

Supplementary data on method for analysis of Valerate (Vlr)

Method based on article

-

Material

Valeric acid (purity $\geq 99\%$) was obtained from Sigma-Aldrich, St. Louis, MO 63103 USA or 89555 Steinheim Germany. Pentanoic acid-d9 (purity 98%) 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 = 5.91 min.

Valerate precursor ion = 192 m/z; product ion = 108 m/z. Valerate-d9
precursor ion = 201 m/z; product ion = 108 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: 4-8 %.