

Supplementary data on method for analysis of Acetate (Ace)

Method based on article

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Material

Acetic acid (purity ≥99%) and Acetic acid-d4 (purity ≥99.9%) was obtained from Sigma-Aldrich, St.Louis, MO 63103 USA or 89555 Steinheim Germany.

Instrumentation

Agilent 7010B GC/TQ and Agilent 8890 GC System

Chromatography and detection

GC-MS/MS; positive-ion multiple reaction monitoring (MRM); retention time = 4.48 min.

Acetate precursor ion = 150 m/z; product ion = 108 m/z. Acetate-d4 precursor ion = 153 m/z; product ion = 109 m/z.

Method performance

Linear range: 5.0 - 1000 µmol/L.

Linearity: r2: 0.99.

LOD (S/N >5): 5.0 µmol/L. Within-day CV: 3-5 %. Between-day CV: 3-7 %.