In-vivo spectra pre-conditioning using PcBc

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INTRODUCTION

In vivo spectra (1H, 13C, 31P, 23Na, ...) are known to be particularly difficult to phase and to correct for baseline drifts. The reasons are multiple: apart from the usual ones encountered typical of in-vitro spectroscopy, such as post-pulse receiver transfer-function distortions (dead-time), filter delays, filter roll, an a few others, there are additional difficulties due to the following specific factors:

- Low signal-to-noise ratio (S/N),
- Unavoidably bad B_1 homogeneity, involving both B_1 amplitude and phase.
- Local magnetic field gradients due to mesoscopic susceptibility variations in tissues.
- Broad solid-tissue background signals.

This makes even manual pre-conditioning (phase and baseline corrections) very difficult and extremely subjective. We present the promising results obtained with a recently developed [1] pre-conditioning method named PcBc which consists in a simultaneous phase and baseline correction using both the in-phase and the out-of-phase parts of a spectrum. Since the method is completely automatic, it bears the promise of being also completely objective – a feature which, according to our opinion, was so far badly missing in the management of in-vivo NMR spectra.

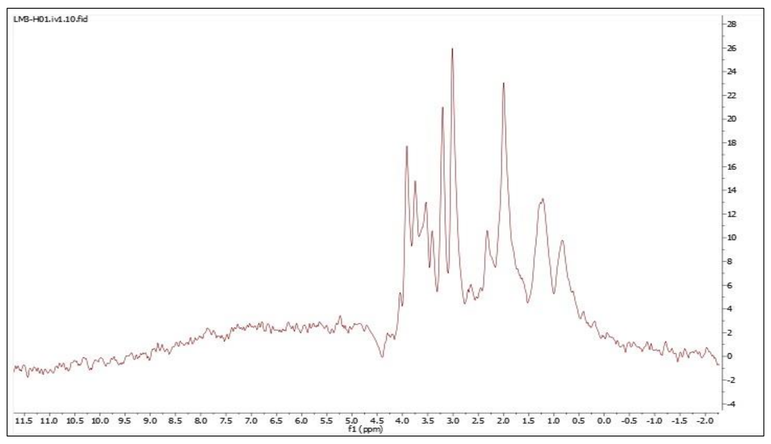
[Here we present recent advances in a novel iterative algorithm in which the 'quality function' is based on the amplitude histograms (real and imaginary) of the spectrum. Apart from the exploitation of some convenient features of histograms, the fully automatic algorithm handles BOTH corrections simultaneously (PcBc rather than Pc + Bc), and it applies the baseline correction to BOTH the real and the imaginary parts of the spectrum.

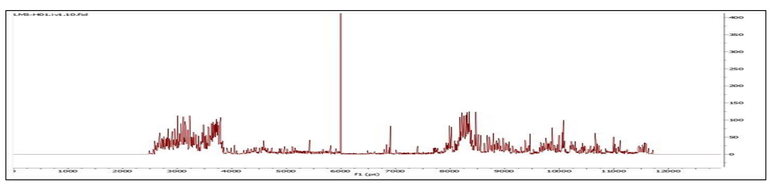
In summary, PcBc permits us to:

- Carry out the phase and baseline corrections *simultaneously;*
- Carry out both corrections (not just the phase) on *both* the in-phase and the out-of-phase parts of a spectrum;
- Enhance the *objectivity* of the corrections, especially considering that in practice one often encounters situations with multiple and/or ill-defined acceptable 'solutions'. Moreover, the manual corrections in current use (especially the phasing procedure) often differ depending of the personal habits of each spectroscopist.

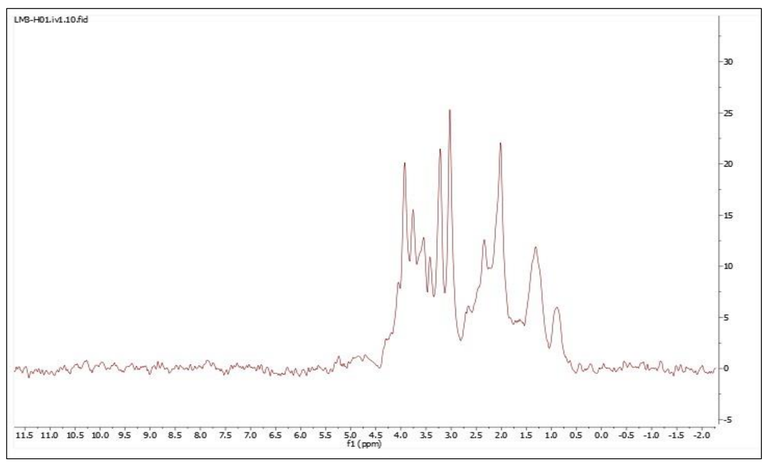
In the following we show some in-vivo sample spectra properly conditioned using PcBC algoritm.

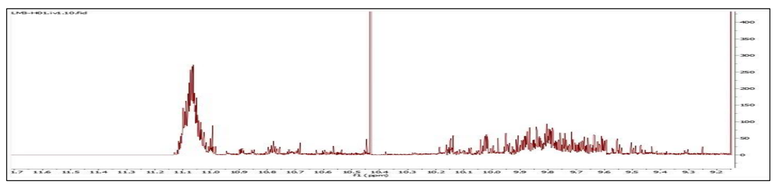
In-vivo brain spectrum # 1 and corresponding histogram



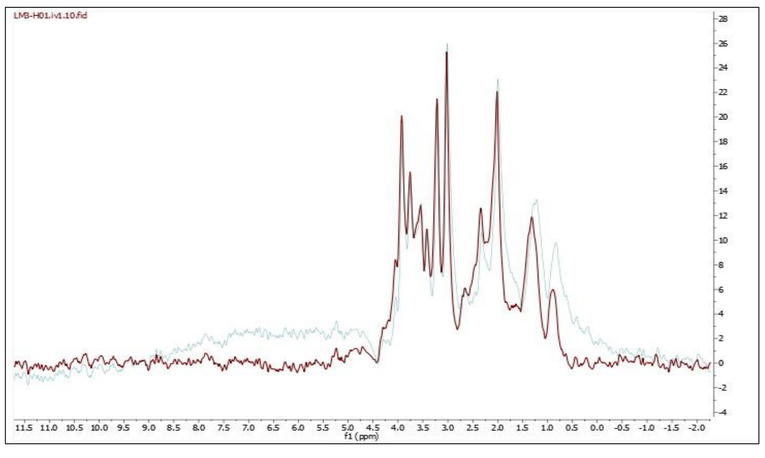


In-vivo brain spectrum # 1 after PcBc correction and corresponding histogram

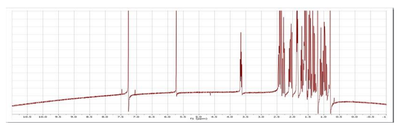




In-vivo brain spectrum # 1 comparison Original (light blue) and PcBc conditioned (red)



Experimental spectrum



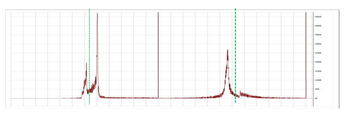
PcBc Correction

Defined by the parameters p:

ph_0, ph_1 , c_0, c_1, c_2, ….

Histogram of the spectrum

For both real and Imaginary part of the resulting spectrum, compute the histogram;



Evaluation

For both histograms of real and imaginary part, evaluate the weighted integral of the histogram (Qr(p) and Qi(p) respectively).

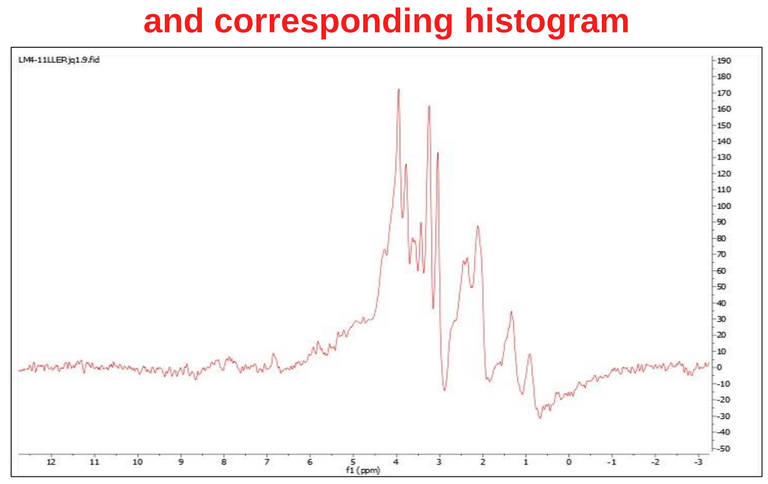
The values of the parameters p are modified in order to minimize Q(p) = Qr(p) + Qi(p) according to the down hill simplex algorithm.

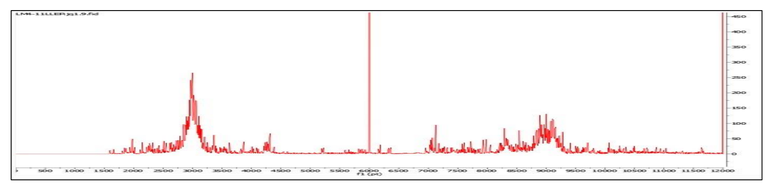
PcBc conditioned spectrum

Corresponding histogram

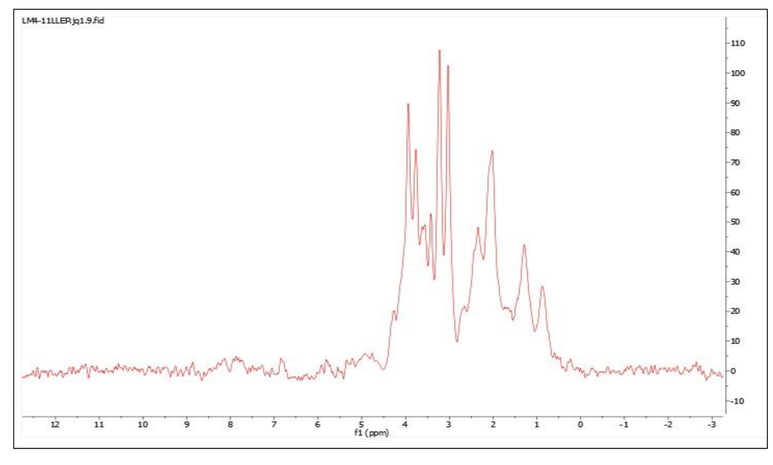
PcBc is a fully automatic procedure

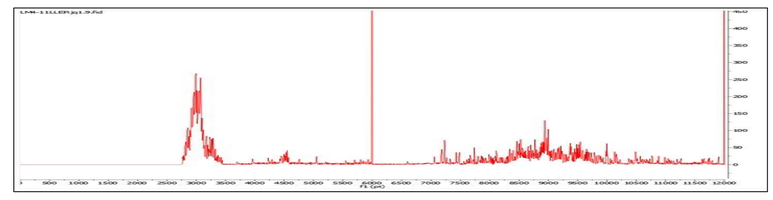
In-vivo brain spectrum # 2 and corresponding histogram



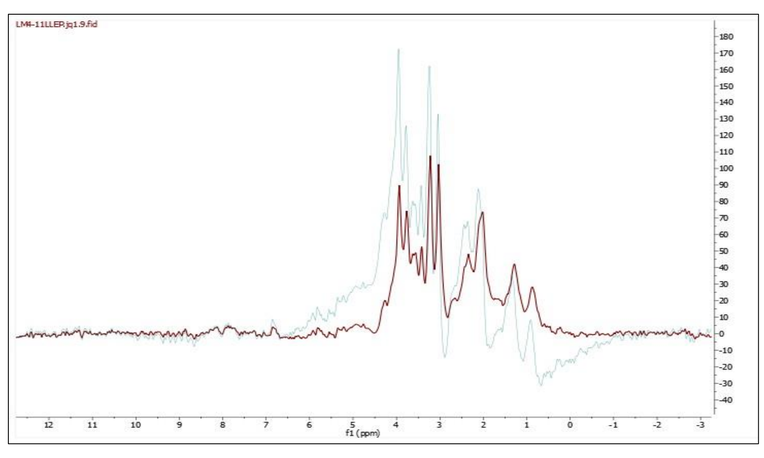


In-vivo brain spectrum # 2 after PcBc correction and corresponding histogram





In-vivo brain spectrum # 2 comparison Original (light blue) and PcBc conditioned (red)



References

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