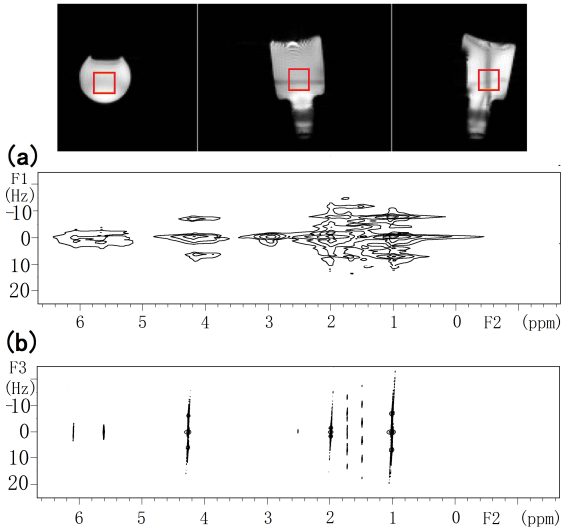

FIG. 2 Localized 2D *J*-resolved spectra of a solution of butyl methacrylate in DMSO under inhomogeneous field. (a) Original *J*PRESS spectrum; (b) high-resolution 2D *J*-resolved spectrum based on iSQCs.

Discussion

The localized voxel is shown in the GRE image on the top of Fig. 2. From Fig. 2a, we can see that high-resolution information is almost lost in the *J*PRESS spectrum. The chemical information can hardly be obtained from the *J* decoupled spectrum obtained by projecting the 2D spectrum along the F2 dimension. Although the inhomogeneous broadening in the F1 dimension can be refocused by spin echo, the overlapping of neighboring signals makes it difficult to obtain exact *J* coupling constants from the F1 dimension. For the iSQC 2D *J*-resolved spectrum shown in Fig. 2b, the influence of field inhomogeneity is greatly eliminated and the spectral line-width is reduced from 80 to 4 Hz. The information of chemical shift and the *J* coupling splitting are clearly shown in F2 and F3 dimensions. The water signal is also effectively suppressed, which is good for the study of biological sample with intensive water resonance.

Conclusion

A new pulse sequence is proposed for high-resolution localized 2D *J*-resolved spectra in inhomogeneous fields. It is potentially useful for metabolites detection of biological tissues.

Acknowledgement

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