Course report
Introduction to Nutritional Metabolomics
Copenhagen, 8-11 February 2016

Mirella Kalafati and Anne Geijsen went to the course 'Introduction to Nutritional metabolomics' in Copenhagen, Denmark. Mirella has a background in computer science and bioinformatics while Anne has a background in Nutrition and Health. The rest of the students also had quite diverse backgrounds however despite this mixed group, the course was very well received by all students.

The first day (Monday February 8th), we were given some general presentations about the related fields in nutritional metabolomics along with some theoretical background knowledge in the principles and techniques of metabolomics. After this introduction day and having given this background information, all of us were able to follow on the same pace.

The second's day (Tuesday February 9th) main focus was the processing and analysis of the metabolomics data. We were given the raw metabolomics data of subjects (both males and females), that have been drinking coffee and water. Urine was collected twice from these subjects, before the test drink and after. We were provided with a lot of information about all the necessary steps of the pre-processing of the data and at this point we were introduced to MZmine, an open source software for mass spectrometry data processing, that mainly focuses on LC-MS data. We did quite some practical work ourselves so we could experience all the difficulties and challenges during these first steps of analysing metabolomics data. In the afternoon, multivariate analysis was introduced. In the evening, we had the most delicious meal at Manfreds with the whole course team and students.

On Wednesday (February 10th) we dipped into multivariate analysis using the pre-processed data of the day before. We used MatLab along with the PLS toolbox to perform the metabolomics data analysis. Principal component analysis (PCA) and Partial least squares Discriminant Analysis (PLS-DA) were used, to obtain a clear distinction between the groups (coffee drinkers and water drinkers) and identify the feature characteristics (possible coffee biomarkers). Apart from multivariate analysis, we were also introduced to univariate analysis, as an alternative solution. The goal of that day, was for us to realize that data analysis is a time-consuming process, that in most of the cases, will need the combination of univariate and multivariate techniques.

Finally, on our last day (February 10th), we performed identification of the metabolites. This was not a trivial procedure, but it helped us learn how to tackle the difficulties of metabolite identification and how to use all the available resources into our advance. By the end of the day, most of us were able to identify coffee related metabolites.

The course "Introduction to Nutritional Metabolomics" that was held at the department of Nutrition, Exercise and Sports in the University of Copenhagen, was a very targeted and informative course. It most certainly met our expectations and gave us an elaborate introduction and hands-on experience on metabolomics analysis. We would like to express our gratitude to all the instructors for their patience, enthusiasm and their constant effort to provide answers to all our questions. We would definitely recommend this course to students who would like to learn about metabolomics and have no prior or basic experience with the field of metabolomics.

Kind regards,
Anne and Mirella