

A method to obtain 2D high resolution MRS under inhomogeneous magnetic fields

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Target audience

Those who are interested in the study of high-resolution MRS on heterogeneous biological tissues are targeted readers.

Purpose

High resolution magnetic resonance spectroscopy (MRS) can provide valuable information in *in vivo* studies. The magnetic field homogeneity *in vivo* is often degraded by magnetic susceptibility variation near, e.g., at air/tissue interfaces. The intermolecular multiple quantum coherence (iMQC) technique can be used to remove the effect caused by inhomogeneous fields and thus offer high resolution spectral information¹⁻². However, intrinsic low signal-to-noise ratio (SNR) of iMQC signals hampers its practical applications. Therefore, in this study a pulse sequence is designed to acquire 2D high-resolution spectra under inhomogeneous fields with high SNRs.

Methods

The pulse sequence is shown in Fig. 1. The coherence transfer module of $[\pi/2-t_1/2-\pi/2-t_1/2]$ can track precession-frequency differences between every two coupled spins and is utilized to obtain high resolution chemical-shift differences information in the F1 dimension. Every single acquisition module records evolutions of chemical shifts in the F3 dimension, and is repeated 2^*N times to trace scalar-coupling evolutions in the F2 dimension. The spectral peaks will broaden along the F3 dimension under inhomogeneous fields. By projecting the 3D data ([F1, F2, F3]) into the F1F2 plane, a high resolution 2D spectrum, with chemical-shift difference information in the F1 dimension and *J*-coupling splitting information in the F2 dimension, can be obtained. The experiments were performed at 298K using an 11.7 T Varian NMR system spectrometer with a 5 mm indirect detection probe and three-dimension gradient coils. A sample of 0.5 M ethyl 3-bromopropionate in CDCl_3 was tested to demonstrate the feasibility of the new sequence. The magnetic field was intentionally deshimmmed to produce a linewidth of ~ 2.5 kHz. The repetition time was 4 s, and the total acquisition time was approximate 10 min.

Results and Discussion

Figure 2c shows the high-resolution 2D spectrum (the F3 dimension is not given) obtained with the sequence in Fig. 1 under an inhomogeneous field of ~ 2.5 kHz. Deliberate aliasing in the F1 dimension was utilized to shorten the experimental duration, and the spectral width in the F1 dimension is 400 Hz. The spectrum in Fig. 2(c) is symmetric with respect to the $F1 = 0$, due to the presence of bipolar spin transfers. The central peak at $F1 = 0$ arises from magnetization that is refocused but not transferred from one spin to another. The F2 spectral width is 42 Hz. High resolution *J*-coupling information is shown in the F2 dimension.

Although this type of 2D high-resolution spectroscopy can be obtained through a 3D acquisition³, the experimental time (several hours) is too long for *in vivo* applications. The experimental duration can be greatly reduced (to about ten minutes) by employing the sequence shown in Fig.1 using a 2D acquisition. The experimental duration can be further reduced through employing the spatiotemporal encoding technique⁴. However, the SNRs and resolutions are significantly reduced in the spatiotemporal encoding spectra.

Conclusion

An efficient method is developed for obtaining 2D high resolution MRS on heterogeneous biological tissues. With the acceptable time cost and elegant performance under inhomogeneous fields, it may potentially useful for studying metabolites *in vivo*.

Acknowledgments

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References

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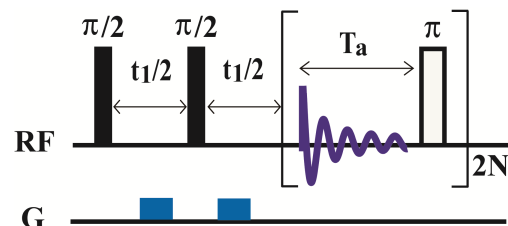


Figure 1. Pulse sequence for high resolution 2D spectroscopy. The filled and open rectangles on the RF line represent the $\pi/2$ and π pulses, respectively. The filled rectangles on the gradient (G) line represent coherence selection gradients. Phases of the repeated 180° pulses are altered by reference to (x, x, -x, -x) for alleviating pulse imperfections.

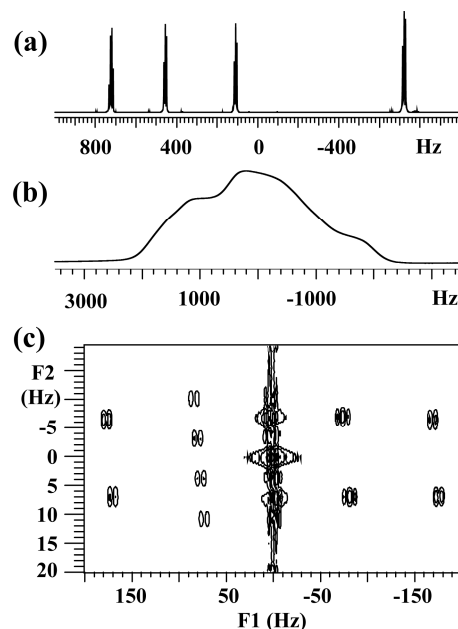


Figure 2. (a) 1D ^1H spectrum under the homogeneous field, (b) 1D ^1H spectrum under the inhomogeneous field (about 2.5 kHz), and (c) 2D high resolution spectrum obtained by the sequence in Fig. 1 under the same inhomogeneous field as (b).