Pipeline Data treatment, CAMERA, QC and reproducibility CV cutoffs

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Xcms and its fellow package CAMERA allow an efficient and reliable analysis of untargeted metabolomics data. This wealth of information have to be further processed in order to answer biological questions. Annotation - the process of going from features to chemical compounds - is a really important element of the data analysis pipeline. Ultimately, however, a meaningful statistical analysis of the data has to be performed in order to identify robust biomarkers.

In the last few years our group has been actively involved in these two tasks. During the presentation I'll show the R based metabolomic data analysis pipeline we have implemented at our institute to analyze and annotate LC-MS and GC-MS metabolomics datasets. In the mean time, I'll also present the results of our recent work on the development of new methods for biomarker selection. The algorithms have been included in our "BioMark" R package.