The influence of chemical shift displacement on ^{1}H MRS quantitation at 3T using a simulated basis set

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Introduction

Accurate and automatic quantitation of ^{1}H MRS is an important requirement for its incorporation into clinical practice. The most robust methods incorporate a high level of prior knowledge into the analysis routine, in the form of a collection of metabolite signals known as a basis set. The use of simulated metabolite basis sets has increased in popularity due to the greater availability of metabolite parameters and software packages with simulation capabilities. Whilst the accuracy of simulation has been demonstrated at 1.5T (Wilson et al NMR Biomed 2010), the influence of chemical shift displacement (CSD) becomes significant at 3T resulting in complex modulations in metabolite signals. Here we show that modelling CSD in basis simulation is required for accurate quantiation on a 3T clinical platform.

Methods

To validate simulation accuracy the following metabolite solution was prepared and stored in a 1L Nalgene bottle: 1L deionised H_2O, 1 PBS sachet (Sigma), 10mM creatine, 10mM glutamine, 10mM alanine, 1g NaN_3. High resolution MRS was performed at 500MHz (Bruker) from a 0.6ml solution and accurate chemical shift and J-coupling values were found for creatine, glutamine and alanine at 20°C using the wxNUTS fitting software. MRS was performed on the full 1L phantom using a 3T Philips Achieva clinical MR system using PRESS localisation (TE=35ms, TR=5s, voxel volume=8cm^3). MRS was also collected from a paediatric patient with an optic pathway glioma brain tumour using the same parameters but with TR=2s. Basis set simulation was performed using two methods: 1) PRESS with ideal pulse properties and 2) PRESS with limited bandwidth 180° pulses. The pulse profile method (Maudsley et al JMR 2005) was used for the limited bandwidth basis simulation. In brief: the tip angle for each spin is calculated over a spatial grid based on the frequency response profile of the pulse, simulations are calculated for each point in the grid and averaged - resulting in a more accurate model incorporating CSD. For the phantom data, basis sets were generated using the metabolite parameters derived from temperature matched high-resolution MRS. For the patient data published values were used (Goverinderaj et al NMR Biomed 2000). Basis simulation, spectral processing and fitting were performed using the TARQUIN software package (Wilson et al MRM 2011).

Results

Figure 1 shows the fit and residual for the phantom data using a basis set simulation incorporating CSD. Improved fitting was evident compared with the ideal pulse simulation (figure insert) and the fit residual was a third less in the realistic model. The greatest improvement in fitting accuracy was for alanine, an expected result due to the large difference in chemical shift between its multiplets. Brain tumour MRS fits are shown in Figures 2 and 3 using the ideal and CSD basis sets respectively. Whilst the fit quality is comparable between the basis sets, the measurement of lactate and lipids at 1.3ppm differ by a factor of 2. To investigate the importance of CSD simulation to other metabolites the spectral difference was calculated between the ideal and CSD simulation methods for each metabolite and expressed as a percentage relative to the metabolite with greatest difference (Table 1).

Metabolite	CSD effect
Lac	100.0%
Ala	98.7%
Asp	61.5%
GABA	55.8%
Gln	33.5%
Glth	32.3%
Glu	26.6%
NAA	20.9%
Glc	12.3%
GPC	9.4%
Ins	7.6%
Tau	4.2%
PCh	3.9%
Cit	3.8%

Table 1. Relative influence of CSD

Discussion

This work highlights the importance of accounting for CSD in the simulation of metabolite basis sets for accurate quantitation of MRS at 3T. Here we show inaccurate lactate simulation may result in an overestimation of the lipid resonances. This is clinically important since MRS lipids are known to be related to patient survival (Wilson et al EJC 2012). In addition we have also shown other coupled metabolites are influenced by CSD and should therefore be simulated fully accounting for CSD to ensure accurate quantitation.

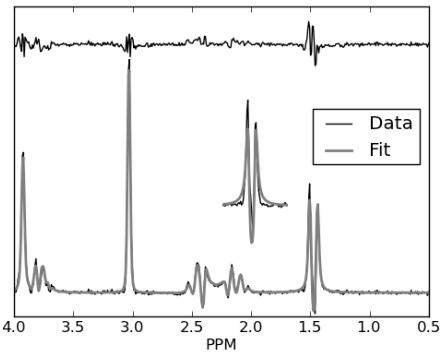

Figure 1. Phantom fit with CSD basis (main) and non-CSD basis (insert).

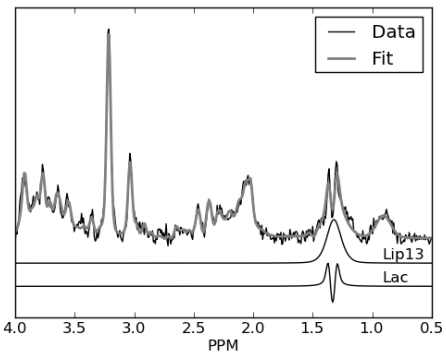

Figure 2. Tumour fit with ideal basis

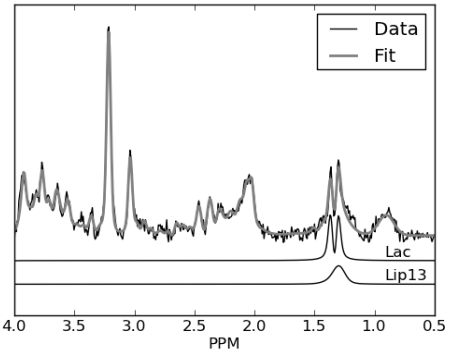

Figure 3. Tumour fit with CSD basis