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NMR based metabolomics in clinical and epidemiology screening

M.Spraul, H.Schäfer and B.Schütz

BrukerBioSpin GmbH, Germany

NMR over many years was used for structure elucidation of pure compounds, however in the last decade NMR established itself as a major tool for metabolomics analysis based on its unmatched reproducibility and transferability properties. This allows to visualize simultaneous smallest changes of concentration of many compounds in mixtures like biofluids.These changes can be observed in untargeted and targeted mode with one experiment. The dynamic range under full quantitative conditions reaches $2*10^5$ with modern digital NMR spectrometers. Calibration for quantification has to be done once for all compounds in the mixture. Sensitivity over the years could be enhanced substantially allowing detection of concentrations of 1mmol/molcreatinine in urines.

Standard operation procedures have been developed and distributed in the Metabolomics NMR community, This secures exchangeability of data created in different NMR centers. In untargeted screening any deviation from a normal model can be detected, if it is visible by NMR. This approach is shown for urine based newborn screening for inborn errors of metabolism. It is also shown, how NMR delivers quantitative information for a multitude of compounds, allowing to rapidly set-up precise concentration distribution curves. Another important aspect is the influence of meta-parameters to the NMR spectrum, spanning from parameters describing the baby like head circumference to parameters of the mother like the body mass increase during pregnancy. In adults the same NMRdependencies from various meta-parameters can be observed.

Moving away from analysis of single samples per person into a longitudinal study allows to generate basically invariant metabolic profiles. These profiles can be used for person recognition, but more importantly allow to detect early deviations from normality and to observe the consequences of personalized drug treatment. In the end an outlook is given, how this technology can be transferred into other metabolomics applications like food and drug quality and safety control.

Examples for all applications mentioned are given and explained.