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Processing and quantification: spectroscopy

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Different quantification algorithms may lead to different results: a comparison on H MRS lipid signals

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Introduction: In vivo, localized Magnetic Resonance (H MRS) spectra are affected by low signal-to-noise (S/N) ratio, presence of background, overlapping peaks and non lorentzian lineshapes. All these characteristics hamper the quantification of chemical compounds within a tissue and require suitable computational algorithms for spectral analysis. Aim of the present work is to establish whether, by analysing spectra with different algorithms, we obtain similar results and how the statistical significance of results is affected. Different quantification algorithms in the time domain implemented in jMRUI [1] have been tested for the analysis of simple lipid spectra (see Fig.1), both simulated and in vivo. High Resolution NMR spectra of lipid extracts was considered as the gold standard [2].

Subjects and Methods: QUEST, HLSVD (jMRUI 4.0), integration and frequency fitting algorithms (Matlab) were applied to the analysis of Monte Carlo simulated spectra (see details in Tab.1). In vivo lipid spectra were acquired from inguinal adipose tissue in Zucker rats (8 obese and 6 lean) using a 4.7 T Bruker Biospec. HR-NMR spectra from the same tissue (extracted according to Folch's protocol [3]) were obtained by a Bruker DRX spectrometer at 500.13 MHz for H nuclei. In vivo spectra from lean and obese subjects were compared through the polyunsaturation index (PI) according to [2].

Results: Fig.2 and 3 show the effect of several parameters in the estimation of peaks amplitude performed by different algorithms. Fig.4 shows the PI index obtained in vivo. For simulated (Fig.2,3) spectra, our results reveal that different quantification methods bring to different averages, especially when different lineshapes occur. Statistically significant difference of PI (see Fig.4) between obese and lean rats is obtained with QUEST analysis, but not by other methods.

Conclusions: More extensive simulations could deepen the reason of such discordance between techniques. This preliminary work suggests that post-processing may alter biological findings.

References:

[1] Naressi A. et al., 2001,Comp.Bio.Med. 31:269-286
[2] Mosconi E., Fontanella M. et al., 2011, J.Lip.Res., 52:330-336
[3] Folch J.,1957, J.Biol.Chem., 226:497-509

TYPE	S/N	Damping factor	Chemical Shift	Lineshape	Phase 1.5 ppm
RANGE	0.02→928	0.04→0.29 ppm	-0.15→+0.15 ppm	L, G, V	-π/2→π/2
number of signals	100*10	100	100	100	100

Tab. 1: Description of simulated signals. (*)100 simulations*10 thresholds. (**) L=Lorentzian, G=Gaussian, V=Voigt

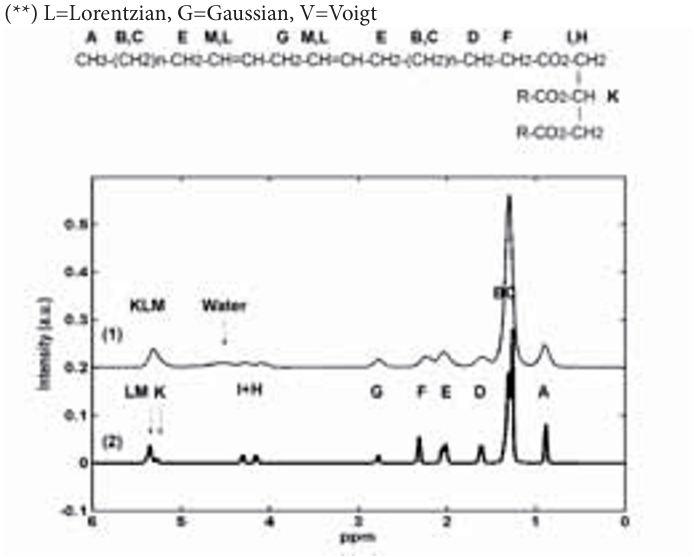

Fig 1: Representation of lipid signal in H-MRS (1) and NMR (2)

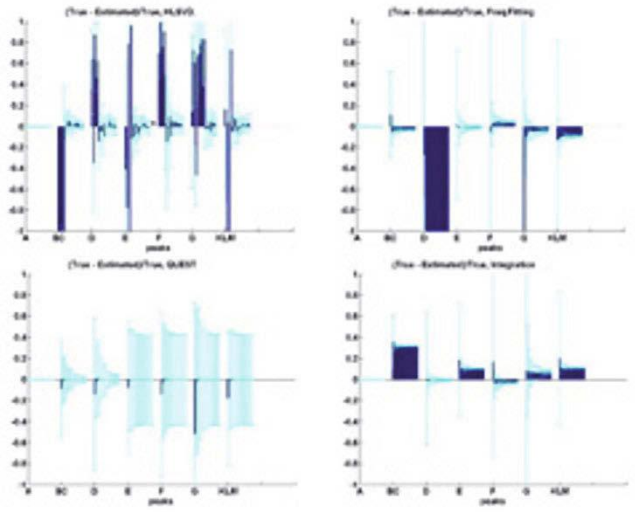

Fig.2: Analysis of simulated signals: peaks estimation ± standard deviation (SD) by changing S/N thresholds