

Supplementary data on method for analysis of Isovalerate (iVlr)

Method based on article

-

Material

Isovaleric acid (purity 99%) was obtained from Sigma-Aldrich, St. Louis, MO 63103 USA or 89555 Steinheim Germany.
3-Methylbutyric-d9 Acid (purity >98.5%-d9) was obtained from CDN isotopes. Ponte-Claire, Quebec, Canada

Instrumentation

Agilent 7010B GC/TQ and Agilent 8890 GC System

Chromatography and detection

GC-MS/MS; positive-ion multiple reaction monitoring (MRM);
retention time = 5.62 min.
Isovalerate precursor ion = 192 m/z; product ion = 108 m/z.
Isovalerate-d9 acid precursor ion = 201 m/z; product ion = 109 m/z.

Method performance

Linear range: 0.02 - 1000 $\mu\text{mol/L}$.
Linearity: r^2 : 0.99.
LOD (S/N >5): 0.02 $\mu\text{mol/L}$.
Within-day CV: 3-6 %.
Between-day CV: 3-8 %.