A method to obtain high resolution MRS through simultaneous acquisition of iZQC and iDQC signals under inhomogeneous magnetic fields

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Target audience

The target audiences of present study are the scientists who are interested in acquiring high resolution MRS in the tissues with field inhomogeneity.

Purpose

High resolution magnetic resonance spectroscopy (MRS) can provide valuable information in in vivo study. Magnetic field homogeneity in vivo is often degraded by magnetic susceptibility variation near, for example, air/tissue interfaces. Intermolecular multiple quantum coherences (iMQCs) have been utilized to acquire high resolution MRS under inhomogeneous fields.[1,2] However, since iMQC signals are phase-modulated, absolute value spectra are usually used for high resolution projections, which introduces unfavorable line broadening. Here, an iMQC pulse sequence is designed, which can be used to simultaneously acquire intermolecular zero quantum coherence (iZQC) and intermolecular double quantum coherence (iDQC) signals under inhomogeneous fields. iZQC and iDQC signals can be combined together to eliminate the dispersion component and to obtain double absorption lineshape, thus doubling the spectral resolution.

Methods

The pulse sequence is shown in Fig. 1. The rectangle pulses are non-selective pulses. The gauss-shaped pulses (the second and third pulses) are selective for solvent. And dash rectangles represent correlation selection gradients. A fixed evolution time is employed. iZQC signal is firstly acquired, and then the iDQC signal. iZQC signal is flipped with respect to t_1=0, and then iZQC and iDQC signals are combined together to form a complete echo in both dimensions of time domain. The experiments were performed at 298K using an 11.7 T Varian NMR system spectrometer and a 5 mm indirect detection probe with three-dimension gradient coils. A sample of mixture of methyl ethyl ketone ($CH_3COCH_2CH_3$, solute) and cyclohexane (C_6H_{12}, solvent) was used to demonstrate the feasibility of the new sequence. The magnetic field was intentionally deshimmed to produce a line width of ~50 Hz (phased mode). To remove the unwanted coherence transfer pathways caused by imperfect pulses, an four-step phase cycling scheme on the second RF pulse (x, y, -x, -y) and the receiver (x, -x, x, -x) was used. The F1 spectral width was 100 Hz with 25 increments, and the F2 spectral width was 2000 Hz. The repetition time was 3 s, and the total acquisition time was about six minutes.

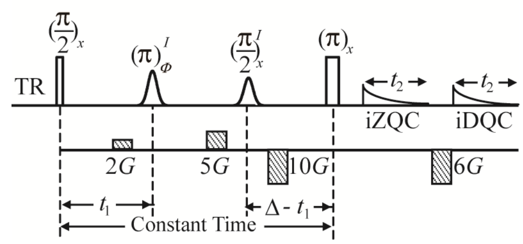

Fig. 1. Pulse sequence for simultaneous acquisition of iZQC and iDQC signals under inhomogeneous fields.

Results and Discussion

From Fig. 2, it can be seen that high resolution information, such as chemical shift and *J* coupling constant, can be obtained from both the separated iZQC spectrum (Fig. 2g) and combined iZQC and iDQC spectrum (Fig. 2h) under inhomogeneous field.

As shown in Fig. 2c, the iZQC and iDQC signal are simultaneous obtained. They can be separated (Fig. 2d and e) and combined to cancel out the dispersive part, thus producing double absorptive lineshape. The linewidths of 1D projection spectra of separated iZQC spectrum (Fig. 2g), iDQC spectrum (not shown here), and combined iZQC and iDQC spectrum (Fig. 2h) are 6.03, 5.71, and 3.42 Hz, respectively. The spectral resolutions are improved by 43% and 40% respectively in comparison of Fig. 2h with Fig. 2g and separated iDQC spectrum. These results are close to the theoretical prediction of doubling spectral resolution.

The solvent signals of cyclohexane almost disappear in the 2D spectra of Fig. 2c~h. This is because the intermolecular double quantum filter module is employed in the sequence of Fig. 1 and it has the ability to suppress the solvent signal.

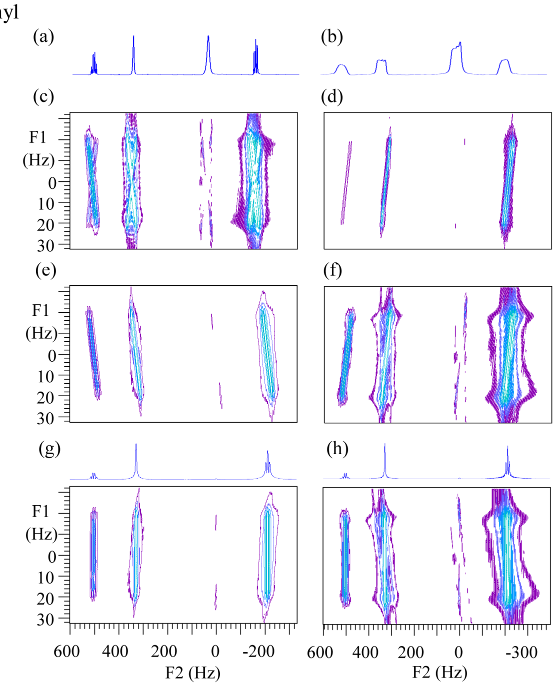

Fig. 2. (a) Conventional 1D ¹H high-resolution spectrum in a well-shimmed field, (b) conventional 1D spectrum acquired in an inhomogeneous field of about 50 Hz line-width, (c) 2D spectrum with both iZQC and iDQC signals acquired using the scheme of Fig. 1 in the same inhomogeneous field as Fig. 2b, (d) separated iDQC signal from (c), (e) separated iZQC signal from (c), (f) 2D spectrum combining together iZQC and iDQC signals, (g) sheared spectrum of (e) after a clockwise rotation of 45° and 1D projection spectrum along F2 dimension, (h) sheared spectrum of (f) after a counterclockwise rotation of 45° and 1D projection spectrum along F2 dimension.

Conclusion

A new iMQC pulse sequence is developed for simultaneous acquisitions of both iZQC and iDQC signals under inhomogeneous magnetic field. These two signals can be combined via data processing to double the spectral resolution. The new scheme can be potentially useful for studying metabolites in in vivo MRS with field inhomogeneity. However, intrinsic low SNR of iMQC singal may be an issue for potential practical applications.

Acknowledgments

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