

Data processing method

All data processing were done using Excel 2013 (Microsoft Inc.) and MetaboAnalyst 3.0 (Xia *et al.*, 2015). Spectral data obtained from the analytical platforms were extracted into matrices. Data matrices were individually inspected (correct peak picking and alignment, batch effect, and data integrity) as well as preprocessed (data filtering, missing value imputation and normalisation). Metabolites were normalised to tissue mass. This was achieved through normalisation with either *N,N*-dimethyl-L-phenylalanine (GC-TOF-MS and LC-MS/MS data) or 3-phenylbutyric acid (¹H-NMR data). In addition, metabolites measured with LC-MS/MS were further normalised to stable isotopes, which were added to samples before derivatisation. Each metabolite was either normalised to its own isotope (where possible) or to an isotope with a similar retention time to which the metabolite strongly correlated. No batch corrections were needed as the QCs showed no significant batch effects. Thereafter, data pretreatment (glog transformation and mean centering) and outlier detection (principal component analysis (PCA) and heatmaps) were done.