Versatile fitting tool for simultaneous modeling of spectral arrays using prior knowledge restrictions in two dimensions

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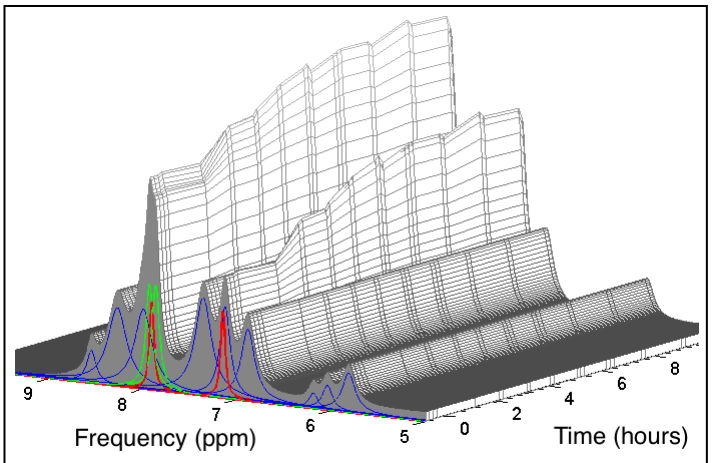

Fig 1. *Fitted time series of spectra obtained after an oral histidine load at time 0. The red signals with varying amplitude originate from histidine, the green doublet from the amide proton of NAA, and the blue lines from the rest of the downfield spectrum.*

Introduction: Most MRS fitting programs are restricted to fit one spectrum at a time and are thus not suited for 2D MRS or linked series of spectra. A versatile MRS fitting tool is introduced that is aimed at general two dimensional spectroscopy experiments [1,2], like J-resolved or saturation recovery spectra, but also kinetic data.

Methods: This software, programmed in JAVA, is designed to allow linear combination model fitting on single, or simultaneously on multiple spectra. A hierarchical spectral model includes the possibility to combine multiple numerical patterns (measured or simulated spectra of metabolites) and Voigt lines. It allows for complex prior knowledge within and between metabolites in the spectral dimension. In the second dimension, simple prior knowledge such as common frequencies, widths or phases can also be enforced, while predefined amplitude relations are available with functions to fit further parameters, like T_2 or T_1. Time and frequency domain fitting is supported. GAVA [3] is used to simulate basis sets. The software can be easily extended for different 2D experiment.

Results: Fig.1 shows the 2D fit for a time series of spectra obtained in a healthy person after an oral histidine load. A total of 24 downfield spectra (scaled by water) were fitted where only histidine was assumed to vary in concentration, while the baseline spectrum remains unchanged. The model enforces a common frequency and Lorentz line width, while allowing for varying phase and Gauss width in consideration of shimming differences. The relationship between the two histidine peaks and within the NAA doublet is also upheld. This complex prior knowledge allows to better model the histidine dynamics without the need to predefine the background spectrum in preload data. Fig. 2 shows a simulated saturation-recovery spectrum with NAA and glutamate. Distinct T_1s were imposed to validate the programs ability to fit additional parameters along the 2nd dimension. While low SNR limits fitting of individual short TR spectra, the 2D fit successfully determines the amplitude of NAA as a whole, with different T_1 values for the two separate sub-patterns (methyl vs. rest), which overlap with glutamate. Fig. 3 shows 2DJ data from lactate, fitted without Fourier transformation in the 2nd dimension. The residues show obvious disagreement, which is mostly due to ideal pulses being used in the simulation. Despite the discrepancy, the software is able to return reasonable T_2 values.

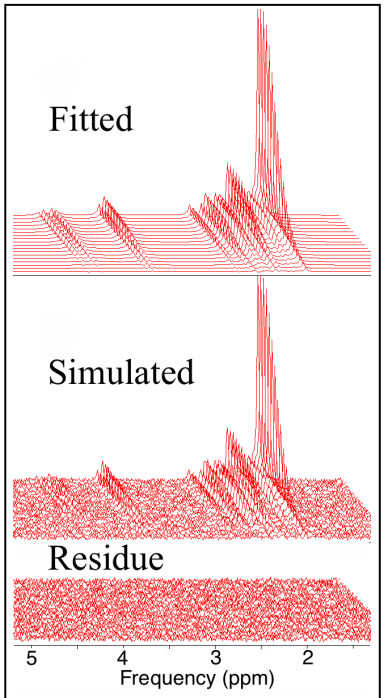

Fig 2. *Simulated and fitted saturation recovery spectra for NAA and glutamate with distinctly different T_1's.*

Conclusions: The developed software framework allows to fit different 2D MRS experiments. It offers fitting of linear combinations of basis spectra in 2D with prior knowledge constraints in both dimensions and options to determine parameters like T_1 or T_2.

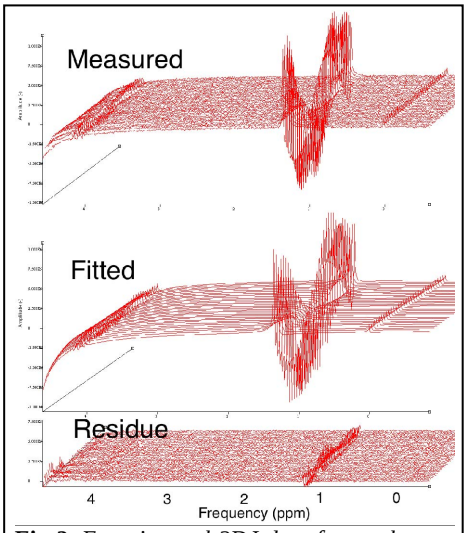

Fig 3. *Experimental 2DJ data from a lactate phantom with 2D fit and residue. PRESS with TE from 21ms to 331ms in steps of 10ms, recorded at 3T.*

References:

[1] Schulte et al. *NMR Biomed* 19:255 (2006). [2] Kreis et al. *MRM* 54:761 (2005). [3] Soher et al. *J Magn Reson* 185:291 (2007).

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