Assessment of the Pade approximant for quantifying Proton MR Spectroscopy data

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Introduction: Recently Belkić1 presented the Padé approximant (PA) as a method of generating magnetic resonance spectra with superior resolution to the standard discrete Fourier transform. The method determines peak frequencies in an identical manner to existing "black-box" quantitation methods2, but has the advantage that the amplitudes are determined analytically. In this work we assess PA as a parametric estimator and compare results from quantifying both simulation and experimental data with results from HLSVD3 and AMARES4.

Methods/Subjects: Simulated signals were generated comprising six separate peaks in the frequency domain. The signals were designed to represent, lactate (doublet), n-acetylaspartate (NAA), creatine (Crn) (2 peaks) and choline (Cho). Signals of varying lineshape (Lorentzian, Voigt) were simulated in the presence of 10% white noise. In addition, single voxel MRS data were acquired form a seven-tube phantom. Each tube contained a different concentration of acetate, Crn and Cho. The data were quantified using the PA, implemented according to the algorithm described by Belkić1, and the results compared with those obtained using the HLSVD and AMARES as implemented in jMRUI5.

Results/Conclusions: Table 1 shows the NAA amplitudes obtained from quantifying the simulated data. For Lorentzian lineshapes all three methods are statistically identical. As the Gaussian character of the Voigt lineshape is increased all three methods show a bias in the mean value. The assumption of a Lorentzian lineshape in the model results in an overestimation of the peak amplitude. This is not a problem if amplitude ratios are required, provided the frequencies are sufficiently well separated and the line broadening is identical across the spectrum. However for closely neighboring frequencies a correlation develops between the peak amplitudes as the peaks broaden (1a and b), invalidating the use of these two amplitudes as an internal standard. Figure 2 shows the ratio of Crn and acetate amplitude determined from the quantification of the phantom data versus the equivalent ratios of metabolite concentrations. Similar results are found for Cho and for acetate where the amplitude of the acetate in tube 1 is used as a reference for the other tubes.

Broadening	PADE	HLSVD	AMARES
0	24.98 ±0.46	24.99 ±0.49	25.00 ±0.42
4	26.42 ±0.44	26.78 ±0.41	26.96 ±0.41
8	28.78 ±0.59	29.03 ±0.60	29.14 ±0.55
12	29.13 ±0.76	31.43 ±2.46	30.20 ±0.70

1Dž. Belkić *et al.* J. Chem Phys., **113**, 6543-6556, 2000. 2L. Vanhamme *et al.* NMR Biomed **14**,233-246, 2001.3W. Pijnappel *et al.* J. Magn. Reson. **97**, 122-134,1992. 4S. Miersova *et al.* NMR Biomed **11**, 32-39, 1998. 5A Naressi *et al.* MAGMA, **12**, 141-152, 2001

Figure 1b: Creatine vs. Choline Amplitudes for Voigt line shape comprising a 2Htz. Lorentzian convolved with a 3Htz. Gaussian.

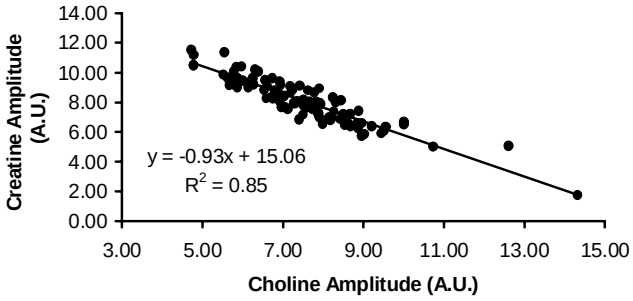

Figure 1a: Creatine Vs. Choline amplitude for a pure 2Htz. Lorentzian lineshape

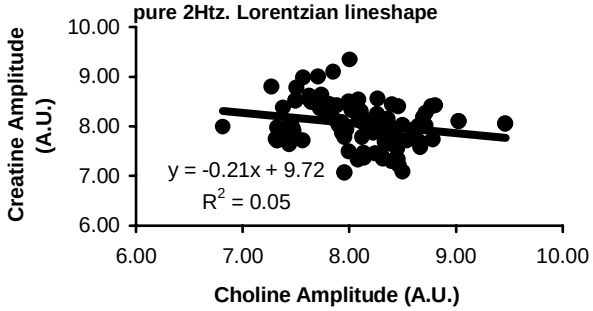

Figure 2a: Creatine (AMARES)

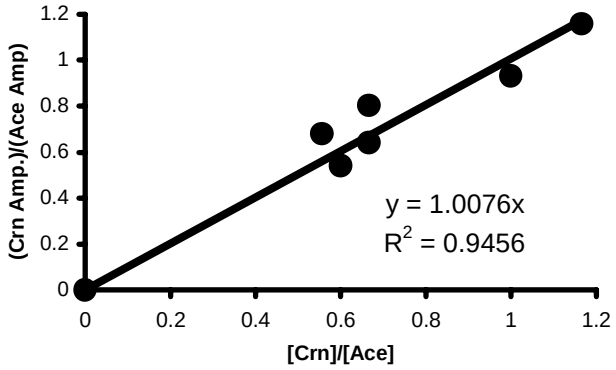

Figure 2b: Creatine (Pade)