Fig. 1

Sample analysis	**Data analysis**			
Measurement and basic data transformation (FID to spectra, m/z records to chromatograms and mass spectra)	Data pre-processing = data coding			Numerical analysis
Delivery of primary data →	Alignment of signals or binning	Normalize data sample wise to unit integral = convert primary data into profiles	Replace missing values by median of reference values, re-code data into deviation profiles with ordinal scale **= scaling by IQRHILO coding**	Model and classify all profiles coded as deviation profiles, predict from deviation profile type
Assure analytical quality	Assure equity of recorded signals	Eliminate global elements of confounding variability (shared variability affecting all samples	Isolate significant treatment related differences between groups (samples) of interest, eliminate confounding individual or time dependent parts of normal variability	Assign meaning to the changes, interpret in the context of the original research question