A Fast Spectral Simulator for in vivo Brain MRS

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Introduction

Simulation in nuclear magnetic resonance (NMR) is a valuable tool towards the development and understanding of NMR techniques. Due to strong coupling of many metabolites on commercial 1.5 T or 3.0 T clinical scanners, numerical simulations have been used to generate *a priori* information for parametric spectral analysis of brain NMR spectra [1] and to predict results of and optimize various editing sequences. However, due to the well-known computational burden in simulating quantum problems, most previous NMR simulation software can only handle one metabolite in an acceptable amount of time. Here, we reported a newly developed simulation package in Matlab, which can simulate the spectrum of any homonuclear proton sequence applyied to human brain. Numerical results for 1D PRESS and 2D L-COSY [2] experiments were obtained with the simulation software and compared to the in vivo spectra on our 3.0 T scanner, revealing good agreement between the two.

Methods

The simulator was written in Matlab with a complete GUI interface. Liouville-von Neumann equation in terms of the density operators was used. The simulation process was optimized to dramatically improve simulation speed instead of keeping a simple and uniform formalism as adopted previously. Both weak and strong J-coupling can be simulated without any approximation. For relaxation process, only the phenomenological exponential decay instead of an exact relaxation superoprator solution was used. Any shaped RF-pulses can be defined and be simulated. Gradient effects were simulated using multiple position approximation. A total of 25 metabolites, which covered the main observable brain metabolites, were chosen as the base molecules for the human brain. The J-coupling constants and the metabolite concentrations for healthy human brains from Ref [3] were used. The protons of a metabolite molecule were further divided into different coupled proton groups. A coupled proton group is defined by a collection of protons that any two protons in the group are J-coupled directly or indirectly through other protons in the same group. Since protons of a metabolite are normally J-coupled to its neighbor protons, a coupled proton group is normally corresponding to one amino-acid unit of a metabolite. The NMR spectroscopy simulator first simulates all independent coupled spin groups separately and then linearly combines all spectra after scaling with their corresponding physiological concentrations. The user is allowed to run a simulation on different levels: a single coupled spin system of a metabolite, a specific metabolite or all 25 metabolites to form a brain spectrum. The base metabolites can be redefined to represent the metabolites of other organs.

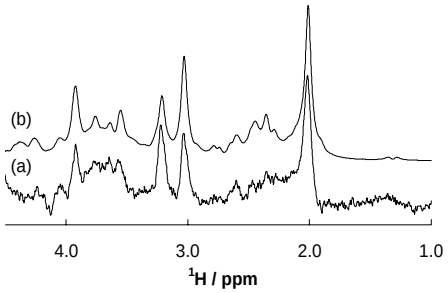

Fig. 1 1D PRESS spectra: (a) in vivo spectrum; (b) simulation spectrum

1D PRESS (VOI: 2.0×2.0×2.0 cm^3) and 2D L-COSY (VOI: 2.7×6.0×7.0 cm^3) were implemented on a 3.0 T scanner (Siemens) with a commercial head coil for excitation and detection. The acquisition parameters for both experiments were as follows: 2048 complex data points in the time domain, TR/TE: 2000/30 ms and 4 dummy scans. 192 averages were used for the 1D PRESS experiment. For t_1-dimension of L-COSY experiment, 64 steps were applied with 8 averages for each step. 4-step and 8-step phase cycling schemes were used for PRESS and L-COSY experiments respectively.

Results and Discussion

Instead of using workstation clusters or supercomputer, the simulations were carried out on a personal laptop with Pentium 4 CPU (2.7 GHz) and 512 MB of RAM. Both water signals and water saturation pulses were not included for the simulation. All other parameters and timings were the same to those used in in vivo studies. The simulation time was around 24 s for the 1D PRESS and was about 1.4 h for 2D L-COSY. On the contrary, for a usual 5-spin system, simulation did not finish even after 36 h for 1D PRESS using previous software: QSim [4]. Fig. 1(a) and Fig. 1(b) show the in vivo and simulation spectra for the 1D PRESS sequence. The left and right figures in Fig. 3 are the in vivo and simulation spectra for the 2D L-COSY experiment. As can be observed in Figs. 1 and 2, the simulated spectra in both cases correctly predicted the main features the corresponding in vivo spectra. Though water saturation pulses were applied for in vivo 2D L-COSY experiment, the residue water is still predominate (Fig. 2 (left)). Since the simulation procedure can be rapidly and conveniently modified to reflect different acquisition parameters and data analysis requirements, new sequences can be developed and be optimized using the simulator without the need to perform human subject studies.

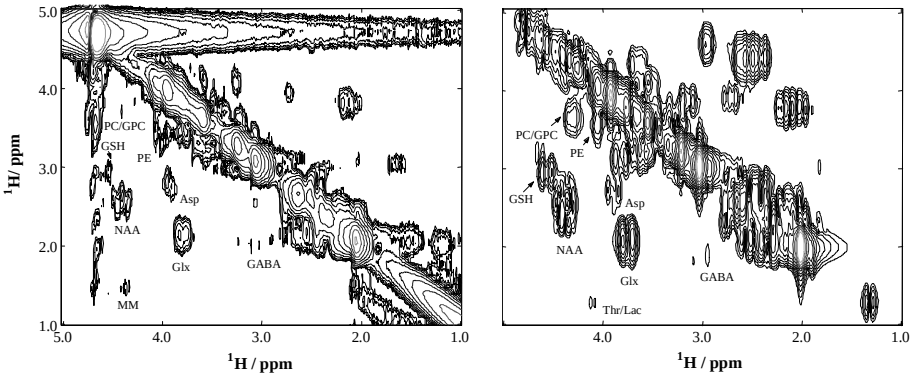

Fig. 2 2D L-COSY spectra: (left) in vivo spectrum; (right) simulation spectrum

Conclusions

A fast brain spectroscopy simulator was developed and was successfully demonstrated for 1D PRESS and 2D L-COSY. The simulator was found to correctly predict the main features of in vivo spectra. The brain simulator is fast enough to allow the simulation of both 1D and 2D proton experiments using a modern personal computer in a reasonable amount of time.

References

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