Bayesian AuTomated Metabolite Analyzer for NMR Spectra: BATMAN

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Introduction

In NMR Spectroscopy often times peaks overlap with one another. BATMAN is a software program that was developed to help with the task to detangle overlap. As the name implies it uses Bayesian statistics to accomplish a best fit of a peak pattern onto an actually measured pattern. It takes advantage of the fact that peak patterns in a compound rely on each other. We applied this to detangle overlapping peaks and determine concentrations of metabolites in rat urine.

Results

This program successfully established this software as a useful method to analyze data. BATMAN is capable of taking a large amount spectra and running them quickly and mostly accurately. Data below show that a large amount of concentrations are close to be identical. In selected cases peak shifts did not allow for an automatic analysis, thus concentrations were underestimated.

Acknowledgements

1. Bayesian Deconvolution and Quantification of Metabolites in Complex 1D NMR Spectra Using BATMAN, Nature Protocols, 9(6), 1416–1427., Hao, J., Liebeke, M., Astle, W., De Iorio, M., Bundy, J. G., & Ebbels, T. M. D.

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References