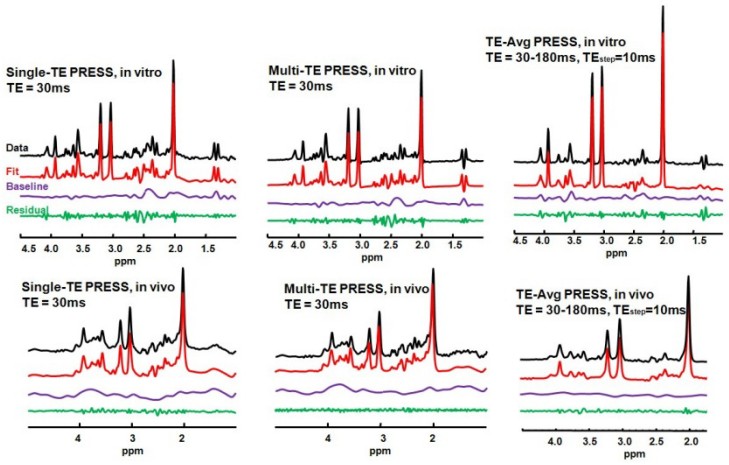
Comparison of Spectral Fitting Methods for Overlapping J-coupled Metabolite Resonances

A. Gonenc[1], V. Govindaraju[1], and A. A. Maudsley[1]
[1]Department of Radiology, University of Miami, Miami, FL, United States

Introduction: Detection of overlapping J-coupled metabolites, in particular glutamate (Glu) and glutamine (Gln), remains a challenge for in vivo proton MRS studies of the brain. Several methods have been developed that provide improved quantitation of these metabolites in comparison to conventional analysis of short-TE spectra analysis; however, to our knowledge no direct comparison of these three methods has been published. In this work, the results of an automated spectral analysis package capable of performing two dimensional prior-knowledge fitting of multi-TE spectra, one dimensional fitting of TE-averaged spectra, and one dimensional fitting of conventional (single-TE) PRESS spectra, are presented for single-voxel data.

Methods and Materials: Data were acquired at 3T (Siemens Trio) with eight-channel phased-array detection. Multi-TE PRESS volume-selected data were acquired with TEs from 30 to 180 ms in steps of 10 ms, TR = 2s, a four-step phase cycling, and a total time of 8 minutes. An additional measurement using conventional PRESS, TE=30 ms was obtained using the same acquisition time as the 2D measurement. Ten measurements were obtained in the same location (the precentral gyrus) in a single subject and a phantom containing typical brain metabolites.

Prior spectral information was generated using computer simulation [1], based on known chemical shifts and coupling constants for N-acetylaspartate (NAA), creatine (Cr), choline (Cho), myo-inositol (mI), Glu, and Gln. This prior information was combined with a time-domain spectral model (amplitude, phase, frequency, T2, and T2* values) using a constrained Levenberg-Marquardt optimization method written in Python. In addition, a wavelet-based baseline model was used. The spectral fitting was performed for: a) the full two-dimensional spectral model; b) the 1D spectrum following summation of all TE data (so-called TE-averaged [2]); and c) for the conventional PRESS spectral fitting. For the TE-averaged fitting, the relaxation effects were accounted for by directly incorporating T2 relaxation into the prior information.



(A)

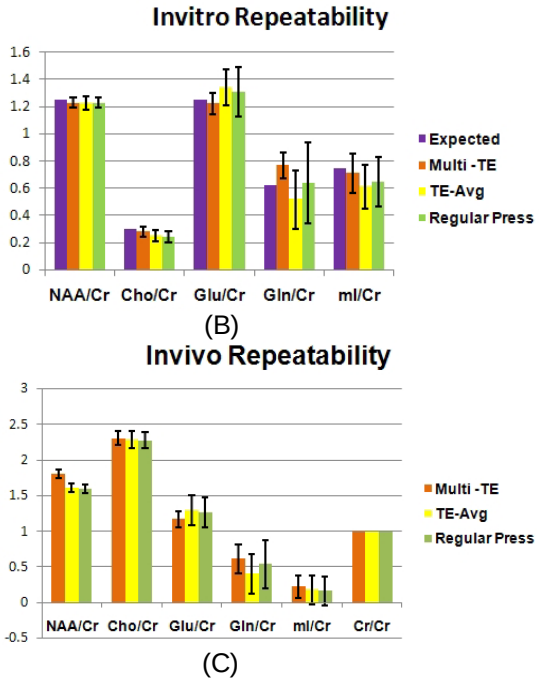


Fig 1. (A): Fit results for *in vitro* (top row) and *in vivo* (bottom row) data, with the columns showing the conventional PRESS, multi-echo 2D model fit, and TE-Averaged fit, respectively. For the multi-echo fit, only the first echo fit is shown. (B): Test-retest characteristic of the fitting methods, as ratios to Cr, using the *in vitro* data. For reference, the known ratio values are also shown in purple. Error bars shown are percent SD. (C): Test-retest characteristic of the fitting methods, again as ratios to Cr, using the *in vivo* data. Error bars are percent SD.

Results and Discussion: The different fitting method results are shown in Fig. 1A for both *in vitro* and *in vivo* data. Both sets of data were first fit 10 times starting with different starting values to test the stability of the fit. The resultant variance of 2% for both Glu and Gln indicated good convergence for all algorithms. The variance of the results across the 10 separate data sets was then obtained, with all spectra fit with the same starting values. The results for the metabolite ratios (corrected for T2 effects) are shown in Figs. 1B and 1C for the *in vitro* and *in vivo* data respectively. This study demonstrates decreased variance with the multi-TE acquisition relative to the conventional PRESS MRS measurement, and improved performance of the spectral fitting using the full 2D model in comparison to the TE-averaged model fit. This finding applied to all metabolites, but with the greatest benefit for the overlapping J-coupled metabolite resonances.

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References: [1] Govindaraju et al., NMR Biomed. 2000;13: 129-153;[2] Hurd et al., Magn Reson Med 2004;51:435–440.