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Application of BATMAN and BAYESIL for quantitative ^{1}H-NMR based metabolomics of urine: discriminant analysis of lean, obese, and obese-diabetic rats (Article)

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Abstract

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Introduction: BATMAN and BAYESIL are software tools, which can provide a solution for automated metabolite quantifications based on the proton nuclear magnetic resonance (^{1}H-NMR) spectral data of bio-fluids. However, their specific application for the quantitative ^{1}H-NMR based metabolomics of urine has not been investigated. Objectives: The aim of this study is to evaluate the performance of BATMAN and BAYESIL in the quantitative metabolite analysis of urine based on its ^{1}H-NMR spectra. Methods: BATMAN and BAYESIL were used for automated metabolite quantification based on the ^{1}H-NMR spectra of the urine from the lean, obese and obese-diabetic rat groups. PLS-DA model was used to discriminate the three different groups based on the results from the quantifications. Results: BATMAN was found to be superior to BAYESIL in identifying and quantifying the metabolites in the urine samples, owing to its flexibility that allows users to define and adjust the relevant signals of the pure standard metabolites in the database in order to fit the signals in the samples, a necessary step since variations and peak shift are natural in most ^{1}H-NMR spectra. The results of BATMAN also agreed well with that of the manual deconvolution method, which indicated the higher accuracy in metabolite quantification, despite the need of pre-processing and longer processing time than BAYESIL. However, in the case where the problems in baseline correction and peak shift of ^{1}H-NMR spectra are absent, the use of BAYESIL is more advantageous. Application of quantitative ^{1}H-NMR based metabolomics of the urine showed that PLS-DA model derived from BATMAN could satisfactorily discriminate the lean, obese, and obese-diabetic rat groups. Conclusion: Both BATMAN and BAYESIL are useful for the quantitative automation of urine metabolites based on its ^{1}H-NMR spectra. The results from BATMAN method is superior to BAYESIL but require expertise in spectroscopy and longer computer time. Both methods help in simplifying the interpretation of metabolite status in the VIP analysis. © 2017, Springer Science+Business Media, LLC.

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Author keywords

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