Data:

The RAW data from the XCMS spreadsheets were feature wise median centered and logarithmised for the statistical analysis.

A T-test model was calculated using Profile.Analysis 2.1 from Bruker Daltonics.

To find the Top 50 changed metabolic features, the data was filtered according to the uncorrected p-value ($p >= 0.001$; 1 out of 1000 is a false positive). Further the remaining features were sorted by their FDR value (Yes $<= 0.05$; No > 0.05) and the absolute ratio. From this list the first 50 were selected.

The absolute ratio was calculated using the data that was normalized to the respective internal standard.

m/z were looked up using excel in a database containing all entries from the HMDB early 2016 (only M+H or M-H).

For visualization RStudio (0.99. 902) with R (3.3.1) was used:

PCA was created using the package pcaMethods 1.64.0