MRS 2D quantification vs 1D quantification

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Introduction

Many studies related to *in vivo* proton Magnetic Resonance Spectroscopy (MRS) led to one dimensional (1D) spectroscopic signal quantification methods including LCModel [1] based on frequency domain or QUEST [2] based on time domain. However, standard in vivo MRS acquisitions in 1D spectroscopy present important limitations. 1D MRS spectra usually present rich in vivo metabolic information through complicated, overlapped spectral signatures with large linewidths especially at moderate field. Accurate concentration quantification remains problematic especially for coupled metabolites such as γ-aminobutyric acid (GABA), Glutamine (Gln), Glutamate (Glu), *myo*-inositol (mI) and Taurine (Tau). To overcome these limitations, the two dimensional (2D) spectroscopy, which is routinely used in organic chemistry, analytical chemistry and structural biology, has great potential to unravel of the spectral information [3] and especially for decorrelation of coupled metabolite concentration. Very few studies (Profit [4]) on 2D spectroscopic signal quantification were performed. This paper introduces a 2D spectroscopic signal quantification based on a global fitting procedure using strong prior-knowledge in the time domain and investigates the correlation between estimate parameters occurring in 1D vs 2D quantification.

Method

Quantification algorithm: A two-dimensional fitting procedure has been developed, allowing quantification of 2D J-resolved magnetic resonance spectroscopic data acquired with J-PRESS sequence. Quantification phase uses complex time domain with a strong prior-knowledge, consisting in a set of M metabolite signals calculated numerically using the GAMMA library [5]. Chemical shifts and J-coupling values have been obtained from literature [6]. A non-linear optimization (MATLAB lsqnonlin function), which allows constrained search, is used in order to determine the following parameters for each metabolite: concentration c_m, relaxation time $T2_m$, damping factor $\Delta\alpha_m$ and frequency shift $\Delta\omega_m$. Additionally, a global phase zero-order phase Φ_0 is determined for the whole metabolite basis. The resulting 2D model function depends nonlinearly on time and Echo Time (TE) and consists of a linear combination of metabolite signals which is given by

$$\hat{x}_{t,TE} = \sum_{m=1}^{M} [c_m \hat{x}^m_{t,TE} \exp\left[(-\frac{TE}{T2_m})(\triangle\alpha_m i \triangle\omega_m)t\right]] \exp(i\triangle\phi_0)$$

Numerical study: To demonstrate the potential of 2D MRS, numerical studies have been carried out in order to compare coupled metabolite intercorrelations between 1D and 2D quantification. A 4.7T metabolite signal was generated. Gaussian random noise was added to simulated signals so as to reach a SNR ratio similar to *in vivo* data. 20 realizations of noisy metabolite signals were used. In order to preserve acquisition time and perform a fair comparison, 1D simulated data is averaged by the number of steps along the TE dimension in 2D simulated data. In this study, the number of steps in the TE dimension was 4, the first echo time being the same for 1D and 2D measurements. The correlation terms were computed from the Fisher matrix [7] of the parameter estimates. At the end the estimated correlation terms were averaged.

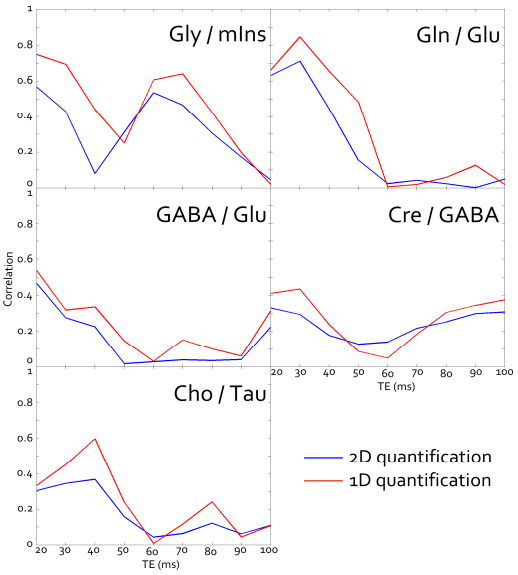

Figure2 : Evolution of the correlation terms between concentration estimates for overlapping metabolite signals.

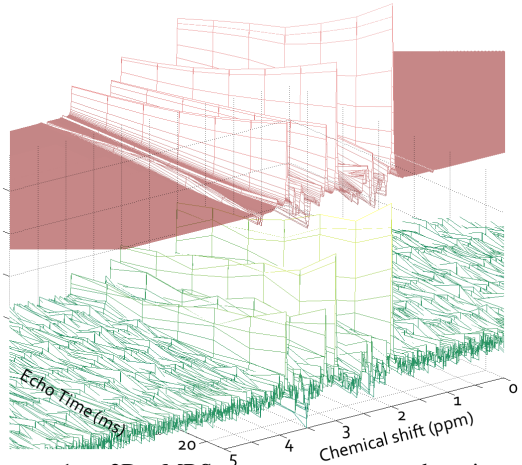

Figure 1 : 2D MRS spectra, generated using GAMMA, mimicking in vivo JPRESS measurements at 4.7T (green), and the corresponding estimated spectra using the proposed two-dimensional algorithm.

Results/Discussions

Figure 1, a 2D quantification fit is represented. Figure 2, the evolution of the correlation terms for different echo time starting points. Overall, the correlation terms are reduced in 2D quantification compared to 1D quantification, with variations that are linked to the J-coupling.

Conclusion

A new fitting algorithm has been set-up for the quantification of 2D in vivo acquisitions. The study of the correlations between the metabolite amplitude parameters demonstrates that starting at short echo time (TE<50 ms), the quantification of the 2D data should beneficiate from the second dimension for the estimation of the concentrations of the strongly coupled metabolites such as GABA, Tau, Glu and Gln. The 2D spectroscopy should alleviate the nuisance effects of the macromolecular contributions on the metabolite concentration estimates.

References

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