

Automatic Phase Correction of Multidimensional NMR Spectra by a Whitening Method

C. Cobas¹, G. Balacco²

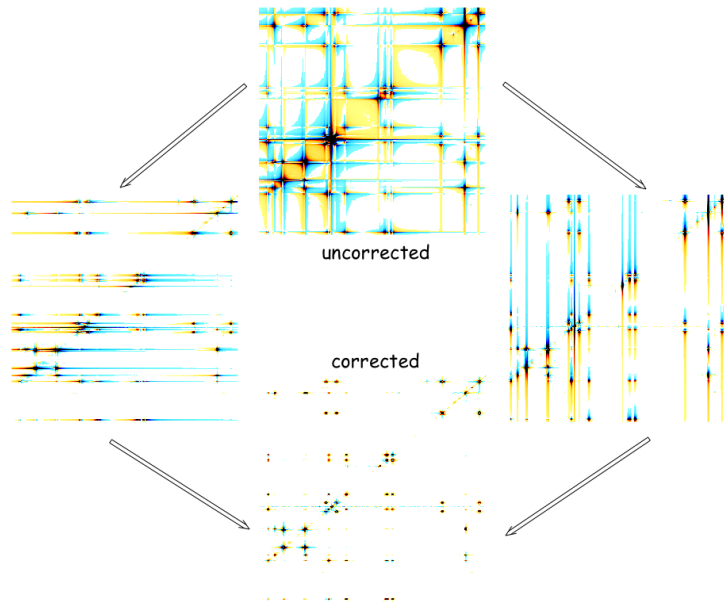
¹ MESTRELAB RESEARCH S.L., 15706 Santiago de Compostela, Spain

²Nucleomatica, 70056, Molfetta BA, Italy

Nowadays, the largest part of multidimensional NMR spectra of liquid samples is routinely acquired in phase-sensitive mode because of its enhanced resolution compared to the power or magnitude modes. These phase-sensitive mode spectra contain both absorption and dispersion components which can be separated by changing the phase of the spectrum.

While 2D manual phase correction, as permitted by today's software, can be extremely accurate, the availability of an automatic method can simplify the job and reduce processing time. In this work we present a novel algorithm for this aim based on the maximization of the white pixels of the 2D spectral map, a process which we call *whitening*. The method exploits the fact that the correction along the orthogonal axis in a multidimensional experiment can be assumed to be independent. This assumption makes the algorithm faster and more likely to succeed.

The algorithm can efficiently phase either homonuclear or heteronuclear experiments and unlike other previous methods,^{1,2} it can also deal automatically with spectra containing positive or negative peaks so that it is not necessary to deal with individual or special cases.



[1] Cieslar, C.; Clore, M.; Gronenborn A.M., *J. Magn. Reson.*, **1988**, 79, 154-157.

[1] Hoffman, R.E.; Delaglio, F.; Levy G.C., *J. Magn. Reson.*, **1992**, 98, 231-237.