Showcasing an open-science environment for rapid benchmarking of new 1H-MRS methods

Helge J. Zöllner[1], Peter B. Barker [1,2], Richard A. E. Edden[1], Georg Oeltzschner[1]

[1]Russell H. Morgan Department of Radiology and Radiological Science, The Johns Hopkins University School of Medicine, Baltimore, MD, United States
[2]F. M. Kirby Research Center for Functional Brain Imaging, Kennedy Krieger Institute, Baltimore, MD, United States

Introduction: Standardized data processing and *linear-combination modelling (LCM) is the expert consensus recommended quantification approach for 1H-MRS[1]. The ability to modify underlying algorithms and or introduce novel quantification approaches may improve transparency, robustness, and accuracy of metabolite estimation, but there is no established framework for rapid prototyping of modelling algorithms and their performance. We present an open-science environment including large publicly available MRS dataset and open-source analysis and visualization software, and demonstrate its utility for 1H-MRS research.*

Methods: *A large-scale multi-vendor, multi-site dataset (GABA-edited MEGA-PRESS and short-TE PRESS) [2,3] forms the data foundation for this environment. Initially conceived to identify sources of measurement variability, it has been used as a benchmark dataset in multiple studies. Osprey (https://github.com/schorschinho/osprey) is a coherent open-source MRS analysis ecosystem streamlining uniform pre-processing, LCM, tissue correction and quantification adhering to recent consensus guidelines[4]. The modular pipeline can be easily modified for rapid method development and benchmarking. Large-scale data visualization was implemented as a repository of R functions (https://github.com/HJZollner/SpecVis). The environment was used to investigate the agreement between the commonly used LCM algorithms for short-TE MRS[5] and to establish a 'best-practice' model for LCM of GABA-edited MRS[6].*

Results: *The established environment (Figure 1A) was successfully used to benchmark the performance of the internal Osprey LCM algorithm against established algorithms LCModel[7] and Tarquin[8] (Figure 1B) and to evaluate different modelling strategies for GABA-edited MRS. Only weak-to-moderate correlations between algorithms were found while mean estimates of the major metabolites broadly agreed. The second study (Figure 1C) investigated different modelling strategies for LCM of GABA-edited MRS. The results suggest that a well-parametrized co-edited 3-ppm macromolecule (MM) basis function with an amplitude constraint to the non-overlapped 0.93-ppm MM performs best in combination with sparse spline knot spacing and a full modelling range (0.5 to 4 ppm).*

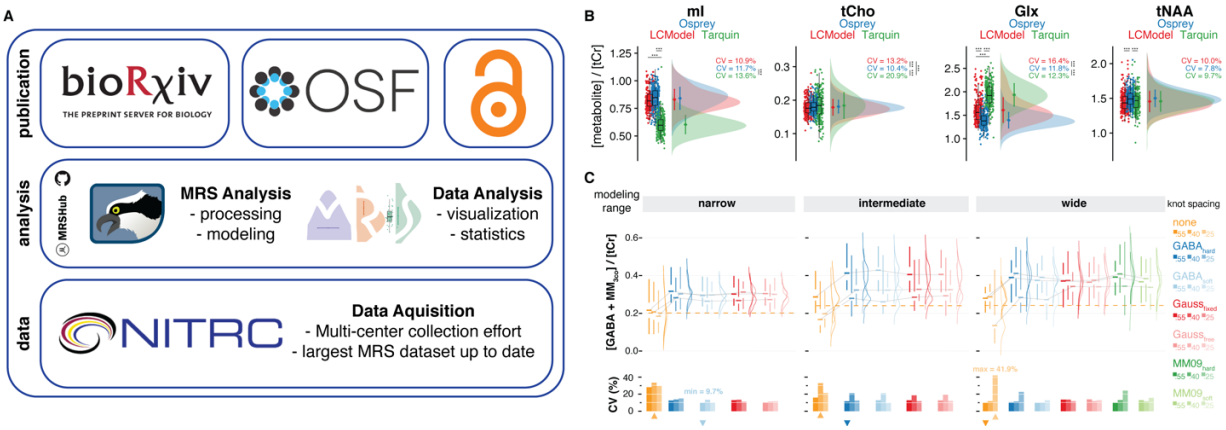

Figure 1. (A) Open-science environment for 1H MRS method development (B) Distribution of metabolite estimates of LCModel, Osprey, and Tarquin benchmarked with the BIG PRESS dataset and analysed with the proposed environment (C) Comparison of LCM strategies for GABA-edited MRS

Discussion: *We present an open-science environment for rapid method development of new 1H MRS methods. The environment was used in two studies demonstrating its flexibility and utility. The results of the first study can be used to benchmark any other modeling algorithms for short-TE MRS and are freely available for such purposes. The second study resulted in general recommendations about LCM of GABA-edited MRS, which are now readily implemented to be used for any application studies of GABA-edited MRS in Osprey.*

Conclusion: *The value of the presented open-science environment for rapid method development of new 1H MRS is showcased with two studies. It allows quick adaption of consensus recommendations for the broader MRS community including application-focused researchers, and quick method benchmarking for MRS methodologists.*

References: [1]Near et al., *NMR Biomed* 2020,[2]Mikkelsen et al., *NeuroImage* 2017,[3]Považan et al., *Radiology* 2020, [4]Oeltzschner et al., *J Neurosci Methods* 2020, [5]Zöllner et al., *NMR Biomed* 2021, [6]Zöllner et al., *NMR Biomed* 2021, [7]Provencher, *NMR Biomed* 2001,[8]Wilson et al., *Magn Reson Med* 2011