Fig. 1

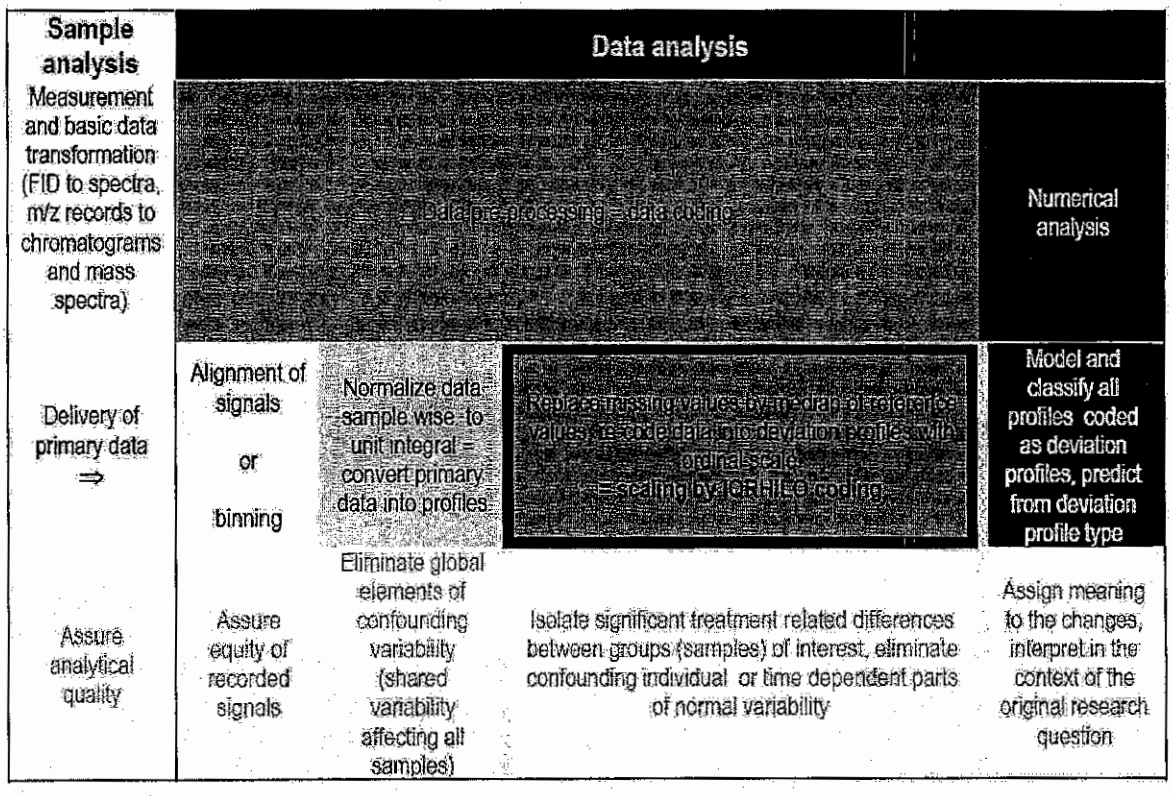

Sample analysis
Data analysis
Measurement and basic data transformation (FID to spectra, m/z records to chromatograms and mass spectra)
Data pre-processing = data coding
Numerical analysis
Delivery of primary data
⇒
Alignment of signals
or
binning
Normalize data sample wise to unit integral = convert primary data into profiles
Replace missing values by median of reference values, re-code data into deviation profiles with original scale
= scaling by (CRITIC) 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

Fig. 2

