Fast high-resolution J-resolved correlation spectroscopy in inhomogeneous fields

Hao Chen[1], Zhiyong Zhang[1], Shuhui Cai[1], and Zhong Chen[1]

[1]*Department of Electronic Science, Xiamen University, Xiamen, Fujian, China*

Target audience

The target audience is basic scientists and clinical scientists who are interested in ultrafast acquisition of high-resolution MRS of biological tissues.

Purpose

Multi-dimensional NMR spectroscopy alleviates the jam or even overlapping of peaks in one-dimensional spectra of biological metabolites, extending the application of NMR spectroscopy. However, the acquisition of high-resolution NMR spectra relies on high homogeneity of magnetic field, which is difficult to achieve in many cases. In this study, we present a fast three-dimensional (3D) NMR approach for high-resolution *J*-resolved spectrum and COSY spectrum simultaneously in inhomogeneous fields via intermolecular zero-quantum coherence (iZQC) and spatial encoding technique.

Methods

The proposed pulse sequence is called 3D JCOSY and shown in Fig. 1. It is a modification of the iZQC *J*-resolved spectroscopy scheme proposed by Lin et al.[1] and the UFJCOSY scheme proposed by Giraudeau et al.[2] After the first π/2 pulse, spins evolve with a linear time incrementation to give ^{1}H chemical shifts information. In this period, the gradient G_1 is introduced to select iZQC, which is not dephased by the field inhomogeneity. Following the π/2 coherence transfer pulse, odd adiabatic π chirp pulses with gradient pulses are applied to spatially encode the phase caused by the iZQC evolution and the inhomogeneous field.[3] In the acquisition period, the *J*-modulated detection scheme is employed to decode the spatially encoded information and sample the *J*-coupling information. Therefore, a high-resolution 3D spectrum can be acquired within the time for a conventional 2D spectrum. Since the chemical shifts are recorded in the conventionally sampled (F1) and spatially encoded (F2) dimensions, a COSY spectrum can be achieved in the F1F2 plane. The *J* couplings can be retrieved from the detection dimension (F3).

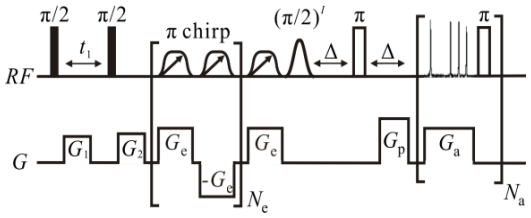

Fig. 1 Fast high-resolution 3D JCOSY sequence via spatial encoding technique and intermolecular zero-quantum coherence.

Results and discussion

Experiments were performed on a Varian NMR System 500 MHz spectrometer. A sample of ethyl 3-bromopropionate in acetone with a molar ratio of 5:1 was used to demonstrate the implementation of the new sequence. A four-step phase cycling was used to improve the spectral quality, and the phases for the second π/2 RF pulse, the Gaussian pulse towards acetone and the receiver were (x, -x, x, -x), (x, x, -x, -x) and (x, -x, x, -x), respectively. As shown in Fig. 2a and Fig. 2b, the spectra were acquired in a well-shimmed field and an intentionally deshimmed inhomogeneous field with a line-width of 200 Hz. The field inhomogeneity demolished the spectral information. Fig. 2c displays the 3D NMR spectrum obtained with the novel sequence within 28 min in the presence of field inhomogeneity. The COSY spectrum achieved by projecting the 3D spectrum along the F3 dimension is shown in Fig. 3a. The linewidths of F1 and F2 dimensions are 27 Hz and 37 Hz, respectively. As shown in Fig. 3b, when the 3D spectrum is projected onto the F2F3 plane, a *J*-resolved spectrum can be achieved, in which the *J* splitting patterns of each chemical sites can be retrieved.

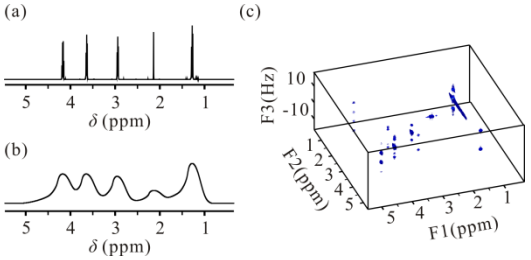

Fig. 2 (a,b) Conventional 1D proton spectrum of the solution of ethyl 3-bromopropionate in acetone in a well-shimmed field (a) and in an intentionally deshimmed field with a line-width of 200 Hz (b); (c) 3D JCOSY spectrum acquired in the same inhomogeneous field as (b) using the proposed sequence.

Conclusion

Spatial encoding technique spares the numerous repetitions with t_1 increments and can shorten the experimental time by several orders of magnitude. With the advantage of intermolecular zero-quantum coherence, the influence of field inhomogeneity can be eliminated. The experimental observations illustrate the acquisition efficiency and the insensitivity to field inhomogeneity of the new sequence. This approach may provide a new way to acquire high-resolution MRS of heterogeneous biological tissues.

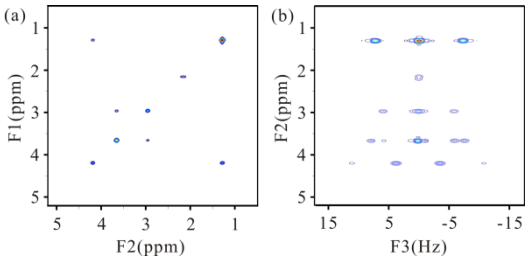

Fig. 3 (a) COSY spectrum extracted from the F1F2 plane of the 3D spectrum; (b) *J*-resolved spectrum gained from the projection of the 3D spectrum onto the F2F3 plane.

Acknowledgement

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References

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