ProFit revised

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Introduction

Reliable and unambiguous detection and quantification of metabolites representing coupled spin systems like Glutamate, Glutamine or GABA, which are of special importance in many psychiatric diseases is impeded by spectral overlap at 3T. Two-dimensional JPRESS spectroscopy showed to significantly reduce the problem of signal overlap by spreading the spectral information of coupled spin systems into a second frequency dimension. A software tool called ProFit [1] was introduced by Schulte et al., which allows two dimensional prior knowledge fitting using fully simulated basis spectra similar to LCModel. However, some drawbacks are still present in the present version of ProFit. **The aim of this work** was to improve ProFit and to tackle problems like macromolecular baselines, residual baseline distortions and lineshape distortions. In addition possibilities for more flexible fine-tuning of the included prior knowledge regarding phase and frequency offsets, line broadening and amplitudes of the resonance lines are provided. The fit quality is finally compared to the original version of ProFit.

Materials & Methods

2D JPRESS spectra were acquired from the human brain on a Philips 3T system (Fig. A). The minimum achievable echo time was 31ms and the TR was set 1600ms. The second frequency dimension was encoded by 100 steps with a t1 increment of 2ms. Maximum echo sampling was used to improve SNR and to produce tilted peak tails in the reconstructed spectrum to prevent overlap [2]. A metabolite nulled 2D macromolecular baseline was measured using a double inversion sequence. A 2D maximum echo sampled basis set of 20 metabolites was simulated in GAMMA using the same acquisition parameters as for the in-vivo scan. The measured macromolecular baseline was denoised and included as an additional metabolite in the basis set (Fig B). The revised version of ProFit was implemented in Matlab (R2010b, The MathWorks, Inc., Natick, MA, USA). Starting values for the different free parameters were estimated from preliminary fit iterations using an increasing number of metabolites and degrees of freedom. Prior to the last fitting iteration a model-free two dimensional lineshape was calculated based on regularized splines and self-deconvolution [3, 4]. Finally all metabolites together with an additional tensor spline baseline and the spline-based lineshape model were used to calculate the final fit. The new algorithm was compared to the old ProFit version applied to the same in-vivo data set.

Results & Discussion

The fit results using the old ProFit tool are shown in Fig. C, E and G corresponding to the fitted spectrum, the residual and a projection along the t1 dimension respectively. Figures D, F and H show the results from the same data set using the proposed improved version of ProFit. Excellent fit quality is achieved due to the inclusion of macromolecular baseline signals as shown in Fig. B and a model-free lineshape model (Fig. I & J). From the comparison of the residuals (Fig. E & F) some of the problems of the previous version of ProFit become apparent. Macromolecular contributions at about 1ppm could not be handled sufficiently well and also residual tails of spectral components like creatine at 3ppm can be still clearly identified within the noise (Fig. E). All these systematic fit problems are drastically reduced in the revised version (Fig. F) and the overall improvement on the fit quality is clearly visible in the projection spectra of Fig (G & H). Another refinement comes from the complex lineshape model, which is able to handle envelope distortions and also phase deviations, which can occur during the whole duration of an experiment (Fig. I & J). In conclusion it could be shown that including features like 2D model-free lineshape and macromolecule signals can significantly improve fitting results for 2 dimensional data.

References

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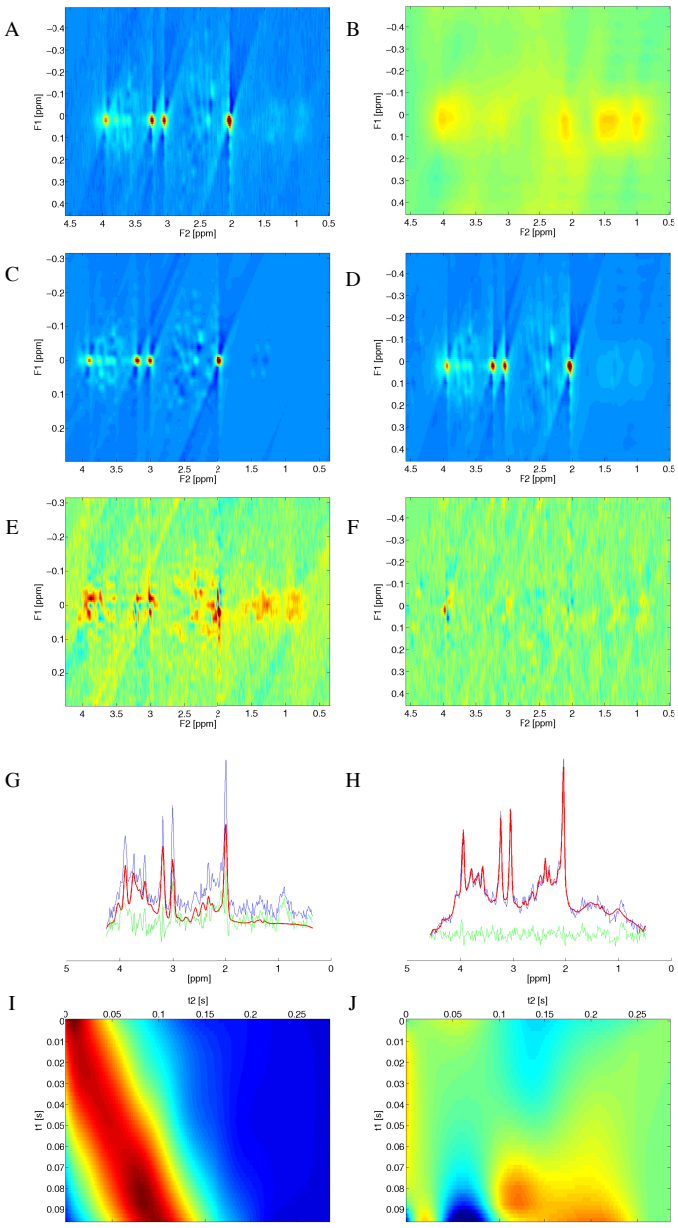

Figures (A-J): (A) shows the measured spectrum from a healthy volunteer. In (B) the final contribution of macromolecules together with surface splines as calculated from the proposed ProFit version is illustrated. In the left column the fitted spectrum of the old ProFit version together with the residual and t1 projected spectrum are shown in (C, E & G). On the right side (D, F & H) the corresponding plots of the newly proposed ProFit version are presented. Subplots (I & J) finally show real and imaginary part of the spline based line shape model used.