Comparison of two approaches to model the macromolecule spectrum for the quantification of short TE ^{1}H MRS spectra at 14.1T

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Introduction:
Accurate assessment of the macromolecule contributions in short echo-time proton MRS spectra is important for a reliable quantification of the neurochemical profile. A biased estimation of the macromolecules can lead to errors in the estimation of the metabolite concentrations (1,2). The aim of the present study was to assess two approaches based on using LCModel (3), which take the macromolecule contributions into account in the quantification step at 14.1 T.

Methods:
Experimental: [1]H spectra were measured on five rats (Sprague-Dawley, VOI=3x4x4mm^3). All data were acquired on a 14.1T/26cm system (Varian/Magnex Scientific) using: a home-built 14 mm quadrature coil as RF transceiver, and the ultra-short-echo time SPECIAL spectroscopy sequence (TE=2.8ms, TR=4s, 320 averages) (4). Field homogeneity was adjusted using FASTMAP (5). For the acquisition of the *in vivo* macromolecule spectra, metabolite nulling was achieved by the inversion recovery method using an adiabatic hyperbolic secant RF pulse (2-ms duration and 8-kHz bandwidth) with 750ms inversion time (TE=2.8ms and TR=2.5s). Residual signals attributed to incompletely nulled metabolites were removed using HLSVD (6).

Data analysis: Metabolite concentrations were estimated using LCModel, combined with a simulated basis-set of metabolites using published spectral parameters and: 1) the spectrum of macromolecules measured *in vivo* using an inversion recovery technique; and 2) the built-in LCModel spline baseline. The water signal was used as an internal reference and average relative differences between the concentration estimates using the two approaches were compared.

Results:
The mean values and standard deviations of the metabolite concentrations obtained using the two approaches are presented in the Figure 1. Although there was overall a reasonable agreement in metabolite concentrations, NAA and Glu concentrations were slightly lower (8-15%) and Cr+PCr, GPC+PCho, Gly concentrations were slightly higher (10-17%) when using the fitted splines. Also an overestimation of Glc, GABA, PCho, GSH, PE, Asp concentrations (~30-70%) and an underestimation of Ala, Asc, NAAG, Lac concentrations (~70-100%) were noted. The built-in LCModel spline baseline obtained from five rats was highly consistent and very well defined from animal to animal, except close to H$_2$O at around 4.5 ppm (Figure 2a).
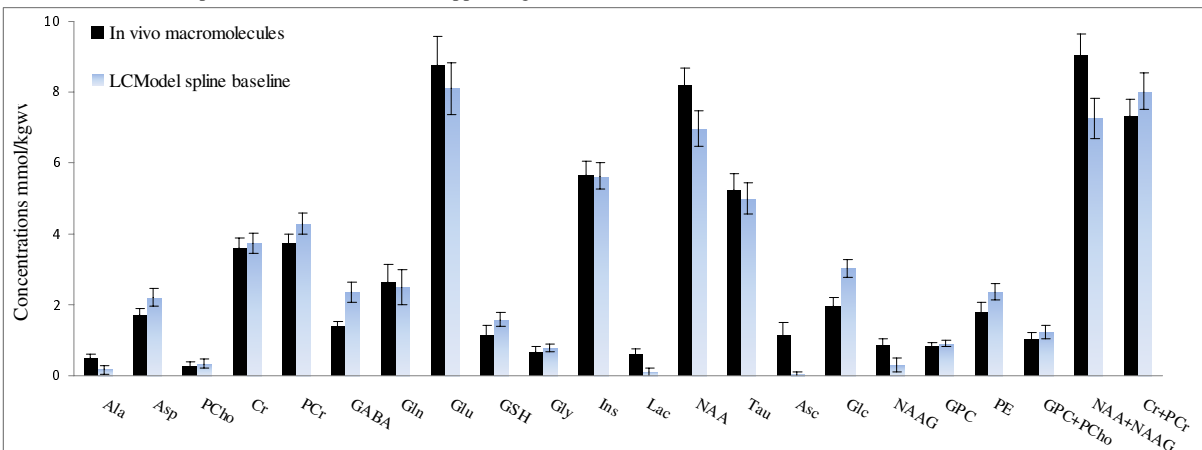

Figure 1: The mean values and standard deviations of the metabolite concentrations obtained using: 1) the spectrum of macromolecules measured *in vivo* (black bars); and 2) the built-in LCModel spline baseline (light blue bars).

Discussions:
The fitted splines (Figure 2a) resulted in a smooth approximation of the *in vivo* macromolecules (Figure 2b), which could not reproduce completely all features of the *in vivo* spectrum of macromolecules at 14.1T (Figure 2b). We can conclude that, as in previous studies using Subtract-QUEST (2), even if the fitted splines reproduce the *in vivo* macromolecules very well, the measured macromolecular "baseline" represents an additional prior knowledge and lead to a more accurate and reliable quantification at higher field strengths, which was attributed to an effectively increased spectral resolution of the macromolecule components.
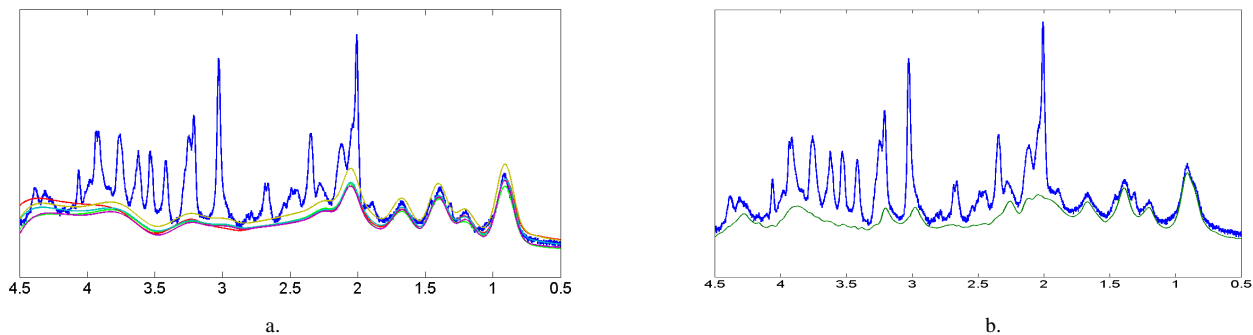

a.   b.

Figure 2: A 14.1T spectrum (320 averages) of rat brain measured from a VOI=3x4x4mm^3 (blue line): a) the built-in LCModel spline baselines obtained from five rats are plotted in colored lines; and b) the *in vivo* measured macromolecules spectrum is plotted in green line.

References
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