



**S1 Fig. Calibration curves, LLOD and LLOQ determination for derivatized SCFA standards.** (A) Calibration curves for the 3 isotopologue pairs of SCFA standards generated from the derivatization of an equimolar standard solution. Concentrations ranged from 20 nM to 100  $\mu\text{M}$ . Dotted lines represent  $^{13}\text{C}$ -standards. Error bars indicate standard deviation, ( $n = 3$  technical replicates). MS signal intensities are plotted in arbitrary units (a. u.). (B) Regression line equations and  $r^2$  corresponding to plots in (A). (C) Signal-to-noise ratio (S/N) from chromatographic peaks for 3 analytes (acetate, propionate and butyrate derivatized with aniline) at five different concentrations (0.02, 0.04, 0.08, 0.16 and 0.31  $\mu\text{M}$ , in  $\text{H}_2\text{O}/\text{ACN}$  (50:50, v/v)). Bold figures indicate the signal-to noise ratios used for the determination of the LLOD and LLOQ for the analytical method ( $\geq 3$  and  $\geq 10$ , respectively).