Course report
Introduction to nutritional metabolomics
13-17 February 2017, Copenhagen, Denmark

The aim of the course was to give us an introduction to all phases in an untargeted nutritional metabolomics study (LC-MS based), and to train us in the use of available software for data handling and data analysis. Specifically, we were taught to evaluate how study design affects sample and data handling, how to use the most common freely available software's, and how to apply common strategies for marker identification. Lars took us briefly through these steps early on day one. In the afternoon, Rastislav gave us an introduction to the different mass spectrometers used in LC-MS, focusing on the exact mechanism of action. On day two, Gözde gave lectures on data pre-processing and analysis using MZmine, including peak detection, deisotoping, alignment and gap filling. Most of the day was spent doing hands-on exercises using a dataset from a coffee intervention performed by Lars' research group. In the afternoon, Mads gave a useful intro to univariate analyses using R, including the use of *for loop* functions. On the morning of day three, Gözde gave a lecture on multivariate approaches, specifically the use of PCA. Again, we used the coffee dataset to perform hands-on exercises with MATLAB and PLS-toolbox. In the afternoon, Gözde gave a lecture on PLS-DA. Again using the same software and dataset, we did further analyses with PLS-DA. On day four, Jan provided nice lectures on the basis for metabolite identification. In this session, we used various web-based tools and MZmine to try and identify coffee metabolites of high importance for projection in the PLS-DA analyses. On the last day of the course, groups gave presentations summarizing their workflow and results.

The *Introduction to nutritional metabolomics* course provided us with useful introductory knowledge on metabolomics, and sparked our interest in doing further metabolomics research. However, since we had no prior knowledge on the topic, the course was very compact and labor-intensive. It was challenging both the overall picture of the workflow, whilst simultaneously performing hands-on analysis using specific softwares. Nevertheless, we had a great time, and got to know scientists from other fields that may open for later collaboration.

Sincerely,
Sunniva Veen Larsen and Jacob Juel Christensen