Assessment of disease risk
by targeted metabolomics

Supplementary data on method for analysis of Trigonelline (Trig)

Method based on article
Midttun et al (2009), PMID 19337982.

Material
Trigonelline HCl (purity >98%) was obtained from
Sigma- Aldrich,St.Louis, MO 63178 USA.
Trigonelline-d3 (purity >99%) was obtained from CDN isotopes.
Ponte-Claire, Quebec, Canada.

Instrumentation
Same as in PMID 19337982.

Chromatography and detection
LC-MS/MS; positive-ion multiple reaction monitoring (MRM);
retention time = 2.4 min.
Trigonelline precursor ion = 138 m/z; product ion = 78 m/z.
Trigonelline-d3 precursor ion = 141 m/z; product ion = 78 m/z.

Method performance
Linear range: 0.01 - 100 µmol/L.
Linearity: r2: 0.99.
LOD (S/N >5): 0.01 µmol/L.
Within-day CV: 3-4 %.
Between-day CV: 3-4 %.