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Title:	Fast profiling of metabolite mixtures using chemometric analysis of a speeded-up 2D heteronuclear correlation NMR experiment
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Abstract:	One-dimensional (1D) NMR spectra of mixtures of metabolites suffer from severe overlap of spectral resonances and hence recent research in NMR-based metabolomics focuses on using two-dimensional (2D) NMR experiments for metabolite fingerprinting. While standard 2D NMR experiments offer an attractive alternative to the problem of overlapping resonances, they suffer from the disadvantages of long experimental time and poor sensitivity. This work uses a fast 2D NMR experiment namely the 2D ASAP-HSQC (acceleration by sharing adjacent polarization heteronuclear single quantum correlation spectroscopy) scheme, which achieves good spectral resolution in a fraction of the experimental time taken by the standard 2D NMR pulse sequences. The experiment is easy to implement on standard NMR spectrometers and does not require specialized hardware, complicated software routines or expensive isotope labeling. The entire metabolomics study, including metabolite identification and preparing input data for multivariate statistical analysis, is performed using the 2D NMR dataset. Integrated 2D cross-peak intensities are used directly as input variables for statistical analysis. The results of the statistical analysis obtained using the 2D ASAP-HSQC spectra were validated by comparing with those obtained by using 1D proton NMR and the standard 2D HSQC NMR datasets, and a good match was obtained.
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