



Assessment of disease risk  
by targeted metabolomics

Supplementary data on method for analysis of IsoCitrate (iCit).

### **Method based on article**

Middtun et al (2016), PMID 27715010.

### **Material**

IsoCitrate (purity  $\geq 95\%$ ) was obtained from Cayman Chemical, 1180 East Ellsworth Road Ann Arbor, Michigan 48108 USA.

IsoCitrate- $^{13}\text{C}_4$  (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 = 4.15 min.

IsoCitrate precursor ion = 157.0 m/z; product ion = 101.0 m/z.

IsoCitrat- $^{13}\text{C}_4$  precursor ion = 161.0 m/z; product ion = 104.0 m/z.

### **Method performance**

Linear range: 0.3 - 500  $\mu\text{mol/L}$ .

Linearity:  $r^2$ : 0.998.

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

Within-day CV: 3-5 %.

Between-day CV: 4-6 %.