Metabolomic spectra pre-conditioning using PcBc

Ester Maria Vasini [1], Carlos Cobas [2] and Stanislav Sýkora [1]

[1] Extra Byte, Via Raffaello Sanzio 22/C, Castano Primo (Mi), Italy I-20022; em.vasini@extrabyte.eu, sykora@extrabyte.eu
[2] Mestrelab Research, Xosé Pasín 6, Santiago de Compostela, 15706 Spain; carlos@mestrec.com

DOI 10.3247/SL7Nmr18.003

INTRODUCTION

Metabolomic spectra are particularly difficult to properly phase and to correct their baseline roll. This is principally due to presence of very large number of heavily overlapping peaks which are therefore difficult to phase and, in addition, leave only limited (or no) gaps between groups of peaks where the baseline can be visually or programmatically assessed. The latter aspect makes inapplicable, or ill applicable, many traditional phase and baseline correction algorithms. Due to the coupling between the phases ph0 and ph1 and the baseline corrections coefficients, this makes the preconditioning of these spectra problematic and, when done manually, extremely subjective. In addition, typical metabolomic studies call for the evaluation of large numbers of spectra. To speed up the pre-processing and at the same time guarantee consistency and objectivity of the results (impossible to guarantee when done manually), it is highly desirable to apply an automatic phase and baseline correction method. We present here preliminary results obtained by the application to metabolomic spectra of a novel [1] automatic method, named PcBc, which allows a simultaneous phase and baseline correction using both the in-phase and out-of-phase parts of a spectrum.

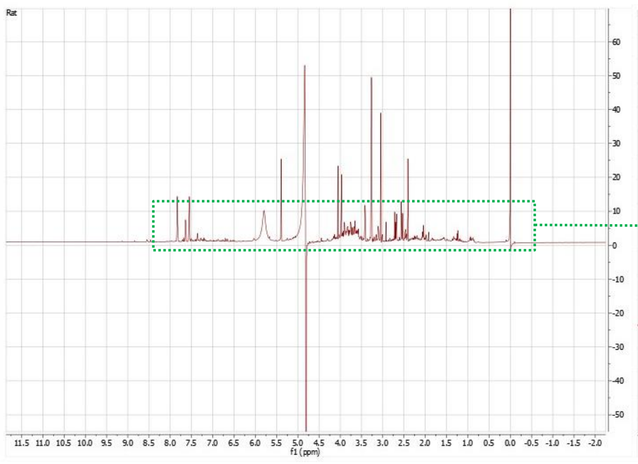
Here we present recent advances in a novel iterative algorithm in which the 'quality function' is based on the amplitude histograms (real and imaginary) of the spectrum. Apart from the exploitation of some convenient features of histograms, the fully automatic algorithm handles BOTH corrections simultaneously (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:

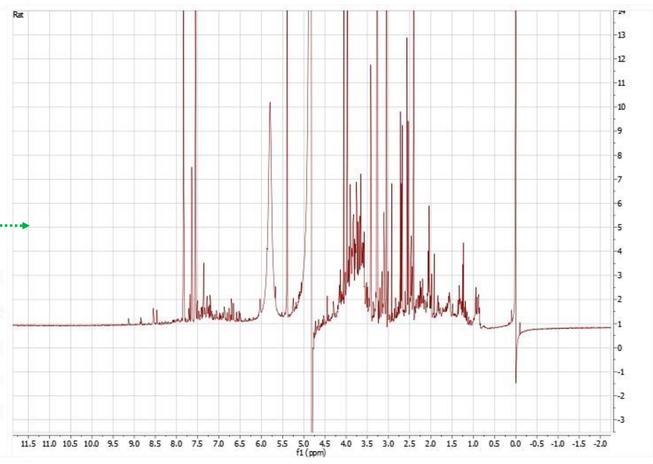
- Carry out the phase and baseline corrections *simultaneously;*
- Carry out both corrections (not just the phase) on *both* the in-phase and the out-of-phase parts of a spectrum;
- Enhance the *objectivity* of the corrections, especially considering that in practice one often encounters situations with 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 metabolomic sample spectra properly conditioned using PcBC algoritm.

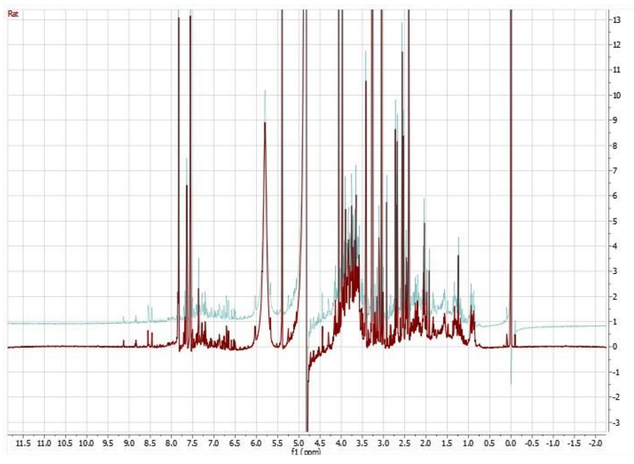
Rat: original spectrum



Rat: original spectrum Zoom on selected area

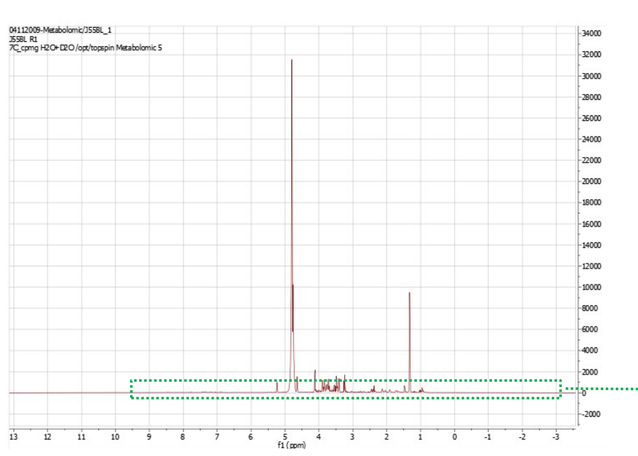


Rat: original (light blue) and PcBc processed spectrum

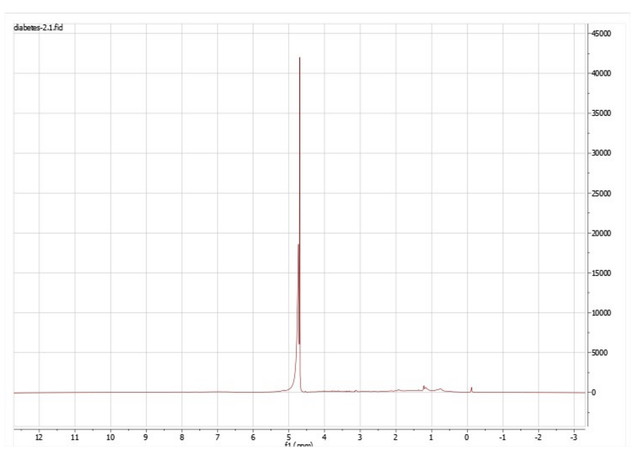


Diabet: original spectrum

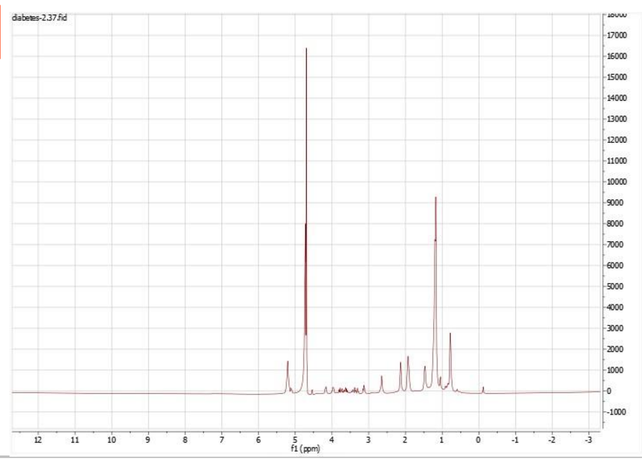
1



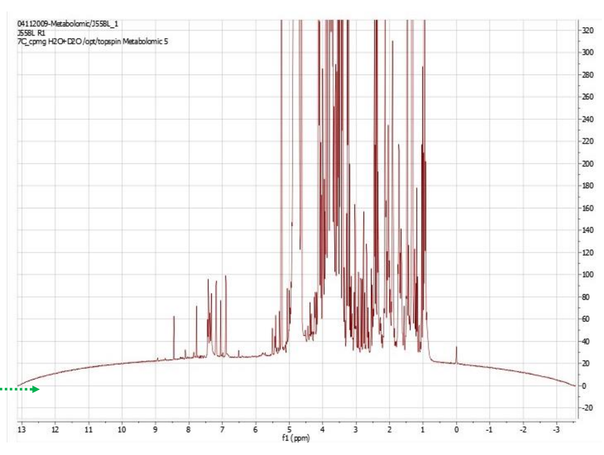
2

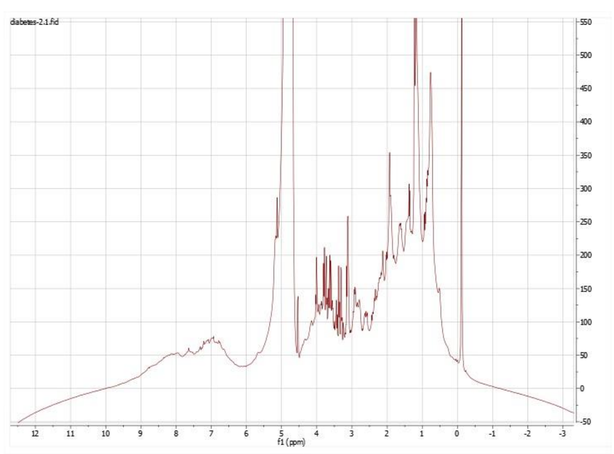


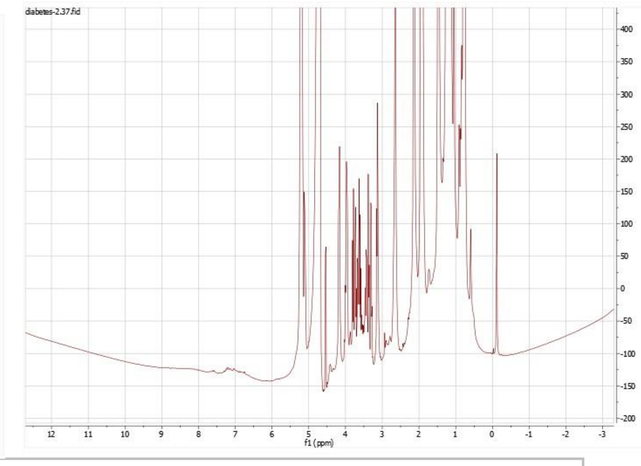
3



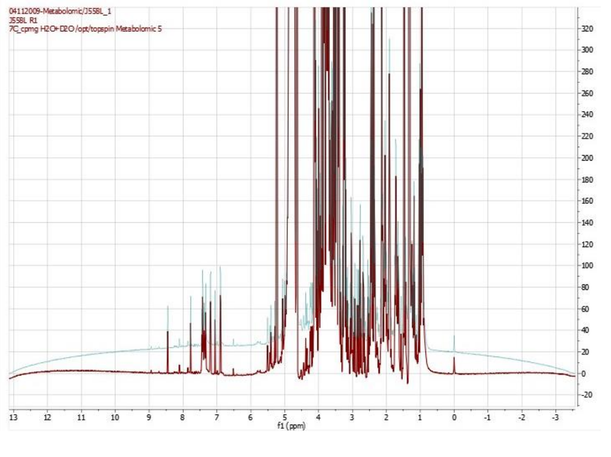
Diabet: original spectrum Zoom on selected area

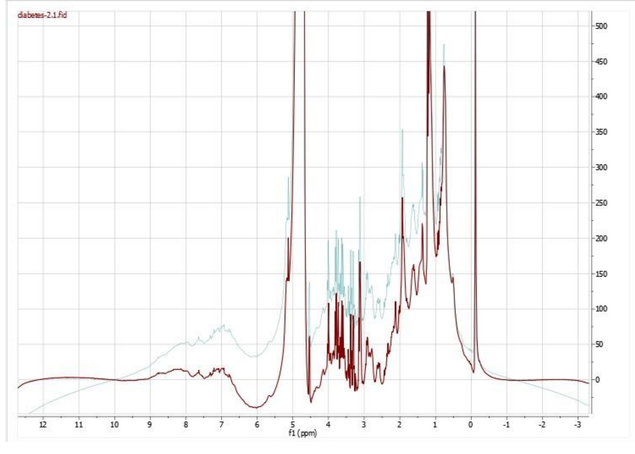


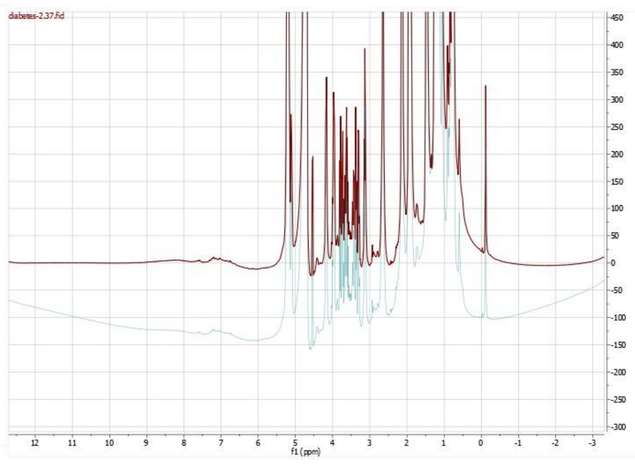




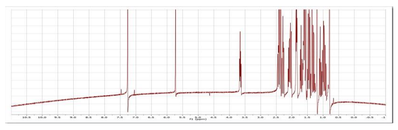
Diabet: original (light blue) and PcBc processed spectrum







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;

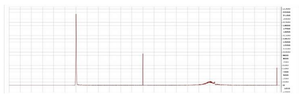
Evaluation

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

References

1. Cobas C., Bernstein M.A, Martìn-Pastor M., Tahoces P.G., 2006. A new general-purpose fully automatic baseline-correction procedure for 1D and 2D NMR data. Journal of Magnetic Resonance 183, 145-151;
2. Binczyk F., Tarnawski R., Polanska J., 2015. Strategies for optimizing the phase correction algorithms in Nuclear Magnetic Resonance spectroscopy. Biomedical Engineering On line 14 (S2);
3. Cobas C. and Sykora S., 2007. Extended DISPersion-Absorption (eDISPA) approach to Automatic Phasing of HR-NMR Spectra. 48th ENC Conference, 2007, DOI: 10.3247/SL2Nmr07.004.
4. Zorin V., Bernstein M.A. and Cobas C., 2017. a robust, general automatic phase correction algorithm for high-resolution NMR data, Magnetic Resonance in Chemistry 55, 738-746.

UNIÓN EUROPEA
Fondo Europeo de Desenvolvemento Rexional

XUNTA DE GALICIA
CONSELLERÍA DE INNOVACIÓN, INDUSTRIA E COMERCIO
Dirección Xeral de Investigación e Desenvolvemento

In collaboration with www.extrabyte.eu