Spectral Simulations Incorporating Spatially-dependent Variables for PRESS Localized Spectroscopy

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Introduction NMR spectral simulations can provide a rapid and convenient method for optimizing acquisition sequence parameters and generating prior spectral information (frequency, amplitude and phase) for parametric spectral analysis [1, 2]. For the PRESS spectroscopic localization method, spatially-dependent variables such as the slice-selective pulse profiles and gradient amplitudes affect the resultant spectral amplitudes and phases. For accurate metabolite quantitation the simulation model must take into account physical parameters that lead to spectral variations of coupled spin systems such as chemical shift offset, tip angle variations in slice-selective RF pulses, and spin evolution during the slice-selection pulses. In this study, numerical simulations of spectra for three different models using the PRESS localization pulse sequence were examined and a comparison made between them. Finally, these simulation models were evaluated for measurement of proton spectra from lactate, and results compared with experimental data.

Methods Spectral simulations were performed for lactate, an AX_3 spin system, and for the CH_3 singlet resonance of acetate. Three models were used: 1) A simple *'4-compartment model'* [3] to account for the chemical shift offset between the A and X spins. 2) A *'tip angle profile'* model that includes the tip angle profiles of the RF refocusing pulses to account for intensity variations across the selected volume, and 3) A realistic *'complete pulse'* model with frequency selective RF pulses modeled as a series of small tip angle, ideal rotations, interleaved with short evolution periods that account for spin evolution occurring during the pulse. Programs were written in C++ using the GAMMA library [4].

Model	Optimized 180°		Sinc 180°	
	144 ms	288 ms	144 ms	288 ms
4-comp.	-0.738	0.541	-0.739	0.544
Tip-angle	-0.747	0.520	-0.690	0.309
Comp. pulse	-0.739	0.528	-0.655	0.269
Experiment	-0.738	0.537	-0.634	0.456

Table 1. Ratios of area of lactate-doublet to acetate-singlet.

Spectra were acquired at 1.5 T using symmetric PRESS sequences with optimized and Sinc 180° pulses at TE = 144 and 288 ms. Phantom parameters: 500 mM lactate and acetate in H_2O, 2×2×2 cm^3 voxel. Ratios of area of lactate-doublet to acetate singlet were obtained by spectral integration. A spectroscopic imaging (SI) acquisition was obtained at 7 T using PRESS volume selection with an optimized pulse for TE = 288 ms, 5×5×3 mm3 volume, FOV 8×8 mm, and 32×32 phase encoding. SI images of both the multiplets were obtained by spectral integration.

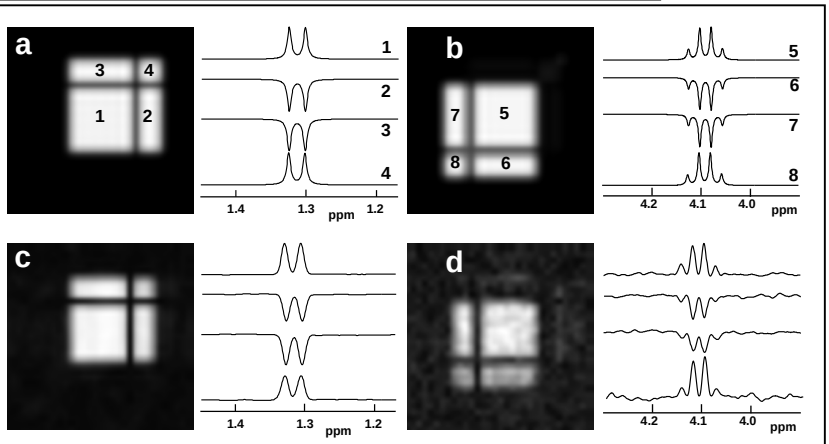

Figure 1. Images and spectra for simulated (a,c) and experimental (b,d) PRESS SI at 7T showing results for the lactate doublet and quartet.

Results and Discussion In Table 1 are shown the ratios of integrated areas of the lactate doublet relative to the acetate singlet for measurements and simulations of the symmetric PRESS sequence using the optimized and Sinc refocusing pulses. The ratios indicate that for numerical simulation of a symmetric PRESS sequence using the optimized refocusing pulse profiles and TE values at increments of 1/*J*, all simulation models result in good agreement with the experimental data; however, results for the poor excitation profiles demonstrated much greater disagreement between simulation and experimental results. For both pulse shapes and TEs examined, the results for the 4-compartment model were in good agreement with experimental results. In Figure 1 are shown 7T PRESS SI images and spectra for the lactate doublet and quartet, demonstrating observation of 4-compartments and the relative phases of the spectra from them.

References [1]. K. Young, et al, Magn. Reson. Med. 40 (1998) 812-815; [2]. K. Young, et al, J. Magn. Reson. 140 (1999) 146-152; [3]. D.A. Yablonskiy, et al, Magn. Reson. Med. 39 (1998) 169-178; [4]. S.A. Smith, et al, J. Magn. Reson. A106 (1994) 75-105.

Acknowledgements This work was supported by PHS grants EB00207 and EB0730.