The potential underestimation of amino acids for the MR spectra analyzed by LCModel: the study of model spectra.

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Introduction

In vivo proton MR spectroscopy (MRS) along with LCModel [1] has been widely used as a reliable modality of diagnosis for brain tumors and abscesses [2]. In the meanwhile, amino acids (AA) such as valine, isoleucine and leucine have been recognized as key metabolites to categorize brain abscesses [2]. Therefore, in this study, we investigated the potential underestimation of amino acids caused by basis spectra for abscess patients. Short TE (35ms) spectra were analyzed by LCModel using basis set of AA (the combination of three metabolites) and that of valine, isoleucine and leucine respectively. Cramér-Rao lower bounds (CRLBs) were used as the criteria to identify the presence of amino acids in MRS.

Materials and Methods

A total of 8 patients with pyogenic brain abscesses were included in this study. All patients underwent MR studies on a 1.5T system (General Electric, Milwaukee, WI) using a quadrature head coil with conventional single voxel MR spectroscopy (MRS) protocol (PRESS, TR/TE = 1600/35 ms, Ave =192, voxel size = 2x2x2 cm^3). Additional acquisitions with two different TEs (136 and 272 ms) were also performed in order to facilitate identifying the presence of amino acids in MRS for radiologists. The MRS data were analyzed by LCModel with two simulated basis sets generated by GAMMA [3] Visual Analysis (GAVA) [4] respectively. Both of the basis sets contained the following metabolites: alanine (Ala), aspartate (Asp), acetate(Ace), succinate (Suc), creatine (Cr), γ-aminobutyric acid (GABA), glucose (Glc), glutamine (Gln), glutamate (Glu), myo-inositol (m-Ins), lactate (Lac), NAA, N-acetylaspartylglutamate (NAAG), scyllo-inositol (s-Ins), glycerophosphorylcholine (GPC) and phosphorylcholine (PC). In addition, one of the basis sets includes separate basis spectra for valine (Val), leucine (Leu) and isoleucine (ILc) simulated with chemical shift and J-coupling values from Tikhonov and Kostromina [5], while the other one basis set included one synthetic AA basis spectrum composed of Val, Leu and ILc (composition ratio = 1:1:1) as illustrated in figure 1. Quantitative results obtained with the two basis sets were compared in terms of CRLBs (SD%). Only when the SD values of either valine, leucine, isoleucine or AA were smaller than or equal to 20%, the AA quantification was considered reliable.

Results and Discussion

All of 8 patients were diagnosed and confirmed the presence of AA in the MR spectra by radiologists. For 3 out of total 8 cases, AA could not be reliably quantified with any of the basis sets due to the poor quality of the short-TE spectra. Table 1 shows the SD values of the other 5 cases. Valine could be reliably quantified in these 5 cases when fitting with individual basis spectra of valine, isoleucine and leucine. On the other hand, when the synthesis spectrum of AA was used as the fitting model, AA could not be detected successfully in two cases. Figure 2 demonstrates the fitted spectra of case no. 4. In figure 2(a), it is obvious that valine and isoleucine can be fitted more precisely with separate basis spectra than fitted with synthesized AA basis spectrum (Fig. 2(b)).

Our example shows that the synthetic basis spectrum of Val, Leu and ILc may reduce the reliability of spectrum fitting because the characteristics of each multiple resonances could become indiscernible due to the summation of three metabolites. Our result suggests that using individual model spectra as basis sets would achieve better fitting than using synthesized multiple model spectra for J-coupled metabolites. Investigators also need to be aware of this potential bias when acquiring the basis spectra from phantom solution.

Table 1. The SD values of fitted results using two different basis sets. SD% >40% indicated by "-". Only SD%≤20% were recognized as reliable fitting (blue).

No	fitted by Basis sets of separate AA spec.			fitted by Basis sets of synthesized AA
	Valine	Isoleucine	Leucine	AA
1	18%	-	-	19%
2	12%	25%	-	8%
3	14%	38%	-	10%
4	12%	20%	24%	26%
5	19%	-	-	37%

References

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Figure 1. Simulated model spectra of valine, leucine, and isoleucine and their synthesized spectrum (AA).

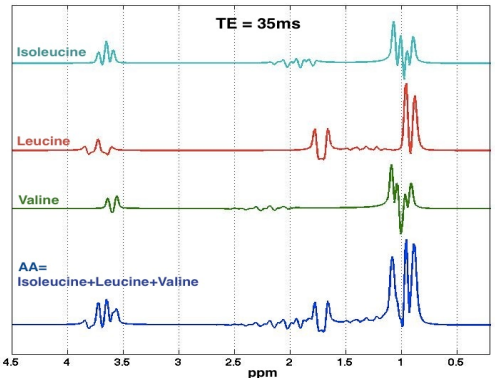

Figure 2. Fitted spectra of case no. 4 by using basis set of (a) separate model spectra (Val, Leu, ILc) and (b) synthesized spectrum (AA).