



Assessment of disease risk
by targeted metabolomics

Supplementary data on method for analysis of Malate (Mal).

Method based on article

Midttun et al (2016), PMID 27715010.

Material

Malate (purity 99%) was obtained from Sigma-Aldrich, St.Louis, MO 63103 USA or 89555 Steinheim Germany.

Malate-d3 (purity 98%) was obtained from Cambridge Isotope Laboratories, Inc., 50 Frontage Road, Andover, MA 01810-5413 USA.

Instrumentation

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

Chromatography and detection

GC-MS/MS; positive-ion multiple reaction monitoring (MRM); retention time = 3.80 min.

Malate precursor ion = 159.0 m/z; product ion = 61.0 m/z.

Malate-d3 precursor ion = 162.0 m/z; product ion = 62.0 m/z.

Method performance

Linear range: 0.4 - 500 $\mu\text{mol/L}$.

Linearity: r^2 : 0.995.

LOD (S/N >5): 0.4 $\mu\text{mol/L}$.

Within-day CV: 2-4 %.

Between-day CV: 3-5 %.