Quantification of ^{31}P NMR Spectra using LCModel

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Introduction

Quantification of ^{31}P NMR spectroscopy is commonly performed using line-fitting techniques with prior knowledge. Currently available ^{31}P analysis software includes AMARES [1] and CFIT [2]. Linear combination modeling with LCModel is another popular approach to fit ^{1}H spectra [3] and has previously been extended to fit ^{13}C *in vivo* spectra [4], but to the best of our knowledge it has not been used to fit ^{31}P spectra. The aim of this study was to evaluate the suitability of LCModel to quantify *in vivo* ^{31}P NMR spectra.

Methods

Healthy volunteers (n = 5) were studied on a Siemens Trio 3 Tesla scanner (Siemens, Erlangen, Germany). *In vivo* ^{31}P NMR spectra (without proton decoupling) were acquired from the occipital cortex using a pulse-acquire sequence (TR = 2 s) and a small ^{31}P surface coil (6 cm diameter). A small sphere filled with water was placed at the center of the coil to verifying the positioning of the ^{31}P RF coil on ^{1}H images. ^{1}H imaging and B_0 shimming was performed with the standard body ^{1}H RF coil.
The baseline in the ^{31}P spectra was removed from each spectrum by subtracting the same spectrum processed with a large exponential filter (LB = 400 Hz). Spectra were then analyzed using LCModel. Basis sets were simulated in Matlab using published and measured ^{31}P chemical shifts and J_{PP} and J_{PH} coupling constants [5, 6]. By default LCModel uses the 0 ppm chemical shift for referencing when generating basis set. However, in ^{31}P NMR, this chemical shift (0 ppm) is generally assigned to PCr singlet peak. Therefore, when generating LCModel basis spectra for ^{31}P, the reference marker was set at -20 ppm (i.e. PPMPK = -20).

Results and Discussion

When using the same T_2 for all resonances, the LCModel fit for an *in vivo* ^{31}P spectrum (Fig. 1A) showed residuals in ATP resonances which resulted from the sharp narrow lineshape estimated by LCModel. By default LCModel assumes similar linewidth (proportional to $1/T_2$) for all resonances. However it is well known that T_2 of ATP is much shorter than the T_2 of PCr [7]. In addition, since no proton decoupling was used, long-range ^{31}P - ^{1}H couplings also broaden the lines for ATP.
As expected, specifying a different expected linewidth for each metabolite resulted in improved residuals in the LCModel fit (Fig. 1B). This was achieved by adjusting the following parameters in LCModel: DEEXT2, DESDT2 and DSSDSH.
The concentrations obtained from the analysis are given in Table 1 assuming a PCr concentration of 4 mM in the brain. These concentrations were consistent with previous studies [8, 9]. Apparent differences in concentration between the three resonances of ATP (fitted separately) are likely due to T_1 relaxation effects as well as the decreased efficiency of the excitation pulse off-resonance. CRLBs were found to be less than 10 % for all metabolites.

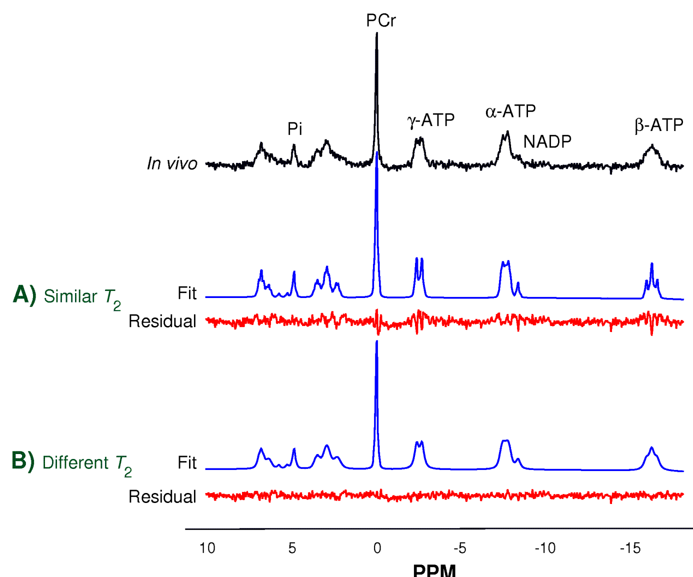

Figure 1: Comparing of LCModel fitted ^{31}P spectrum (nt = 600, TR = 2 s) with similar (A) and different (B) T_2 values for each resonance.

Metabolites	Rel. Conc. (mM)	CRLB (%)
PCr	4.0 ± 0.0	1
α-ATP	4.5 ± 0.4	2
β-ATP	3.7 ± 0.2	2
γ-ATP	3.9 ± 0.3	2
Pi	1.4 ± 0.2	4
NADP	0.8 ± 0.1	7
MP	1.9 ± 0.4	5
PE + PC	3.2 ± 0.5	2
GPE + GPC	3.5 ± 0.2	3

Table 1: Concentration and CRLB of metabolites from 5 subjects obtained with LCModel.

In summary, this study shows the feasibility to quantify *in vivo* ^{31}P spectrum using the LCModel software.

References

[1] van deen Boogaart et al. ESMRMB 1996; [2] Gabr et al. JMR 2006; [3] Provencher NMRB 2001; [4] Henry et al. NMRB 2003; [5] Jung et al. MRM 1997; [6] Jensen et al. NMRB 2002; [7] Merboldt et al. JMR 1990; [8] Reyngoudt et al. Cephalagia 2011; [9] Pan et al. AJP 2007.

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