Spatially encoded ultrafast 2D SECSY in inhomogeneous fields

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Introduction

The ultrafast method based on spatial encoding enables a two-dimensional (2D) or multi-dimensional (mD) acquisition to be completed with a single scan [1]. It has been successfully used in NMR spectroscopy including COSY, TOCSY, *J*-resolved spectroscopy, HSQC, HMQC and DOSY. It also shows great potential in the applications of MRI. Recently, Frydman and co-workers applied RF pulses to compensate the influence of magnetic field inhomogeneities on ultrafast method but the distributions of magnetic fields should be mapped in advance [2]. Pelupessy et al. proposed a heterogeneity removing method based on spatial encoding to get high-resolution NMR information in magnetic fields with unknown spatiotemporal variations [3]. However, it is not straightforward to get absolute chemical shift values. In this abstract, an ultrafast pulse sequence for acquiring 2D spin-echo correlated spectroscopy (SECSY) spectrum in inhomogeneous fields was proposed and experiments were performed to verify its feasibility.

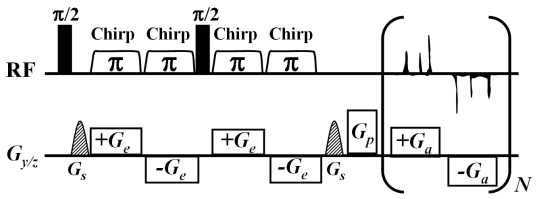

Fig. 1 Ultrafast 2D SECSY sequence

Experiments and Results

The sequence for ultrafast 2D SECSY spectrum is shown in Fig. 1. All gradients are applied along both *z* and *y* directions simultaneously with the same durations and strengths. Experiments were performed at 298 K on a Varian NMR System 500 MHz spectrometer using a 5 mm indirect detection probe. A sample of $CH_3CH_2CH_2OH$ and C_5H_5N in $CDCl_3$ with a volume ration 1:1:2 was used. Experiments were first carried out using the ultrafast sequence shown in Fig. 1 and the conventional SECSY sequence respectively in a well-shimmed magnetic field to demonstrate the validity of the new sequence. For the ultrafast experiment, two consecutive scans were performed to double the spectral width in F2 to avoid peak folding. The results are shown in Fig. 2. To demonstrate the feasibility of the ultrafast sequence in inhomogeneous field, we acquired another three spectra with the sequence under different kinds of inhomogeneous fields. The spectra shown in Fig. 3a~c were obtained in inhomogeneous fields with linewidths of 800, 300 and 650 Hz respectively through deshimming the Z_1-Z_5 shim coils (I), the X_1, Y_1, X_1Y_1 and X_2Y_2 shim coils (II), and the Z_1-Z_5, X_1, Y_1, X_1Y_1 and X_2Y_2 shim coils (III). The experimental time for each ultrafast experiment and the conventional SECSY experiment were 2.5 s and 10 min, respectively. All data were processed using our custom-written program with Matlab 7.1.0 (The Math Works Inc.)

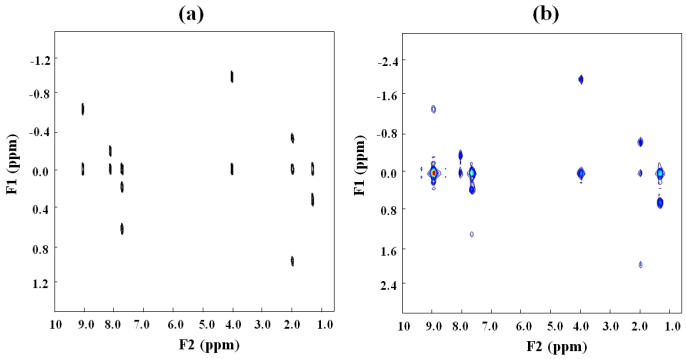

Fig. 2 (a) Conventional 2D SECSY spectrum, and (b) ultrafast 2D SECSY spectrum acquired with the sequence shown in Fig. 1.

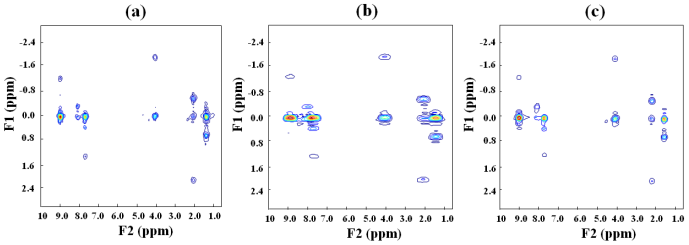

Fig. 3 Ultrafast 2D SECSY spectra obtained with the sequence in Fig. 1 under inhomogeneous fields (I) (a), (II) (b), and (III) (c) described in text respectively.

Discussion

The effects of field inhomogeneities on spins evolution in the indirect dimension (F1) will be eliminated before data acquisition. In the decoding period, field inhomogeneities still affect spins' evolution in the direct dimension (F2). However, line broadening mainly results from the field inhomogeneities along *z*-orientation which can be addressed by circularly shifting the acquired 2D t_2-v_1 data matrix. A comparison of the spectra shown in Fig. 2a and b indicates that the ultrafast sequence in Fig. 1 does give a correct SECSY spectrum. The only difference is that the chemical shifts of coupled spins in the indirect dimension (F1) are twice as large as those in the conventional SECSY spectrum. We can obtain the absolute chemical shift information from the direct dimension (F2) and the *J*-coupling information from the cross peaks of the coupled spins. The ^{1}H signal of the hydroxyl group in propyl alcohol was too weak to be displayed. From Fig. 3a, we can come to a conclusion that the sequence in Fig. 1 is insusceptible to the field heterogeneities along the *z* direction. As expected from Fig. 2b, the influence of field heterogeneities along the *x* and *y* directions cannot be completely eliminated in the detection period, which result in line broadening along the F2. In such cases, the ultrafast sequence is only effective within certain amount of field inhomogeneities. Fig. 3c shows that the ultrafast sequence still works quite well under a highly inhomogeneous field where *z*-orientation field inhomogeneities play a major role. The SECSY spectrum can be converted to corresponding COSY spectrum through mathematical manipulation of the final 2D data matrix. In conclusion, the proposed sequence provides an ultrafast way of obtaining chemical shift and *J*-coupling information under inhomogeneous fields mainly resulting from *z*-orientation heterogeneities.

Acknowledgment

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References

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