MRS quantification; practicalities in the simulation of basis sets by Topspin.

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Introduction

MR Spectroscopy (MRS) and Spectroscopic Imaging (MRSI) have substantial diagnostic potential. However, reliable and efficient data analysis is challenging, especially of ^{1}H MRS(I) data obtained at short echo times and with dedicated measurements like spectral editing [1]. The analysis of spectra is commonly done using a program like LCModel [2], in which a linear combination of metabolite spectra is fitted to the experimental data. This requires the separate measurement of individual compounds under the specific experimental conditions of the '*in vivo*' measurement, in which field strength, acquisition sequences and applied pulse shapes have to be taken into account. However, this is cumbersome and inflexible as for every type of MRS(I) measurement and field strength the individual compounds need to be re-measured, which may also be prone to chemical degradation.
In this **educational poster presentation** we will show how this can be circumvented by using the easy applicable and flexible program Topspin that can simulate spectra of individual compounds under a wide variety of conditions. Its usefulness will be demonstrated in the analysis of MRS data acquired at different field strengths and with multiple MRS(I) sequences.

Materials and methods

For this demonstration we will show how to program sequences like semi-LASER, including adiabatic refocusing pulses for localization and realization of variable echo times and MEGA-PRESS, optimized for GABA and lactate editing in Bruker's Topspin software (NMRSIM) [3] to generate simulated metabolite spectra. This software is based on a density matrix approach using the Liouville equation [4]. We then show how spectral profiles [5] of glycerophosphocholine (GPC), choline (Cho), phosphoryl choline (PC), creatine (Cr), phosphocreatine (Pcr), glutamate (Glu), glutamine (Gln), taurine (Tau), myo-inositol (mI), glucose (Glc), n-acetyl-aspartate(glutamate) (NAA(G)), alanine (Ala), gamma-Aminobutyric acid (GABA), aspartate (Asp), glutatione (GSH), 2-hydroxyglutarate (2HG) and lactate (Lac) are simulated and sampled into basis sets. It is then shown how, '*in vivo*' spectra are analyzed by LCModel with this basis set, including the determination of absolute tissue concentrations by scaling to tissue water.
Subsequently, we demonstrate how MR spectra of the human brain acquired by semi-LASER at TE=30 ms are satisfactorily fitted by LCModel with the simulated basis set (Fig 1A). In addition. we show how to use this set to fit GABA edited spectra of volunteers performing a functional task in the magnet (Fig 1B) and how to quantify lactate in an edited spectrum of a patient during an euglycemic clamp (Fig 1C). Chemical shift artifacts in editing are accounted for by scalar product normalization.

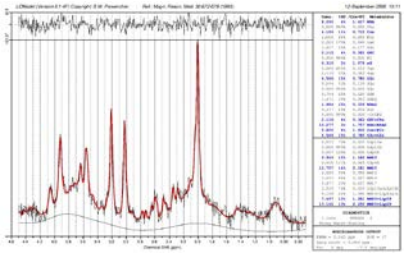

Figure 1A: MRS brain, sLASER (TE=30ms)

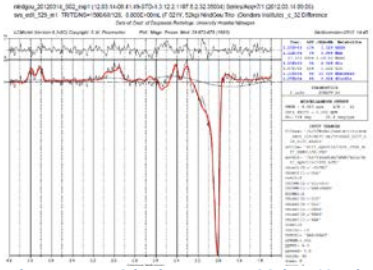

Figure 1B: MRS brain, MegaPRESS (TE=68ms)

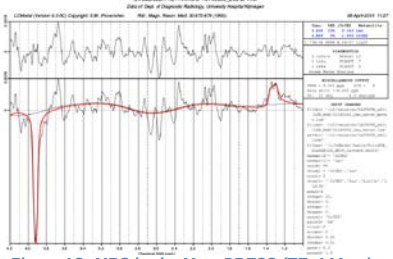

Figure 1C: MRS brain, MegaPRESS (TE=144ms)

Conclusion

Topspin software offers a complete and comprehensive environment to perform 'virtual' NMR experiments. It enables to generate basis sets for any field strength and measured with any pulse sequence used in the clinic or for research, including the generation and evaluation of a variety of shaped pulses. In this way it facilitates (absolute) quantification of MRS(I) in clinical practice. The software also offers the possibility to generate spectra for X-nuclei like carbon, phosphor or fluor.

References

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