

Supplemental Materials

Addressing the accuracy of reference values in a large-scale cohort by kit-based metabolomics compared to other methodologies

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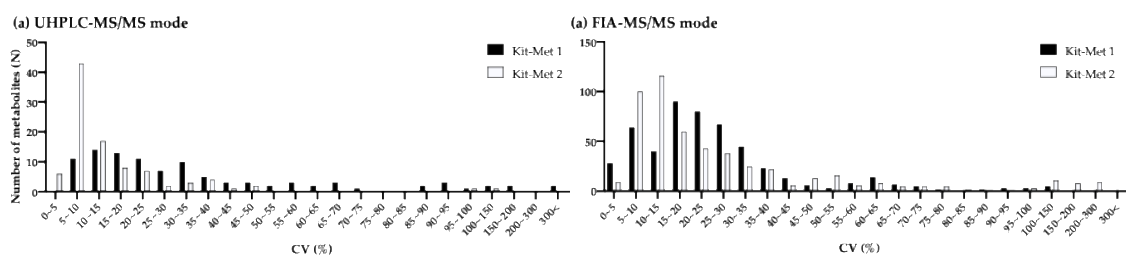


Figure S1. Frequency of detected metabolites along with the range of coefficient variation (CV, %) in gQC plasma at UHPLC-MS/MS mode (a, left panel), and FIA-MS/MS mode (b, right panel) by Kit-Met 1 (black bar) and Kit-Met 2 (white bar).

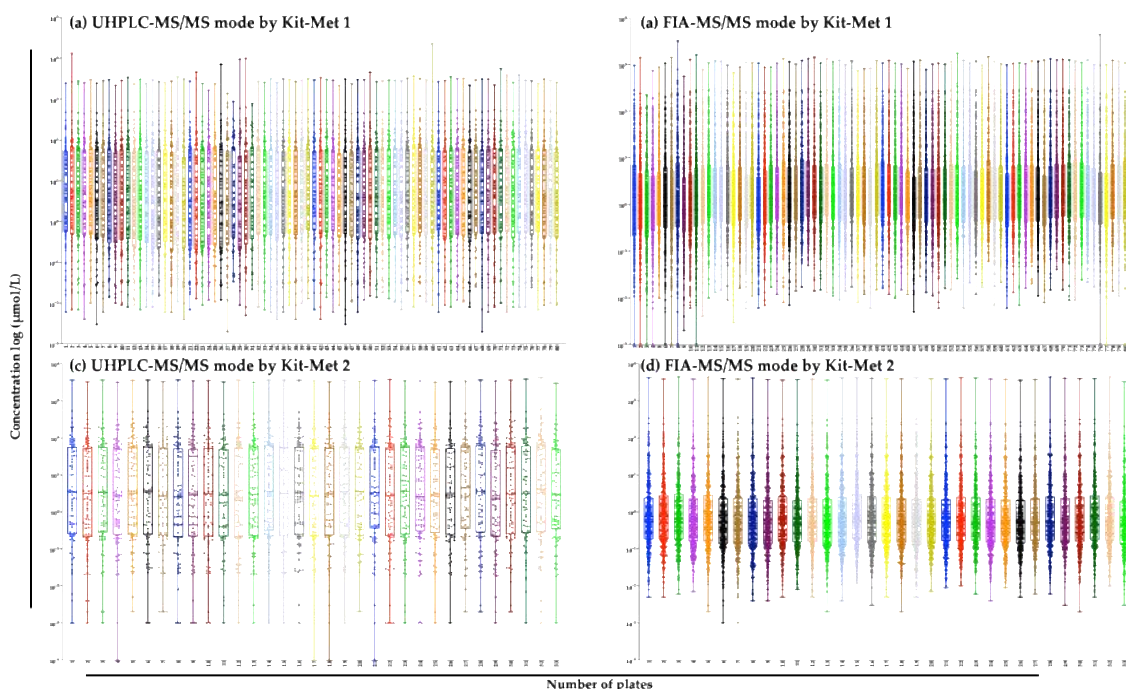


Figure S2. The median intensities of boxplot for detected metabolites in NIST plasma. The boxplots of 80 plates by Kit-Met 1 by UHPLC-MS/MS mode (a, upper left panel) and FIA-MS/MS mode (b, right panel), and the 33 plates by Kit-Met 2 by UHPLC-MS/MS mode (c, bottom left panel) and FIA-MS/MS mode (d, bottom right panel) were created and colored for each plate by GraphPad Prism 8.4.3.. Kit-Met 1 and Kit-Met 2 were performed by the Xevo® TQ-S and Xevo® TQ-XS MS system (Waters, Wilmslow, Manchester, UK), respectively. Both MS systems were conducted with the UHPLC system, which were consisted with dual pumps (ACQUITY UPLC H-Class, Waters) and an autosampler with a column compartment (ACQUITY UPLC I-Class, Waters).

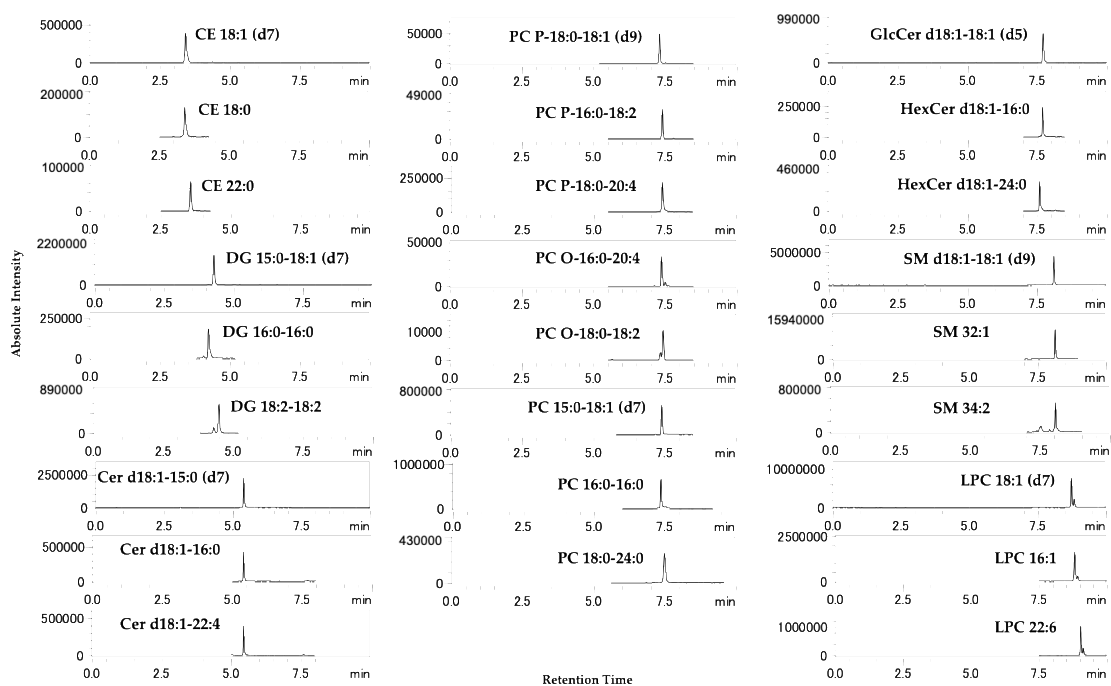
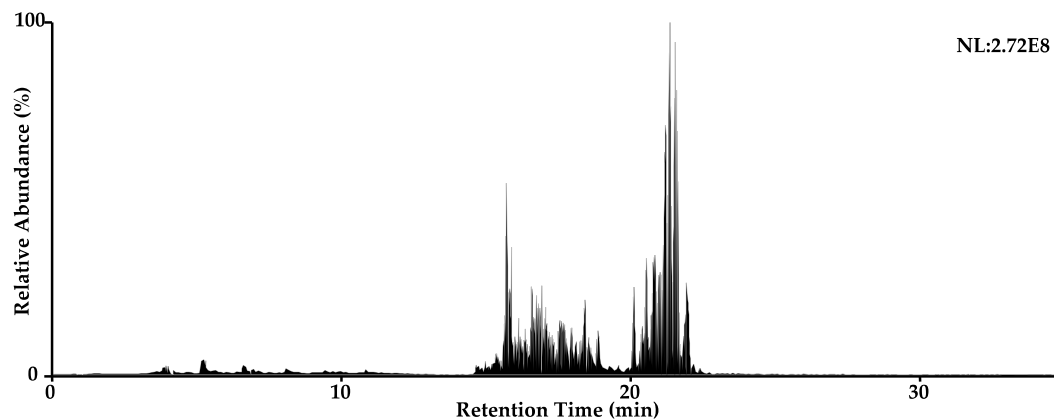
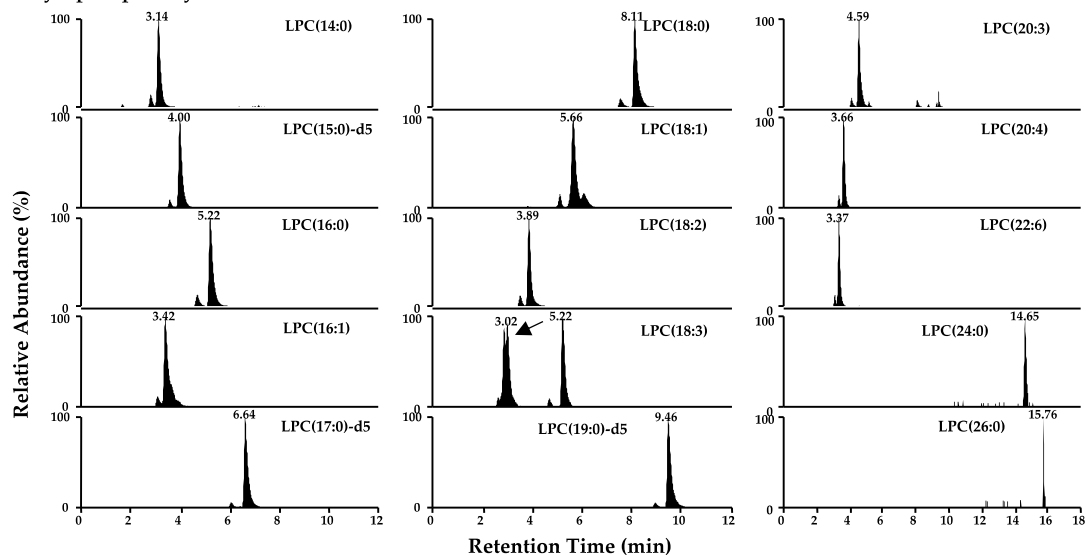


Figure S3. Multiple reaction monitoring chromatograms of representative lipid species detected in the NIST plasma samples by SFC-MS/MS.

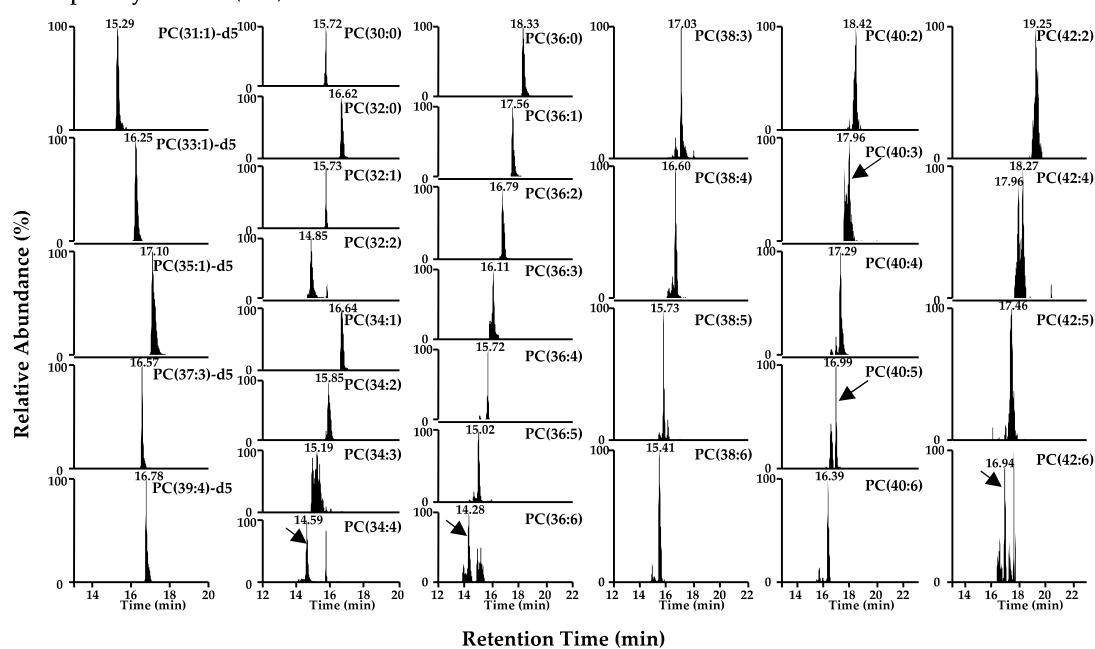
Total ion current (TIC)



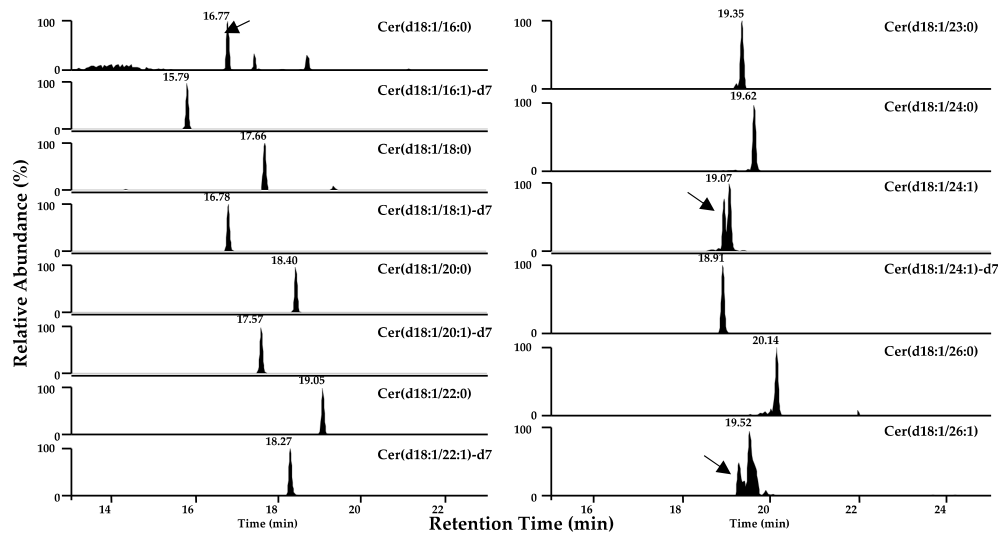
Lysophosphatidylcholines (LPCs)



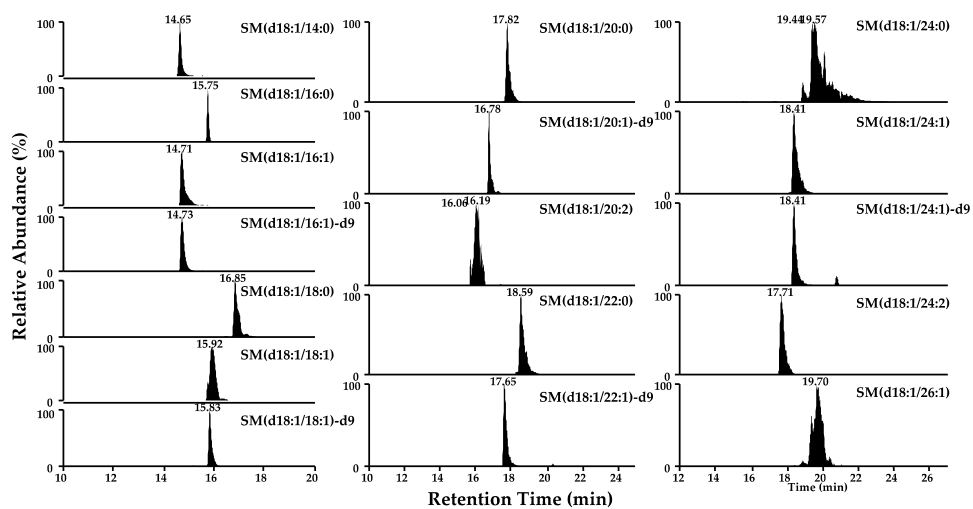
Phosphatidylcholines (PCs)



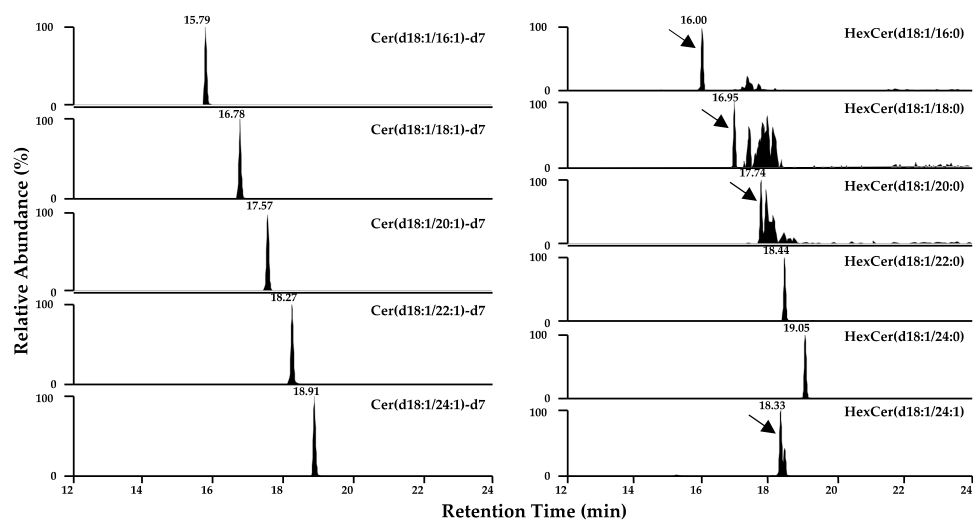
Ceramides (Cers)



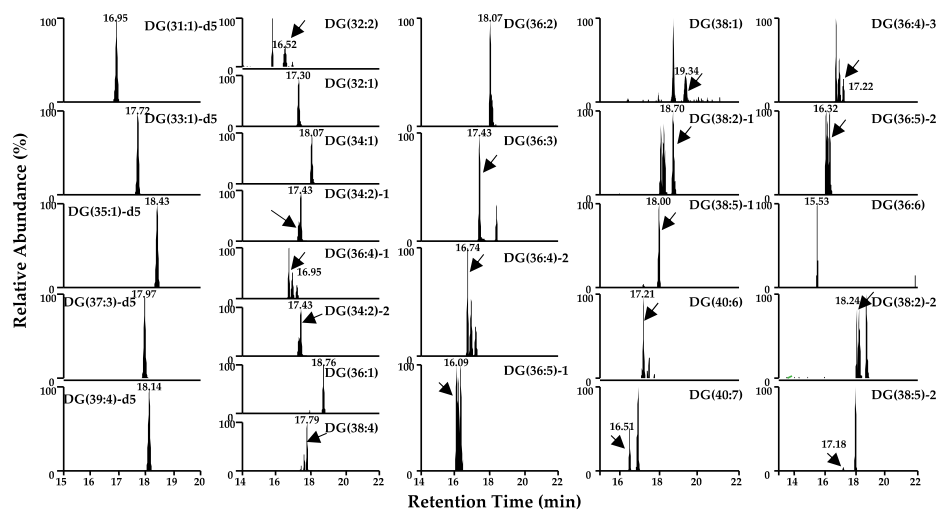
Sphingomyelins (SMs)



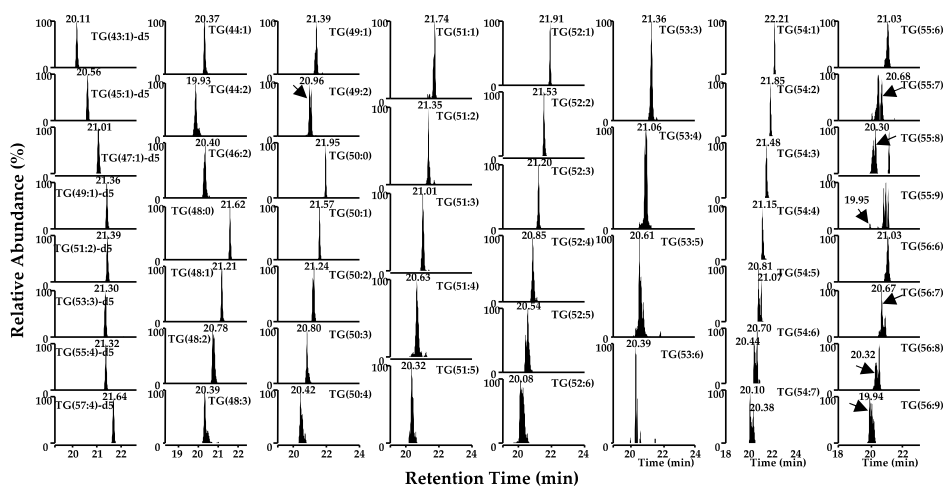
hexosylceramides (HexCers)



Diacylglycerols (DGs)



Triacylglycerols (TGs)



Cholesterol esters (CEs)

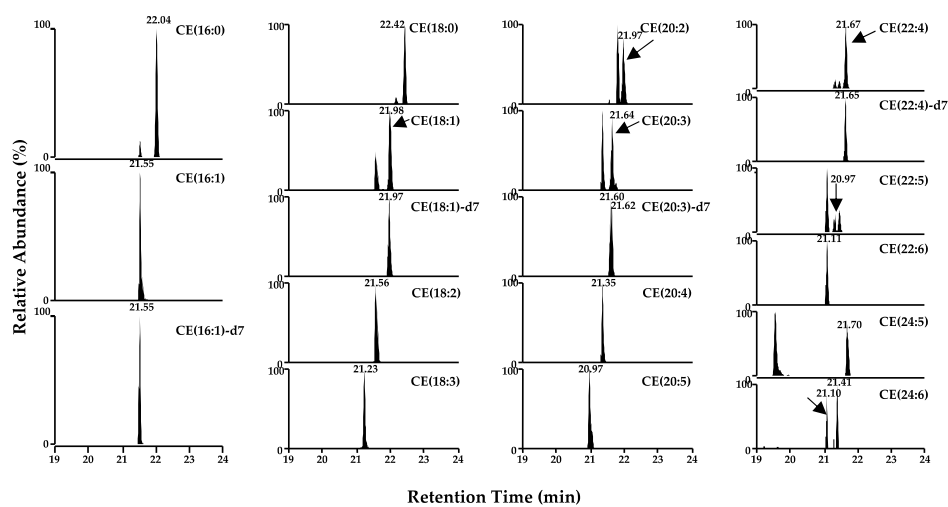
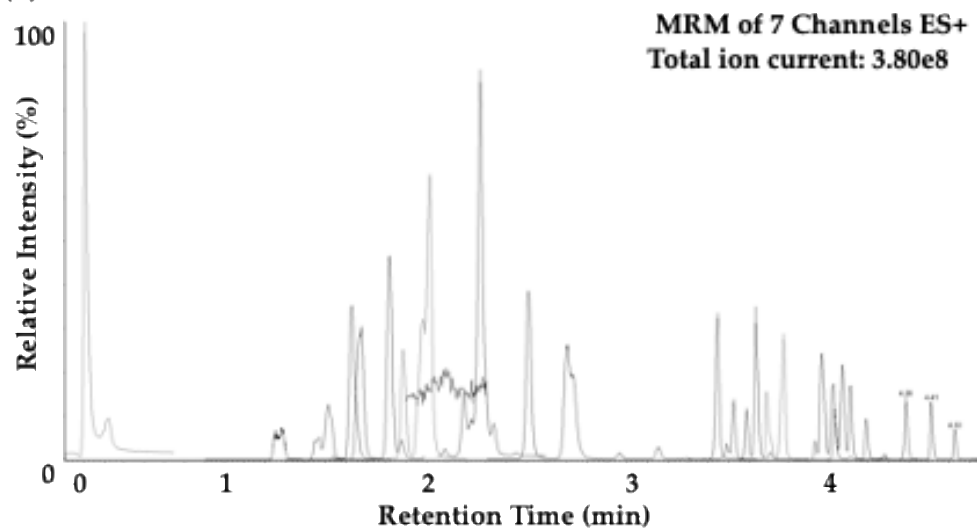


Figure S4. Total ion current (TIC) and mass chromatograms of 148 lipid species with ISs detected in the NIST plasma samples by UHPLC-FTMS at positive ion mode.

(a) LC mode



(a) FIA mode

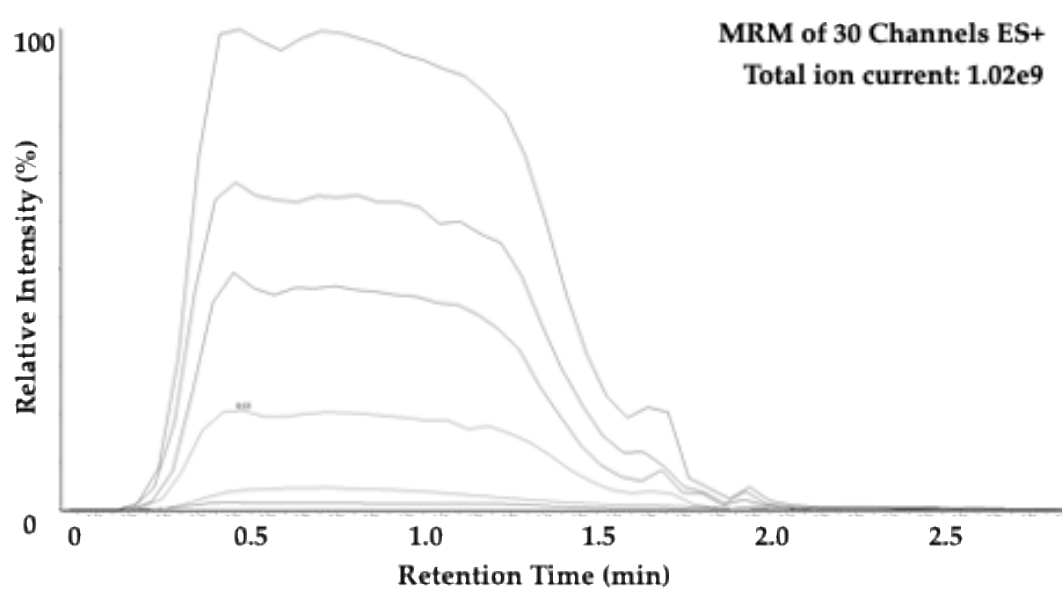


Figure S5. Examples for typical MRM chromatograms of NIST plasma sample analysis by Kit-Met 2 in UHPLC-MS/MS mode (a) and FIA-MS/MS mode (b).

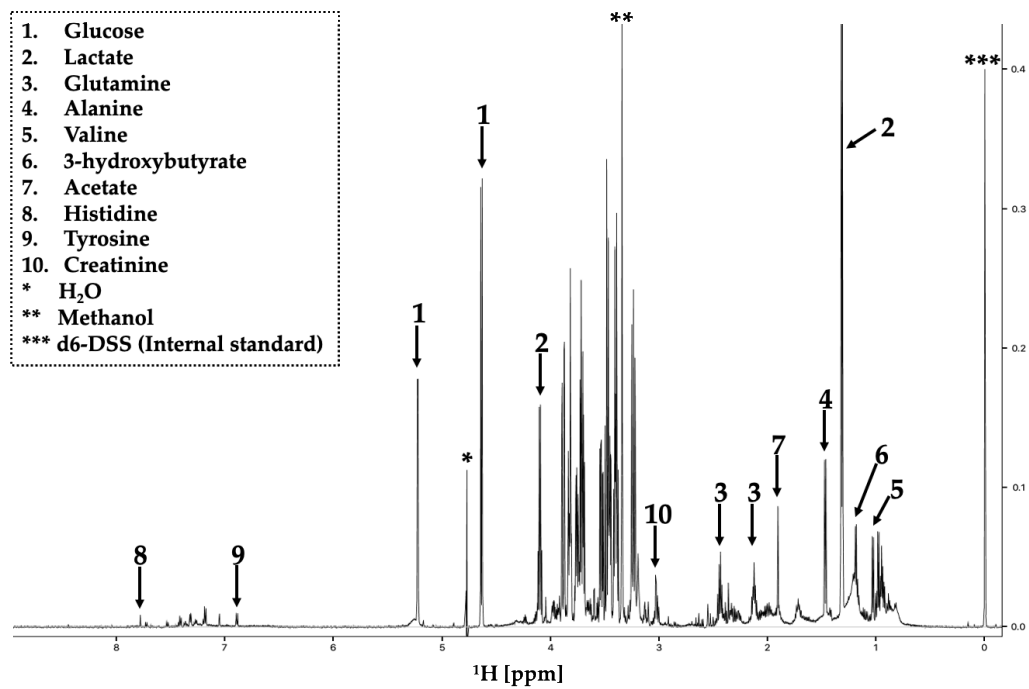


Figure S6. ¹H-NMR spectrum of detected metabolites in NIST plasma sample.