Simulation Study for Suppression of Myo-inositol for Glycine Measurement by PRESS at Various Field Strengths

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INTRODUCTION The glycine (Gly) singlet at 3.55 ppm is difficult to measure because of the low concentration (< 1 mM) and the abundant overlapping multiplet that arises primarily from myo-inositol (mI). The mI resonances at ~3.55 ppm are strongly coupled, and as a result the signal evolves with time in a complex fashion. Here, we present a preliminary result of a density-matrix simulation study that was carried out to search for optimal echo times of PRESS (point-resolved spectroscopy) for detection of Gly at various magnetic fields.

METHOD Density-matrix formalism [1] was employed to calculate the responses of the spin systems to the single-voxel localized PRESS sequence. The time evolution of the density operator over the sequence was calculated numerically for the Hamiltonian that includes the Zeeman, chemical shift and scalar coupling terms, and the gradient and shaped RF pulses. The space resolution for the slice selection gradient was set at 1% with respect to the slice thickness. Namely, 200 pixels along each of the three orthogonal directions were set within a sample-size length set at double the slice thickness, defined at half amplitude of the frequency profile of the RF pulses. The carrier of the slice-selection RF pulses was set at 3.65 ppm, ensuring that spatial localization for the resonances of mI and Gly spin systems was all within the sample dimension, especially for the small bandwidth (BW) of the 180° pulse at the highest field (7.0T). The PRESS sequence used in the simulation consisted of a 90° RF pulse (9 lobes; 3.0 ms; BW = 3.8 kHz) and two 180° RF pulses (9 lobes; 7.6 ms; BW = 1.0 kHz). The waveforms of these pulses were generated from MATPULSE [2] at an RF field intensity of B_1 = 0.235 G, for all field strengths (B_0 = 1.5T, 3.0T, 4.0T, 4.7T and 7.0T), ignoring the potential decrease of the maximum available B_1 intensity with increasing B_0. The effects of T_1 and T_2 relaxation were not included in the simulation. The published chemical shift and coupling constants [3] were used. The density-matrix simulation was programmed with Matlab (The MathWorks, Inc.).

RESULTS and DISCUSSION Fig. 1 illustrates the pattern of the echo time dependence of the PRESS mI multiplet at ~3.55 ppm, for 1.5T, 3.0T and 7.0T. The signal degrades with increasing TE drastically at all field strengths. At 1.5T, the lineshape is most upright, but the peak height is not necessarily greatest. At this field, the mI multiplet reduces substantially at total TE (= $TE_1 + TE_2$) > 250 ms, and it is predicted that the Gly singlet is readily visible at, e.g., {TE_1, TE_2} = {120, 170} ms. When calculated from 0.06 ppm width, indicated by vertical dotted lines in Fig. 2, the peak height and area of mI at this echo time pair are 21% and 10% relative to those of the Gly singlet, respectively. For 3.0T, the mI signal is small at TE ≈ 160 or 280 ms. An echo time pair {TE_1, TE_2} = {100, 60} ms is likely a good option for Gly measurement at this field. The mI peak height and area are 15% and 4% relative to those of Gly, respectively (see Fig. 2). Despite these smaller ratios, the resolution of Gly at 3.0T is lower than at 1.5T because of the mI downward peak at 3.7 ppm. It is unlikely that at higher fields the Gly peak is well resolved from the mI background. For comparison, calculated spectra for the published TE-averaged-PRESS method at 4.0T [4] are shown on the right. The simulation indicated that, when applied similarly, 4.0T is the most appropriate field strength for this type of TE-averaging method. In conclusion, for PRESS, Gly is better resolved from the mI background at 1.5T or 3.0T than at higher fields.

REFERENCES: 1. Slitchter CP, "Principles of Magnetic Resonance". 3rd ed., Berlin, pp.157-169; 1990. **2**. Matson GB. Magn Reson Imaging 1994;12:1205-1225. **3**. Govindaraju V *et. al.* NMR Biomed 2000;13:129-153. **4**. Prescot AP *et. al.* Magn Reson Med 2006;55:681-686.

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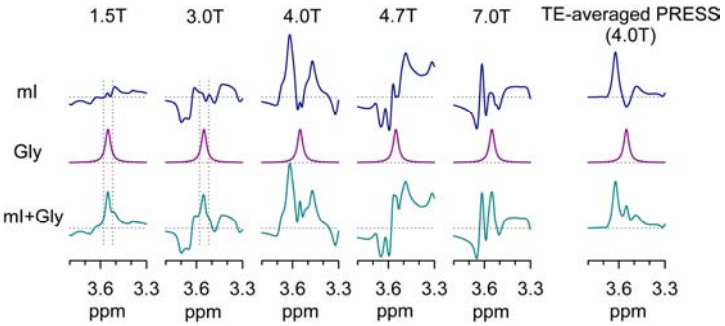

FIG 2. Calculated PRESS spectra of mI, Gly and mI+Gly, scaled with [mI]/[Gly] = 8, are displayed for 1.5T, 3.0T, 4.0T, 4.7T and 7.0T, for which the echo times used are {TE_1, TE_2} = {120, 170}, {100, 60}, {140, 30}, {70, 50}, and {100, 50}, respectively. At these echo times, the absolute value of the mI peak height between the vertical dotted lines (0.06 ppm wide) is smallest for total TE < 300 ms. Calculated spectra for the published TE-averaged-PRESS method at 4.0T [4] are shown on the right, for comparison. Spectra are broadened to 0.04 ppm.

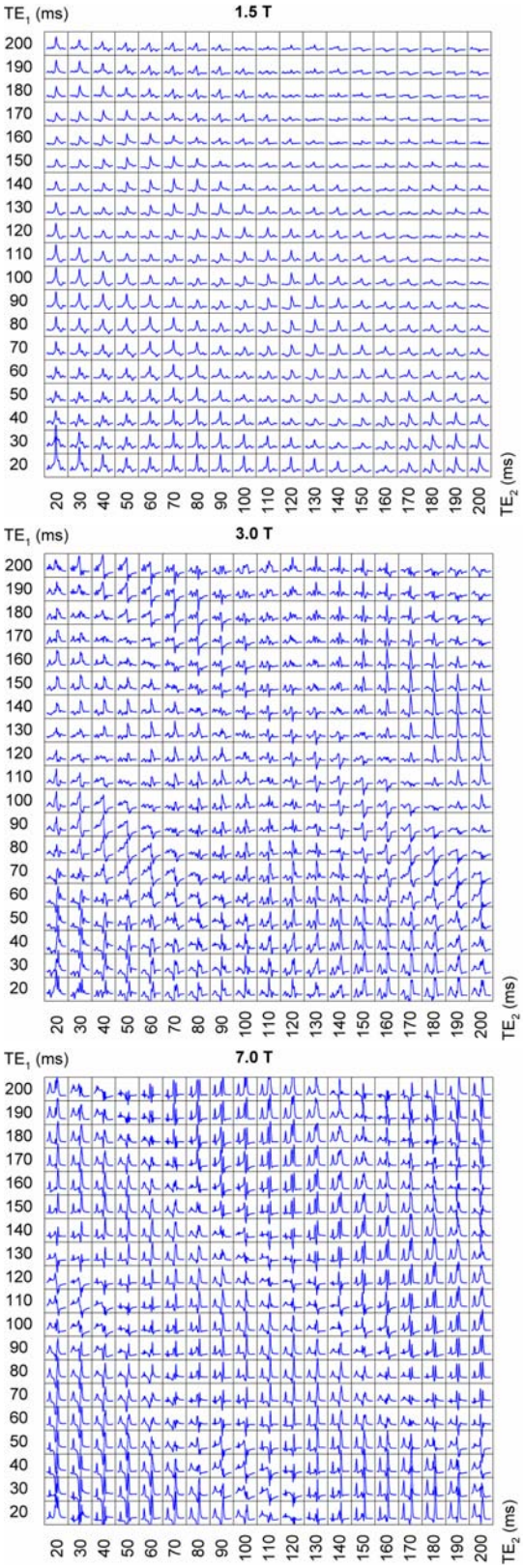

FIG 1. The pattern of the echo time dependence of PRESS mI spectra is illustrated for 1.5T, 3.0T and 7.0T. TE_1 and TE_2 denote the echo times for the first and second 180° pulses of PRESS. For each square partition, the spectrum is plotted for 3.05 - 4.05 ppm, centered at the 3.55-ppm Gly resonance. The mI spectra are normalized with respect to the Gly peak height, for [mI]/[Gly] = 8. The height of the partitioned squares is four times the Gly peak height. Spectra are broadened to 0.04 ppm.