FID-A: An open-source, MATLAB-based toolbox for magnetic resonance spectroscopy simulation and data processing

Jamie Near[1,2], Gabriel A. Devenyi[3], and Robin Simpson[4]

[1]Department of Psychiatry, McGill University, Montreal, Quebec, Canada, [2]Centre d'Imagerie Cérébrale, Douglas Institute, Montreal, Quebec, Canada, [3]Centre d'Imagerie Cérébrale, Douglas Institute, Montréal, Quebec, Canada, [4]Department of Medical Physics, Freiburg University, Freiburg, Freiburg, Germany

Target Audience. This work is aimed at those involved in simulation and processing of in-vivo magnetic resonance spectroscopy (MRS) data.

Purpose. MRS enables non-invasive measurement of tissue metabolite levels in-vivo. Performing in-vivo MRS metabolite measurements usually involves a number of steps, including quantum mechanical simulations of metabolite model spectra, data processing to prepare the acquired data for analysis, and spectral analysis to estimate peak intensities. While tools for spectral analysis are well established [1,2], the availability of tools for MRS simulation and data processing is limited. For example, processing of MRS data typically consists of a few routine operations (eddy-current correction, removal of motion corrupted averages, frequency/phase drift correction, etc.), however, few (if any) software packages can achieve all of these steps, forcing many users to implement "home-grown" solutions. This lack of availability of processing tools may contribute to a lag in the uptake of MRS methods in both research and in the clinic, and it may also contribute to a lack of consistency or replicability of results in the MRS literature. Motivated by the need for improved access to tools for simulation and processing of MRS data, this abstract introduces a new, open-source software package for simulation of MRS experiments, design and analysis of radiofrequency (RF) pulses, and processing of MRS data. The software is called 'FID Appliance' (FID-A), and is freely available for download (www.github.com/CIC-methods/FID-A).

Methods. The FID-A software package is implemented in MATLAB (Natick MA, USA). Within FID-A, a simulated or experimental MRS dataset is stored in a uniquely formatted data structure that encapsulates all of the data and relevant header information. Each data structure stores both time-domain and frequency-domain data arrays. When multiple averages, coil channels, or subspectra of data are present, they are stored in separate dimensions of the arrays, and indexed within the header. By encapsulating data and header information in this way, processing operations have access to all relevant information and thus require as few input arguments as possible. S*imulation Toolbox*: The FID-A simulation toolbox is based on an implementation of the density matrix formalism, where the evolution of the spin system in a given experiment is described by successive evolutions of the density matrix by time-independent Hamiltonian operators [3]. The simulation toolbox contains built-in functions for simulating common in-vivo MRS pulse sequences (FID, PRESS, STEAM and spin-echo) by specifying the pulse timings and the chemical shifts and coupling constants of the spin-system of interest. A full set of common metabolite spin-system definitions is provided based on previously published values [4,5]. Excitation and refocusing RF pulses can be modeled as ideal (instantaneous) rotations, or fully shaped RF waveforms, depending on the user's requirements. In the case of shaped RF pulses, phase cycling is performed to remove unwanted coherences. To demonstrate the functionality of the FID-A simulation toolbox, the MEGA-PRESS experiment was simulated on the GABA spin system with ideal localization pulses and shaped editing pulses. The effect of varying the editing pulse duration with values of 8, 14, 20 and 26 ms was investigated. *RF-Pulse Toolbox*: The FID-A RF toolbox enables the creation of basic RF pulse waveforms, and Bloch simulation to determine the resulting excitation/refocusing/inversion profiles. *Processing Toolbox*: The FID-A processing toolbox contains 'load' functions to accept MRS data in MRI vendor data formats (Siemens, Agilent, others in development), and store them in MATLAB as described above. The data can then be operated on using any of the over 50 different processing operations, including (but not limited to) filtering, zeropadding, time domain truncation, frequency domain truncation, eddy current correction, removal motion corrupted averages, retrospective frequency and phase drift correction [6], combination of multi-element RF coil data, and zero- and first-order phase corrections. Finally, the FID-A processing toolbox contains 'write' functions to output the data into the formats accepted by leading MRS data processing packages. To demonstrate the functionality of the FID-A processing toolbox, an in-vivo MRS dataset was acquired from a 8 cm^3 region of interest in the motor cortex of a healthy female volunteer on a 3T Siemens (Erlangen, Germany) Trio MRI system using the SPECIAL sequence and a 32 channel receive array head coil and 192 averages. Processing was performed using the FID-A processing toolbox, with steps including weighted recombination of receiver array data, removal of motion corrupted averages, frequency and phase drifts correction, and eddy current correction.

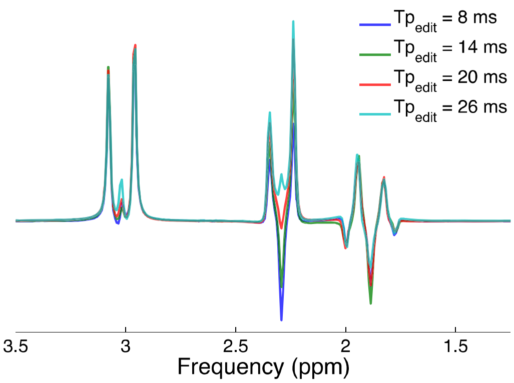

Figure 1. Simulations of the MEGA-PRESS sequence using the FID-A simulation toolbox, and incorporating shaped editing pulses with various editing pulse durations.

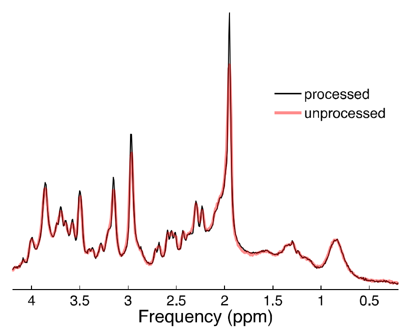

Figure 2. In-vivo SPECIAL MRS data with and without processing using the FID-A processing toolbox.

Results. The results of the MEGA-PRESS simulations with different editing pulse durations are shown in Figure 1. The effect of the editing pulse is most clearly observed on the 2.28 ppm GABA resonance, with longer editing pulse durations resulting in less suppression of the 2.28 ppm GABA resonance. Figure 2 shows the acquired in-vivo spectrum with and without the processing steps described above. Compared to the unprocessed spectrum, the processed spectrum has increased peak amplitudes and narrower linewidths.

Discussion. From Figure 1, it is clear that the editing pulse duration has a pronounced effect on the observed GABA signal in edited MEGA-PRESS data. This demonstrates the importance of accounting for the full shape of the editing pulses when generating simulated metabolite model spectra. Finally, the results shown in Figure 2 illustrate the importance of spectral processing for optimal spectral quality. The examples shown here illustrate some of the functionality provided by the FID-A software package, which may be difficult to achieve using existing software packages.

Conclusion. The FID-A software package provides a powerful and versatile platform for simulation and processing of MRS data, and RF pulse design and analysis. The open-source nature of the package enables users to easily customize their own simulation and processing routines.

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