An Open-Source Platform for Routine Clinical 1H Magnetic Resonance Spectroscopy Processing

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Introduction: 1H Magnetic Resonance Spectroscopy (MRS) is an invaluable tool for the clinical diagnosis of many neuropathological conditions [1,2]. However, routine use of 1H MRS either clinically or in research has been complicated by lack of standardization regarding data processing. Current research tools for processing spectroscopic data (e.g. [3-5]) are often too complex, expensive, or unwieldy for the average clinical end-user to employ on a routine basis, and for this reason the MR manufacturer-provided programs are the default choice for MRS processing in clinical settings. This dependence on manufacturer software has lead to a black-box approach to 1H MRS data processing, with flexibility of processing, understanding of artifacts, and cross-institution comparability suffering as the result. Though spectral fitting has improved tremendously, one could argue that the critical problems facing clinical use of MRS are not completely answered by better methods, but also by greater consistency and usability. In this abstract we discuss a platform for processing 1H MRS data which shifts the emphasis away from the complex format preferred by expert MR engineers and physicists, towards a tool which even new-comers to 1H MRS will find natural and intuitive-- without sacrificing flexibility or power. The advantages of this system, and the ideals guiding its development, include: 1) completeness; 2) usability; 3) transparency; 4) availability; and 5) reliability.

Completeness: The software is based on algorithms from [6-8]. The order of steps in 1H processing include: 1) data selection (Siemens .rda and GE probe formats supported; extensions for other formats can easily be added); 2) data labeling (e.g. overriding or setting transmitter frequency; labeling patient information); 3) water referencing; 4) eddy current correction; 5) water filtering; 6) zero-order phasing; 7) creatine referencing and baseline calculation; 8) apodization; 9) quantitative ratio calculations and reporting. See Figures 1-3 for screens and [11] for videos. Quantification of exact chemical concentrations via an external standard and assessment of water compartments is supported [6,7], but not required, and the open source nature of the application supports extensions to other quantification techniques (e.g. [3-5]).
Usability: The unique feature of this platform is the focus on usability [9]. At every step, the user can choose to override parameters and make adjustments— however, appropriate defaults are provided so a less seasoned user can easily skip adjustments he does not fully understand. At one extreme, to obtain quantitative measures on all key metabolites, the user need only hit the "Next" button (or hit the spacebar) until processing is complete. An additional benefit is that the single-track structure of the application provides ample opportunity for education regarding the subtleties of 1H MRS processing, and facilitates remote help, debugging, and support.
Transparency: To prevent a "black-box" mentality, every manipulation to the data is explicitly visualized via reporting screens. This allows users to understand, if they so desire, every change to the data in a step-by-step manner, facilitating the discovery of artifacts of processing and system instabilities. The system thus provides all the information and capabilities an advanced user requires, without overloading the newcomer or less technical user.
Availability: The system is an open-source, publically available software package (http://www.spectroscopy.org/Proton-Torpedo), written in IDL and executable through IDL Virtual Machine [10]. IDL was chosen for historical reasons, but planning for porting the system to free languages such as R or Java is underway.
Reliability: The system has been in daily use in a clinical setting for 9 years, having been applied to thousands of individual spectral data sets for hundreds of subjects. "Default" operability of the system has zero variability, as processing without changing presets leads to deterministic results. Employing the software on data from a 1.5T GE Signa (STEAM, TE=30ms, TR=1500ms, voxel size= 11.34cc, NEX=64 (*in vitro*)/128 (*in vivo*)) we examined the coefficients of variation (CV) of serial scans over a two year period on a "brain metabolite" phantom and in an occipital grey matter brain location in 4 young adults (age: M=24.7 years, SD=1.4). The results (Table 1) are upper limits of variation factoring in not only inter-operator variability in data analysis, but also variability in data acquisition and changes in system stability. The low CVs, combined with the continual use of the software for almost a decade, suggest the software is reliable, stable, and ready for mass dissemination.

Conclusions: We report on a 1H MRS processing platform that is powerful, reliable, and easy-to-use, reflecting on a much overlooked aspect of 1H MRS: the end-user experience. We believe that difficulties in navigating the myriad options and subtleties of spectroscopic data processing have limited the use of 1H MRS, and believe that this new focus on widely accessible, easily adopted, and usable tools is a critical, and too-often overlooked, aspect of MR research.

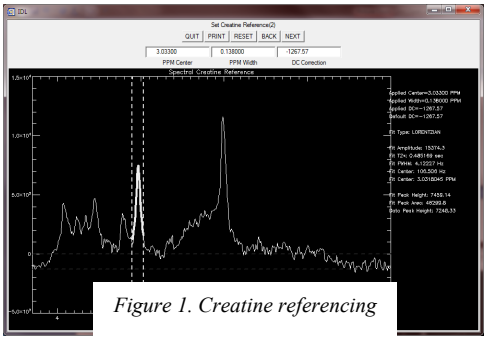

Figure 1. Creatine referencing

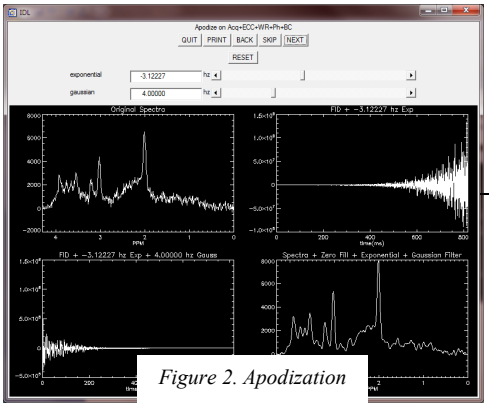

Figure 2. Apodization

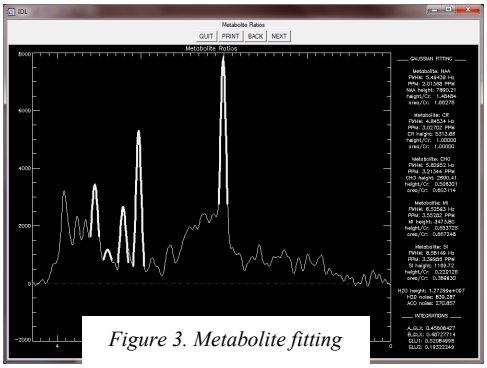

Figure 3. Metabolite fitting

Table 1: in vitro & vivo 2-year exam variability

	N	Exams/ Subject	Coefficient of variation NAA/ Cr	Cho/ Cr	mI/ Cr
Phantom	1	22	2.1%	1.9%	3.6%
Controls	4	4,4,5,6	5.3%	5.2%	7.4%

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