Nutritional metabolomics
Mikkelsen, Mette Skau; Savorani, Francesco; Rasmussen, Morten Arendt; Jespersen, Birthe P Møller; Kristensen, Mette; Engelsen, Søren Balling

Publication date:
2013

Document version
Early version, also known as pre-print

Citation for published version (APA):
**Nutritional Metabolomics**

- Object specific lipoprotein profiles and fat boosting

**Nutritional metabolomics**

Nutritional metabolomics seeks to relate the intake of a particular dietary component to specific metabolic fingerprints.

The workflow of a nutritional metabolomics study involves hypothesis, experimental design, sampling of biofluids, the analytical platform, the sample spectra, data preprocessing, the multivariate data analysis and last but not least the biological interpretation.

**Motivation**

By using nutritional metabolomics techniques, it may be possible to detect additional nutritional responses to those found with the traditional biomarkers.

In this study, NMR spectroscopy in combination with multivariate data analysis is applied to investigate the full blood metabolic effects of daily supplementation of mixed linkage β-glucans from oat and barley.

Both targeted and exploratory metabolomics approaches are used.

**Lipoprotein profiles**

The second most influential variation in the data is due to gender and characteristic lipoprotein profiles are found for male and female samples.

**1H NMR spectroscopy**

Proton nuclear magnetic resonance profiling of blood plasma reveals hundreds of small metabolites.

Assignment of the spectra is made according to previous investigations with the most important resonances for this study being the broad signals from the CH$_2$ and CH$_3$ protons in the lipoproteins (VLDL and LDL) at 0.9 and 1.3 ppm.

**Multivariate data analysis**

The complexity of metabolomics data makes interpretation complicated.

Multivariate data analysis can decompose data into simpler and more interpretable structures.

Principal component analysis (PCA) on plasma NMR spectra demonstrate that the main variance among samples is due to subject specific metabolomes.

**Conclusions**

No significant blood metabolic exposure and effect markers were identified for intake of β-glucans from oat and barley as studied by targeted metabolomics.

Explorative metabolomics revealed the existence of subject unique lipoprotein profiles, which especially are dependent on gender and diet.

This leaves a potential for improvement of design in future nutritional metabolomics studies.

**References**

3. bOgger, S et al. (submitted), J Nutr.