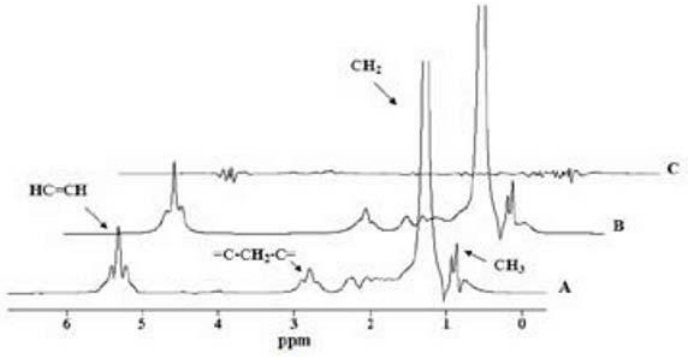
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The omega-3 polyunsaturated fatty acid methyl protons exhibit characterisctic inphase antiphase echo time behavior. Towards determining adipose tissue omega-3 PUFA content by proton spectroscopy in vivo

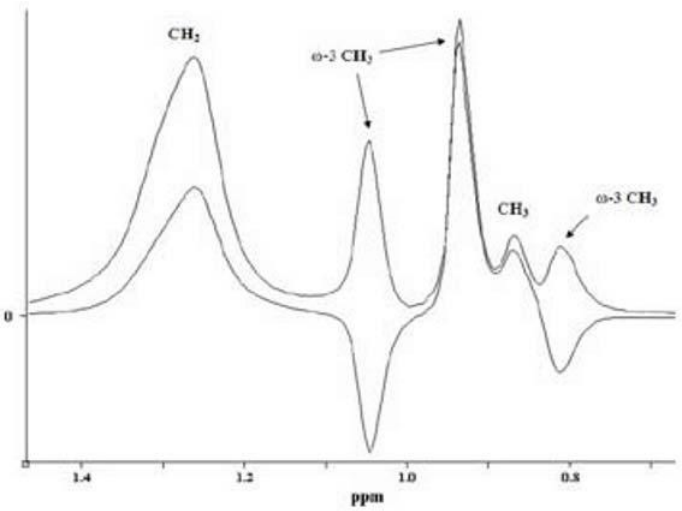
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Introduction: Omega-3 polyunsaturated fatty acids (PUFA) are considered to have numerous health benefits when incorporated into a diet (1). Carbon-13 NMR spectroscopy has been shown to be useful for the analysis of human adipose tissue fatty acids (FA) *in vivo*, but the equipment is not normally found in clinical imagers and cannot identify omega-3 PUFAs (2). Noninvasive assesment of human adipose tissue omega-3 PUFA content would be a valuable clinical application. The aim of this study is to determine using proton NMR spectroscopy 1) to what extent the FA composition of triglycerides can be determined on a clinical 1.5 Tesla MR imager, and 2) how the individual FA resonances behave with increasing echo time.
Subjects and Methods: Ten different edible oils (FA compositions determined by gas chromatography (GC)) were measured on a clinical 1.5 Tesla MR Imager (Avanto, Siemens, Erlangen, Germany) with the PRESS sequence with TE/TR = 50-300/1500 ms and analyzed by AMARES (jMRUIv3.0). The spectrum (TE = 50) of Cod Liver oil (**A**) is shown in Figure 1, along with the peak fitting estimate (**B**) and residue (**C**).
Figure 1:



Results: For TE = 50 ms the olefinic and diallylic proton resonance areas correlated with the olefinic **H**C=C**H** (R = 0.993, 0.33 standard error of estimate (SE)) and diallylic =C-C**H**$_2$-C= (R = 0.997, 0.19 SE) proton contents calculated from the GC data. The TE series revealed differences in the J-coupled evolution of the individual resonances. The omega-3 PUFA methyl resonance exhibited a characteristic echo time evolution, which could be attributed to the inphase antiphase behavior of the omega-3 Methyl Outer Triplet Lines (omega-3 MOTL). The omega-3 MOTL were found to be inphase every TE = 135 ms. The omega-3 MOTL at 1.04 ppm was found to be useful for determining the omega-3 content of the oils (R = 0.999, 0.80 SE). Figure 2 shows the proton spectra of Linseed oil (62% omega-3 PUFA) when the omega-3 MOTL are inphase (TE=140) and antiphase (TE=200).

Figure 2:



Conclusions: This study demonstrated that the omega-3 PUFA methyl outer triplet lines are modulated by the PRESS TE parameter and exhibited characteristic inphase antiphase behavior with a period of 135 ms. The left outer triplet line at 1.04 ppm could be used to determine omega-3 PUFA content *in vivo* using long TE.
References:
(1) Seidelin K.N.(1995) Prog Lipid Res 34:199-217
(2) Hwang J.H., Bluml S., Leaf A., Ross B.D.(2003) NMR Biomed 16:160-167

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Nonparametric modelling of the macromolecular background in Nuclear Magnetic Resonance spectroscopic signals

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Purpose/Introduction: Nuclear Magnetic Resonance (NMR) spectroscopy can be used as a non-invasive technique to quantify metabolite concentrations in human tissue. NMR spectra are hampered by a nuisance background, coming from some unknown macromolecules.
Subjects and Methods: Our motivation is the method QUEST [1], where a noisy background obtained from the NMR signal needs to be de-noised. In [1] this is done by fitting several Lorentzian peaks. We extend this approach to splines and wavelets focusing on the robustness with respect to hyperparameters.We start from a realistically simulated noiseless background to which we add white noise of various Signal-to-Noise Ratios (SNR). The criterion used for selecting the smoothing method is maximizing the Relative SNR, which shows the SNR improvement.
We study 3 different methods for modelling the macromolecular background:
a) Spline study, which aims at finding the range of the smoothing parameter *p* that gives the best RSNR for each SNR.
b) Wavelet study, where a rigorous procedure was followed for choosing the best wavelet from a variety of wavelet families and hyperparameters.

c) Lorentzians, where the HLSVDPRO method [2] was used. The aim was finding the optimal number of Lorentzians that gives the best results in terms of RSNR for different SNR.

Results: For **splines**, the results show that the optimal *p* is proportional to the SNR. Moreover, the standard deviation of *p* grows with the SNR. We also found out that the improvement in terms of RSNR is linear. The improvement is bigger when the signal is noisier, but in general the global improvement is around 10dB.The optimal results for each family of **wavelets** in terms of RSNR are very similar. The best thresholding criterion is Soft Thresholding. The best vanishing moment for each family of wavelets and the level of wavelet decomposition do not depend on the SNR. The average improvement is around 10dB in the denoising process.

The results for **Lorentzians** show that the optimal number of Lorentzians is very dependent on the noise level. They show an average improvement of around 10dB.

Discussion/Conclusion: Our study proves that spline- or wavelet-based modelling of the background can replace the Lorentzian-based modelling in a quantification method such as QUEST.

References:

[1] Ratiney et al. *NMR Biomed.* 18(1)**,** 1-13. 2005.

[2] Laudadio et al. *J. Magn. Reson.*, 157, 292-297. 2002.

Acknowledgment: ETUMOUR (FP6-2002-LIFESCIHEALTH 503094), Healthagents (IST-2004-27214), FAST (FP6-MC-RTN-035801), Neuromath (COST-BM0601)

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Absolute quantification of LCModel water scaled metabolite concentration of 1H magnetic resonance spectroscopy (MRS) using quantitative magnetic resonance imaging (qMRI)

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Purpose/Introduction: The purpose of this work was to develop a clinically useful procedure for absolute quantification of 1H MRS on clinical scanners. Here a method is presented that utilize the unsuppressed water signal as internal reference, thereby circumventing the quantification errors caused by field inhomogeneities [1]. The water signal from the VOI was quantified by using a qMRI method [2], which provided T1 and T2 for the whole brain in 6 minutes.

Subjects and Methods: SVS MRS (PRESS, TE 30, TR 3000, NSA 80) in parietal white matter from 15 healthy volunteers (m = 6; f = 9) were acquired and analyzed using the procedures described below.

The metabolite concentrations were calculated using the water scaling function provided in LCModel, in which the MRS signal is scaled using a scaling factor fscale (Eq. 1) [3].

$$f_{scale} = Basis_{norm} \frac{2 * WCONC * ATTH2O}{Area_{water}}$$

Equation 1

ATTH2O corrected for relaxation effects of the water signal. The quantitative T1 and T2 values of each VOI were used to calculate the attenuation (Eq 2).

$$ATTH2O = e^{-\frac{TE}{T2}}\left(1 - e^{-\frac{TR}{T1}}\right)$$

Equation 2

The quantitative T1 and T2 values of the VOI were obtained by registration of the VOI into T1 and T2 volumes, which were acquired using QRAPMASTER using a resolution of 0.84x0.84x3 mm3.

By placing the VOIs such that no CSF was included, the water signal was mainly derived from the intracellular fluid, thus the water scaled concentration by definition provided the aqueous fraction.

The factor Basisnorm normalized the signals to absolute concentrations (correcting for system dependent differences). Since the basis spectra were obtained on a different scanner, the method also had to be calibrated using WCONC as a calibration factor (scaled to a Cr concentration of 7.34 mM).

Results: The results are presented in Table 1. A repetitive number of measurements were performed on one healthy volunteer; two MRS VOI were placed in parietal white matter, one left and one right (PRESS, TE 30, TR 3000, NSA 128). The experiment was repeated four times on two separate days. These results are also presented in Table 1.

Table 1:

Mean metabolite concentration in mM ± standard deviation (Relative standard deviation mean/std in %). LCM std are the mean Cramér-Rao Lower bound of the LCModel fits.

	Healthy controls Parietal WM (n=15) mean ± std (std%)	LCM std	Repetitive study Parietal WM (n=2*4)	LCM std
Cr				
Abs conc.*	7.34 ± 0.52 (7.1)	0.64	7.26 ± 0.23 (3.1)	0.41
WS conc.**	7.51 ± 0.58 (7.7)	0.66	7.35 ± 0.24 (3.3)	0.41
LCM***	7.35 ± 1.45 (19.7)	0.65	7.35 ± 0.31 (4.3)	0.41
Cho				
Abs conc.	2.78 ± 0.29 (10.5)	0.25	2.72 ± 0.15 (5.3)	0.15
WS conc.	2.84 ± 0.31 (10.8)	0.25	2.75 ± 0.15 (5.3)	0.15
LCM	2.78 ± 0.57 (20.6)	0.25	2.76 ± 0.20 (7.3)	0.15
tNAA				
Abs conc.	12.33 ± 1.21 (9.9)	0.83	13.24 ± 0.45 (5.1)	0.59
WS conc.	12.60 ± 1.26 (10.0)	0.85	13.41 ± 0.69 (5.2)	0.60
LCM	12.46 ± 2.78 (22.3)	0.81	13.41 ± 0.72 (5.4)	0.60
Ins				
Abs conc.	6.81 ± 1.54 (22.6)	0.90	5.57 ± 0.45 (8.1)	0.51
WS conc.	6.96 ± 1.57 (22.6)	0.92	5.64 ± 0.46 (8.1)	0.52
LCM	6.69 ± 1.65 (24.8)	0.90	5.65 ± 0.49 (8.8)	0.52

* Absolute concentrations calculated with the method presented. ** Water scaled concentrations calculated with LCModel without any correction for individual attenuation differences between subjects. *** Concentrations calculated with LCModel without using water scaling.

Discussion/Conclusion: The repeated measurements showed that the method gave consistent results, independent of changes of system parameters, such as shimming, coil load, voxel position.