Real-time tool to forecast the adequacy of shim and to define the number of acquisitions needed to answer the clinical question at hand with the prescribed 1H MR spectroscopy exam

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Introduction: Spectral quality and quantitation errors can strictly only be assessed after recording the water suppressed (WS) spectrum. If data quality is then found to be insufficient, the scan time used is wasted and in the clinic there is often no time to re-record the spectrum with more suited acquisition parameters. However, a single-shot water spectrum (nWS) recorded anyway for referencing could serve as basis to forecast the error bounds that can be expected at best given the SNR and linewidth found in this water scan. Hence, we developed and evaluated such a tool by generating simulated normal brain spectra of varying line widths and SNR to characterize quantification errors of the main metabolites for long and short echo time spectra as a function of the water SNR and linewidth.

Method: Brain spectra were simulated [1] for short and long echo time PRESS (TE 30 ms and 136ms) and scaled to yield a normal spectrum based on concentrations and T_2 values from Refs [2, 3]. A macromolecular baseline (MMBL) spectrum was added at short TE (fitted MMBL extracted from experimental averaged metabolite-nulled gray matter spectra of 10 subjects). These in silico spectra were then used as basis to generate spectra with different Gaussian broadening (13 sets with FWHM from 3 to 15 Hz). For each width, 100 spectra of different noise were created to obtain sets at 15 SNRs ranging from 5 to 100 (5,10, .. ,50,60, .. 100). (SNR defined as intensity of NAA_{CH3} divided by two standard deviations of the noise in frequency domain). Quantification was done with the two most widely used fit packages (LCModel [4] and jMRUI (QUEST) [5]). Using the true variance found over the sets of 100 spectra for each case, a toolbox was created that takes the nWS spectrum, number of averages, TE and brain matter type as input to predict the SNR and error bounds (SD% of normal values) for specific metabolites associated with QUEST and LCModel fits of the metabolite spectrum. Finally, we tested the tool (Figure 1) on experimental spectra from 5 subjects comparing the variance forecast from the tool with the error bounds found when actually fitting subsequently recorded WS spectra.

Figure1: Prognosis tool

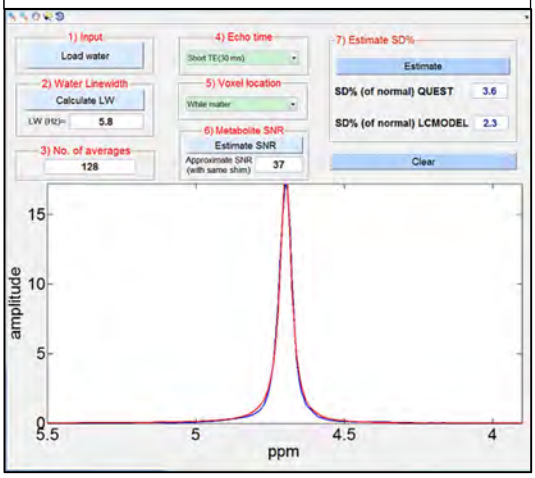
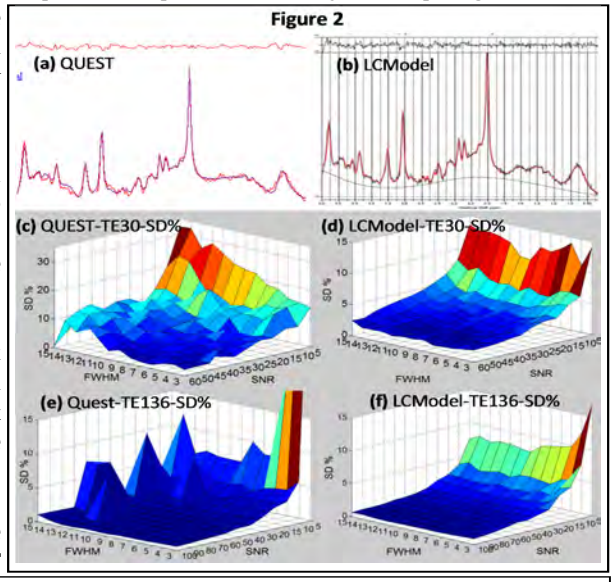


Figure 2



Results and Discussion: Example fits in QUEST and LCModel for one of the synthetic short TE spectra (5 Hz broadening, SNR 50) are shown in Figure 2(a-b). Figure 2(c-f) illustrates the variance found across fit results for total creatine in 100 spectra each with respect to FWHM and SNR. This variance was compared to the error bounds given by the fitting tools. It was found that the indicated error in general overestimates the variance of fitting results (modestly for LCModel with 35 and 18% for TE 30 and 136; more so for QUEST at long TE with 56%). This is expected since in both algorithms the noise was (over-)estimated from fitting residues, rather than the original data. For QUEST at short TE, we found very large variance (2.2 times more than for LCModel), which is underestimated by the indicated error and probably due to large fluctuations in the estimated baseline. Table 1 illustrates the success of forecasting the error for creatine based on the unsuppressed water signal for 12 short TE spectra. The prognoses are quite good for LCModel, while for QUEST the forecasted error is at least twice the actual error indicated, reflecting in part the mismatch mentioned above.

Table 1: Forecast error values for total creatine using the developed tool

# Sub	Voxel location	TE ms	Voxel Size (mm³)	# avg	LW (Hz)	SNR	Forecast SD% for LCModel	SD% from LCModel	Forecast SD% for QUEST	SD% from QUEST
1	Frontal	30	7.7	128	4.2	44.1	2.3	2	3.7	1.1
2	Supraventricular	30	6.7	64	4.4	33.0	3.3	3	5	1.2
3	Supraventricular	30	6.7	64	4.7	33.9	3.2	3	5.1	1.6
	Occipital	30	2.7	64	4.2	20.8	4.6	4	9.2	2.2
	Frontal	30	1.6	64	4.9	8.2	8.1	7	13	5.0
4	Supraventricular	30	6.7	64	4.5	32.1	3.3	3	5	1.5
	Occipital	30	3.5	64	5.9	14.6	4.7	4	9.9	2.6
	Frontal	30	3.5	64	5.0	16.3	4.6	4	9.1	2.3
5	Supraventricular	30	5.3	64	4.0	31.9	3.3	3	4.8	1.5
	Occipital	30	4.5	64	6.3	34.0	3.3	3	5.6	1.5
	Frontal	30	3.3	64	5.3	18.3	4.6	4	10	2.4
	Supraventricular	30	8.2	64	4.4	23.2	3.9	4	5.8	1.9

Conclusions: Our first results indicate that it will be possible to forecast the errors associated with specific metabolites to be found in model fits of WS spectra based on a single shot water signal. Thus, the clinical MRS user will be able to judge ahead of time whether the planned acquisition will be of sufficient quality to answer the question at hand or whether it needs more averages or improved shimming.

References: [1] https://scion.duhs.duke.edu/vespa/; [2] Mlynarik et al. *NMR Biomed* 14:325(2001); [3] Mekle et al. *Magn Reson Med* 61:1279 (2005); [4] Provencher *Magn Reson Med* 30:6(1993); [5] Naressi et al. *Comput Biol Med* 31:4 (2001)

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