



Assessment of disease risk
by targeted metabolomics

Supplementary data on method for analysis of β -Alanine (bALA).

Method based on article

Midttun et al (2016), PMID 27715010.

Material

β -Alanine (purity 99%) and β -Alanine $^{13}\text{C}_3,^{15}\text{N}$ (purity 98 atom% ^{15}N , 99 atom% ^{13}C) was obtained from Sigma-Aldrich, St.Louis, MO 63103 USA or 89555 Steinheim Germany.

Instrumentation

Agilent 7010B GC/TQ and Agilent 8890 GC System.

Chromatography and detection

GC-MS/MS; positive-ion multiple reaction monitoring (MRM); retention time = 3.27 min.

β -Alanine precursor ion = 130.0 m/z; product ion = 88.0 m/z.

β -Alanine $^{13}\text{C}_3,^{15}\text{N}$ precursor ion = 134.0 m/z; product ion = 92.0 m/z.

Method performance

Linear range: 0.3 - 1000 $\mu\text{mol/L}$.

Linearity: r^2 : 0.996.

LOD (S/N >5): 0.3 $\mu\text{mol/L}$.

Within-day CV: 3-5 %.

Between-day CV: 3-5 %.