

Supplementary data on method for analysis of Isobutyrate (iBut)

Method based on article

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Material

Isobutyric acid (purity 99%) was obtained from Sigma-Aldrich, St. Louis, MO 63103 USA or 89555 Steinheim Germany.
2-Methylpropionic-d7 Acid (purity >98.8%-d7) 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 = 5.13 min.

Isobutyrate precursor ion = 178 m/z; product ion = 108 m/z.

Isobutyrate-d7 precursor ion = 185 m/z; product ion = 109 m/z.

Method performance

Linear range: 0.05 - 1000 $\mu\text{mol/L}$.

Linearity: r^2 : 0.99.

LOD (S/N >5): 0.05 $\mu\text{mol/L}$.

Within-day CV: 3-6 %.

Between-day CV: 3-8 %.