

3D Localized 2D J-Resolved MR Spectrum in a single scan

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Introduction

Recently, original ultrafast 2D acquisition schemes have been proposed to collect the 2D NMR data within a single scan [4]. Up to now, these techniques have been applied mainly to organic chemistry [5], analytical chemistry [6] and structural biology [7]. Until now, ultrafast spectroscopic sequences have been implemented on standard spectrometers equipped with one or two magnetic field gradients. In this work, for the first time, we present a 3D localized 2D ultrafast J-resolved spectroscopic sequence.

Method

The proposed ultrafast JPRESS sequence, named ufJPRESS, is based on constant-time phase-modulated spatial encoding (Fig. 1) and was developed on Paravision 5.1 (7T Bruker Biospec). The pulse sequence starts with a water suppression module (VAPOR) combined with a slice saturation module (OVS). These modules are followed by the proposed 3D localized 2D ultrafast J-resolved excitation scheme which is based on the PRESS scheme nested in a modified version of the ultrafast excitation scheme proposed by Pelupessy et al. [8]. The combination of the two 180° chirp pulses, applied during inverted magnetic field gradients ($\pm G_e$), spatially encodes the chemical shift information along the third spatial dimension. The “shifting” gradient pulse (G_c) is necessary to move the peaks inside the acquisition window. The excitation scheme is followed by a modified EPI detection scheme [9]. The acquisition gradients G_a are separated by non-selective 180° pulses that refocus the effect of internal chemical shifts while the homonuclear J evolution remains unaffected. Two phase cycles Φ_1 and Φ_2 were introduced in order to reduce undesired signals. This scheme, repeated N_2 times, results in a $2^*N_1^*T_a$ total digitization time. Data reconstruction was processed by a home-made Matlab algorithm. We developed an automatic procedure based on spatial apodization window [10] in order to reduce the asymmetric *sinc* wiggles inherent to ultrafast MR experiment [11].

A comparative study was carried out to evaluate spectral resolution of conventional and ultrafast 2D J-resolved spectra. 128 transients were acquired using conventional spectroscopy (Echo Times from 20 to 320 ms, NA=1). 128 transients were acquired using ultrafast spectroscopy ($G_e=22$ mT/m, 128 detection gradients $G_a=70$ mT/m, $T_a=4$ ms, $G_c=-156$ mT/m, $T_c=600$ ms, NA=2). The model sample consisted of a concentrated ethanol solution (10% w/w in water). The voxel size was 8 mm x 8 mm x 8 mm. To evaluate the localization efficiency of the ufJPRESS sequence, tests were performed on a GABA *in vitro* phantom. This phantom consisted of a 1.5 mL tube containing a GABA solution (10% w/w in water) placed at the center of a 50 mL tube of pure ethanol. The localization test consisted in collecting the ultrafast signal from a voxel (5 mm x 5 mm x 5 mm) placed in the 1.5 mL tube and checking the residual signal of ethanol on the 2D spectrum of GABA. The following parameters were used: $G_e=35$ mT/m, 128 detection gradients $G_a=62$ mT/m, $T_a=6$ ms, $G_c=-117$ mT/m, $T_c=700$ ms, NA=16 and 3 mm OVS bands with a 0.5 mm gap to voxel. All acquisitions were performed using the following parameters: $T_e=30$ ms, $\zeta=15$ ms, 9 kHz chirp sweep range, TR=10 s and VAPOR water suppression. The signal (2048 x 128 points) was collected using a quadrature coil (transmit/receive, 32 mm diameter, Rapid Biomed).

Results

As expected, the conventional 2D J-resolved MRS experiment, performed in 21 min, led to a well resolved 2D spectrum with linewidth of less than 2 Hz along the 2 dimensions. The ultrafast 2D J-resolved MRS spectrum, obtained in 20 s, was much better resolved in the conventional F_1 dimension (2.3 Hz linewidth) than in the ultrafast F_2 dimension (17 Hz linewidth). The measured chemical shifts (1.89, 2.28 and 3.01 ppm) and the J-coupling values of GABA obtained for the localization test (Fig. 2) are in good agreement with literature [12]. Very low intensity ethanol peaks (at 1.19 ppm) were reported.

Discussion/Conclusion

These results are in good agreement with the resolution performances of ultrafast NMR experiments which were recently described [13]. The localization test results demonstrate the efficient 3D localization of the ufJPRESS excitation scheme. This paper presents the first 3D localized 2D ultrafast MRS experiment developed on a small animal imaging system. This sequence offers an efficient signal localization allowing the acquisition of a whole 2D J-resolved spectrum in a single scan which is of great interest for investigations on moving organs. Moreover, this sequence acquisition technique could be combined to existing high SNR *in vivo* spectroscopy applications such as ^{13}C hyperpolarized acquisitions. The time saved using this technique opens new perspectives for *in vivo* dynamic spectroscopy.

References

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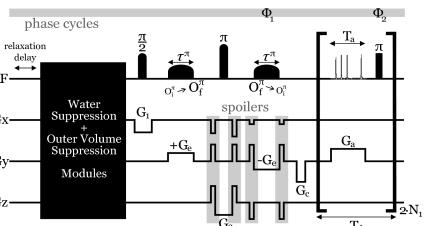


Fig. 1: Proposed ultrafast JPRESS pulse sequence (ufJPRESS) for *in vivo* localized 2D J-resolved ultrafast spectroscopy.

The excitation scheme is followed by a modified EPI detection scheme [9]. The acquisition gradients G_a are separated by non-selective 180° pulses that refocus the effect of internal chemical shifts while the homonuclear J evolution remains unaffected. Two phase cycles Φ_1 and Φ_2 were introduced in order to reduce undesired signals. This scheme, repeated N_2 times, results in a $2^*N_1^*T_a$ total digitization time. Data reconstruction was processed by a home-made Matlab algorithm. We developed an automatic procedure based on spatial apodization window [10] in order to reduce the asymmetric *sinc* wiggles inherent to ultrafast MR experiment [11].

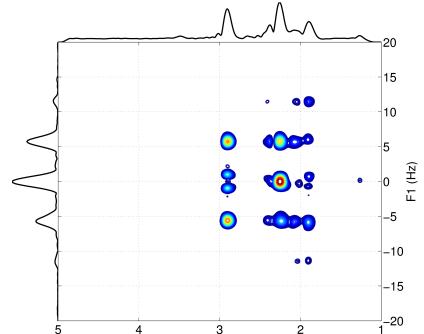


Fig. 2: 3D localized 2D ultrafast J-resolved spectrum of the GABA phantom acquired in 2 min 40s. A column was extracted from the 2D spectrum (at 2.28 ppm) and projected on F_1 axis.