



Item Number: 18224		Short-Chain Fatty Acid LC-MS Mixture			
Label	Item Name	Formula	[MH] ⁻ Theoretical m/z	[MH] ⁻ Measured m/z	Mass Accuracy (ppm)
A	Propionic Acid	C ₃ H ₆ O ₂	73.02950	73.02948	-0.274
B	Butyric Acid	C ₄ H ₈ O ₂	87.04515	87.04511	-0.460
C	Hexanoic Adid	C ₆ H ₁₂ O ₂	115.07645	115.07646	0.087
D	Heptanoic Acid	C ₇ H ₁₄ O ₂	129.09210	129.09222	0.930
E	Octanoic Acid	C ₈ H ₁₆ O ₂	143.10775	143.10788	0.908
F	Nonanoic Acid	C ₉ H ₁₈ O ₂	157.12340	157.12356	1.02
G	Decanoic Acid	C ₁₀ H ₂₀ O ₂	171.13905	171.13928	1.34
H	Dodecanoic Acid	C ₁₂ H ₂₄ O ₂	199.17035	199.17058	1.15

Direct Infusion Negative ESI-FTMS Analysis on a Q Exactive Plus mass spectrometer (Thermo Scientific)

Mass Range: 62-500 m/z	Mass Resolution: 140,000	Concentration: 5 µg/ml
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Solvent: 80:10:10 Methanol:Acetonitrile:Water with 1 mM Ammonium Acetate