AQuA: An Automated Quantification Algorithm for ^{1}H NMR-based metabolomics of human plasma

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Although ^{1}H NMR-based metabolomics is very useful – e.g., to identify disease biomarkers – spectra generated by NMR are complex as signals from many different metabolites are observed. Some of these signals are typically located within close proximity and interferences are therefore encountered. Such interferences must be accounted for in the quantitative process to yield accurate results. This process can be very time-consuming, especially in large-scale studies. Hence, development of accurate and rapid quantification tools is desired. In response to this, an Automated Quantification Algorithm (AQuA)[1] was designed as a final step of the ^{1}H NMR-based metabolomics workflow (Figure 1). One preselected NMR signal per metabolite is used in AQuA and interferences, which affect these signals, are modelled from a spectral library. The quantifications are done in a two-step procedure (data reduction and an AQuA computation). Data generated in this process, such as signal positions, heights and interferences, can be used to evaluate AQuA. This was demonstrated in an implementation of AQuA that quantified 67 human plasma metabolites in 1342 human samples collected using heparin as an anticoagulant. AQuA performed all quantifications within one second on a standard personal computer and it generated concentrations that were in excellent agreement with the results from a more time-consuming software for manual deconvolution of metabolite signals (ChenomX[2]; ca. 30 minutes per spectrum). The accuracy and speed of AQuA is desired for metabolite quantifications in large-scale NMR-based metabolomics studies. Further development for spectra from other sample types can facilitate a broader use of AQuA.

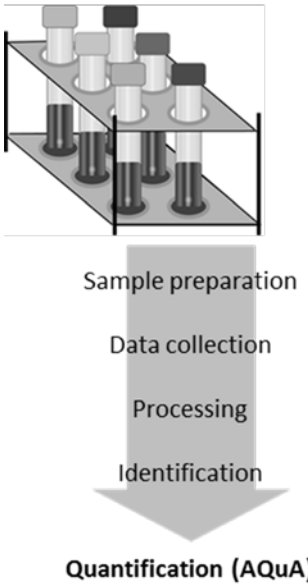

Figure 1. Workflow for ^{1}H NMR-based metabolomics

[1] HE. Röhnisch et al. *Anal. Chem* **2018**, *90*, 2095-2102.

[2] AM. Welije et al. *Anal. Chem* **2006**, *78*, 4430-4442.