Modelling, Optimization & QA for Magnetic Resonance Spectroscopy

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Motivation

In-vivo magnetic resonance spectroscopy (MRS), can potentially give information on the chemical level – allowing quantification of relative concentrations of chemical biomarkers of disease. However, using standard single voxel spectroscopy sequences such as PRESS (Fig1) we find in-vivo spectra to be a convolution of many constituent signals (Fig2), and separating them into their components is not always possible.

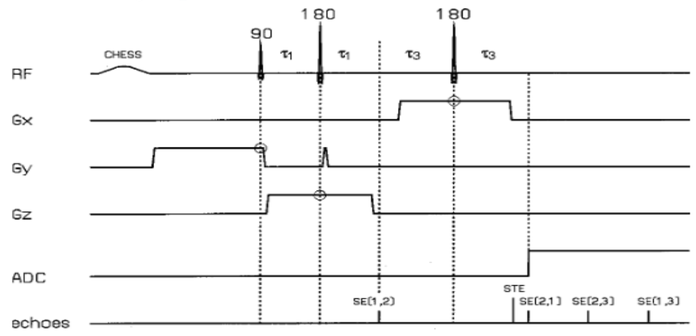
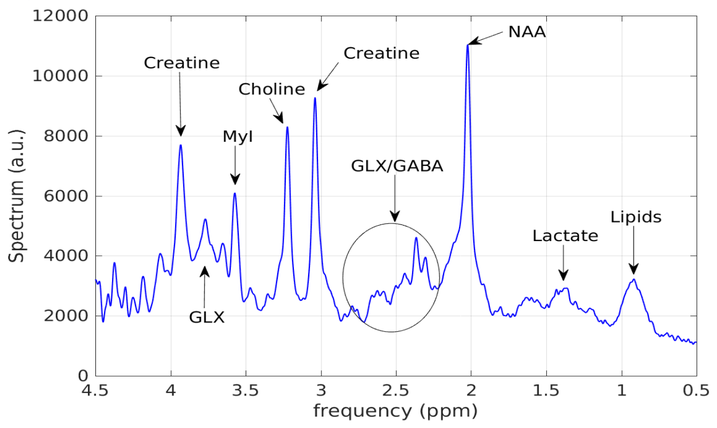


Fig1. Pulse sequence diagram for Point RESolved Spectroscopy (PRESS)

Fig2 – In-vivo brain spectrum



Signal of individual metabolites is obscured by ***overlapping signals*** of other molecules.

2D Spectroscopy

- Enables resolution of overlapping peaks and ***J-coupling*** by acquiring several spectra, varying a single parameter as shown in (Fig3).
- Many individual acquisitions add up to a long scan time – generally too slow for in vivo use.
- Difficult to interpret – Variation in parameter space could have many causes – coupling, relaxation, etc.

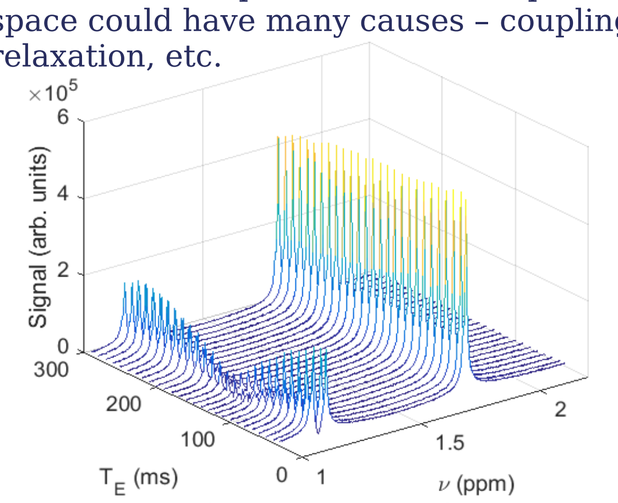


Fig3 – T_E series for QA spectroscopy phantom.

Editing – MEGA-PRESS

MEshcher–GArwood Point RESolved Spectroscopy (MEGA-PRESS) is a J-difference editing technique for MRS.

- Exploits structure of targets to allows detection of previously obscured peaks
- Limited applicability – This technique can't be applied to all situations

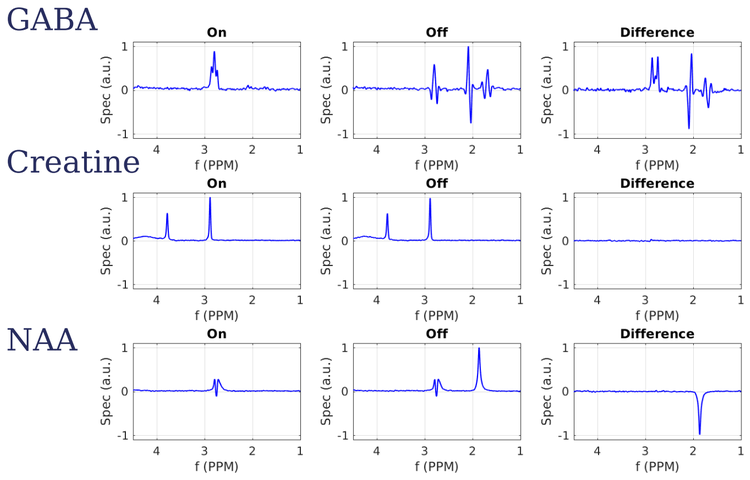


Fig4 – MEGA-PRESS for a range of metabolite phantoms.

Optimised pulses

Optimisation enables us to find pulses that can ***exploit minor differences*** in chemical shifts and couplings of molecules to discriminate.

- Flexible – Many potential applications in MR
- Fast – No need for multiple acquisitions
- Requires experimental verification

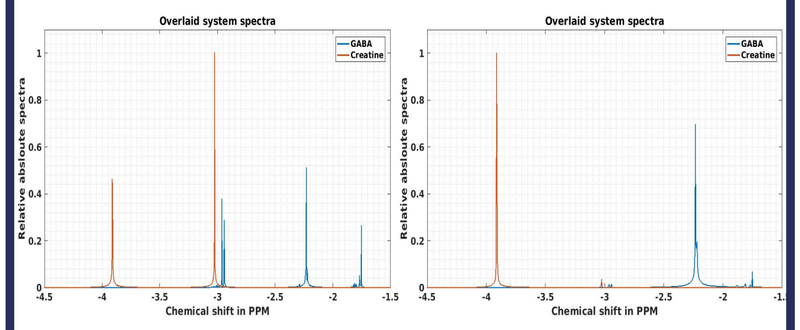


Fig5 - Spectra resulting from 90 pulse (left), and optimised pulse (right). Notice separation of features.

Calibration and testing

Experimental verification of these controls requires careful calibration and testing. We need to test in tissue mimicking phantoms.

- Essential for validation of pulses.
- Known tissue composition – Allows verification of pulses. This is not possible in-vivo!
- Reproducibility – The results need to be reproducible!
- Also allows optimisation of existing protocols

Tissue mimicking phantoms

Fig6 - Spherical spectroscopy phantom (left) and plain agar phantom for calibration (right)

We want phantoms to have:

- Same spectroscopic features as real tissue.
- In-vivo ranges of T_1 & T_2 values.
- Long shelf lives to enable to repeat measurements on the same phantom.
- Characterised and consistent properties that allow calibration of sequences

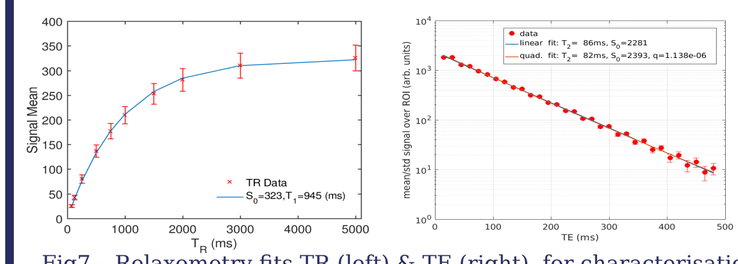
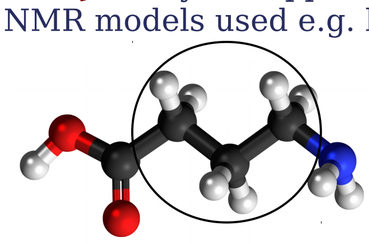


Fig7 – Relaxometry fits TR (left) & TE (right), for characterisation of relaxation properties

Modelling

The controls produced by optimisation are only as good as the models used for simulation!

Experimental GABA spectra below show that ***peaks are shifted*** by 0.12 ppm compared to standard NMR models used e.g. by TARQUIN.



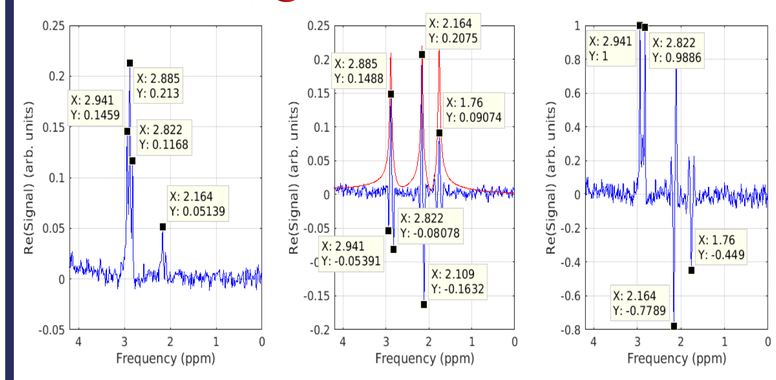


Fig8 - Simulated GABA spectrum (red), fitted over experimental data. Uncoupled model of 6 Hydrogens shown in image.

Future work

- Modelling of tissue mimicking phantoms.
- Generation of new pulses from these models.
- Experimental verification of pulses.
- Identification of new targets. Have a target in mind? We would like to collaborate!

References & acknowledgements

- Solvent suppression using selective echo dephasing. Mescher M, Tannus A, O'Neil Johnson M, Garwood M. J Magn Reson A 1996
- Proton NMR chemical shifts and coupling constants for brain metabolites. Govindaraju V, Young K, Maudsley AA NMR Biomed. 2000
- Design and Characterization of Tissue-Mimicking Gel Phantoms for Diffusion Kurtosis Imaging. Portakal Z G, Shermer S, Spezi E, Perrett T, Tuncel N ,Phillips J
- Scans performed at Swansea Clinical imaging facility

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