

Course Description

Recent years have seen rapid development in biological mass spectrometry and proteomics. In particular, the quantitative performance has taken a huge leap forward, both as a label-free (LF) approach and as multiplexed quantitative mass spectrometry. This development has enabled new technologies for unbiased characterization of drug molecules with protein targets, which is one of the major challenges in drug development. Here we will explain the basic principle of protein quantification by mass spectrometry. A pragmatic description of strengths and weaknesses of both label-free as well as the multiplexed methodology will be presented. A novel technology, thermal proteome profiling (TPP), will be explained that detects protein drug interactions in living cells. A practical session will take the students through the analysis and interpretation of quantitative mass spectrometry data stemming from the TPP experiment using an R package. In the LF part of the course, we will explain the basics of the identification software DeMix that performs deconvolution of the naturally multiplexed tandem mass spectra, thus significantly improving the identification aspects. An extension to quantification, DeMix Q, introduces the false discovery rate (FDR) for peptide identity transfer between the LC-MS runs, and greatly improves the quantification performance. Both DeMix and DeMix Q are realized based on Open MS package. The participants will learn how to use these programs and process their data.

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