Metabolomic Analysis of Human Fecal Microbiota: A Comparison of Feces-Derived Communities and Defined Mixed Communities

Supporting Information

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This document provides extra information concerning the choice of compound groupings based on concentrations (Figure S1); and loading plot associated with PCA of samples (Figure S2).

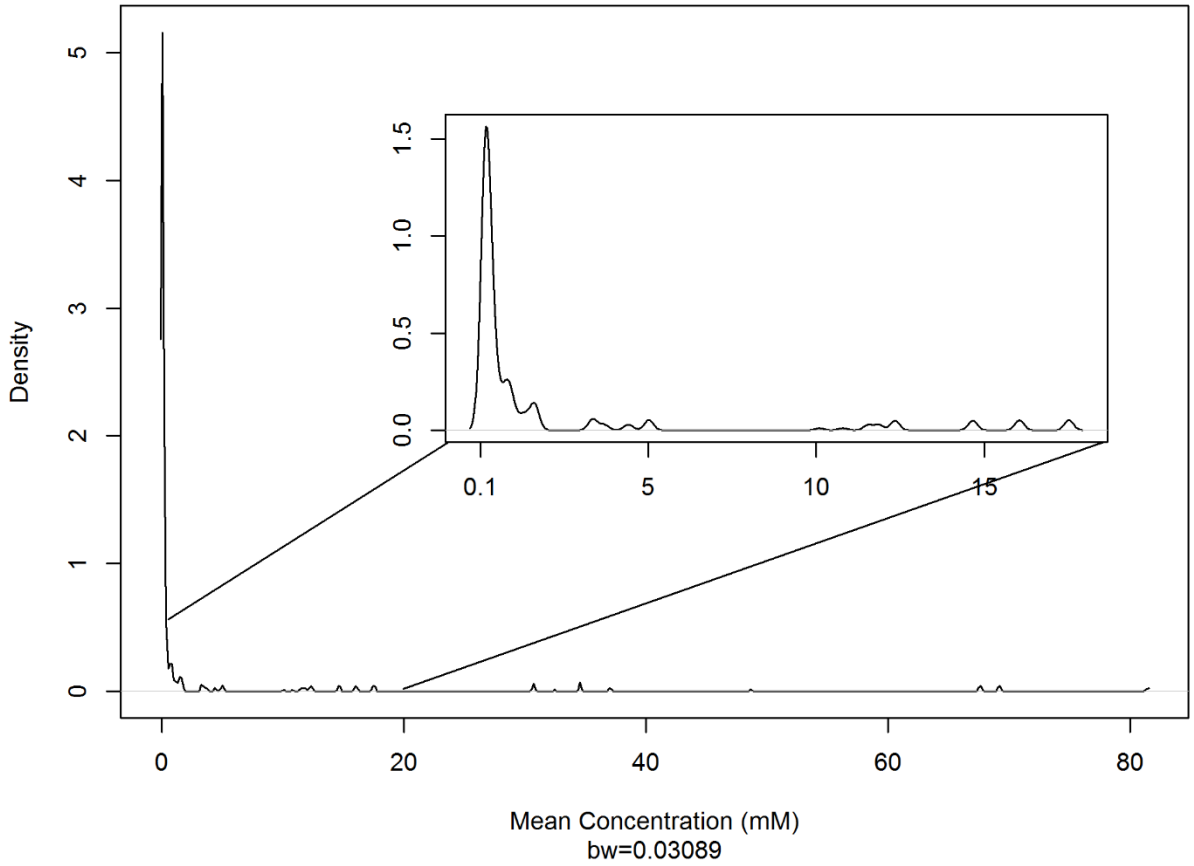

Figure S1. Kernel density plot of mean concentrations of untreated samples collected during steady state, bandwidth=0.03043. Inset is the kernel density plot of mean concentrations greater than or equal to 0.1 mM and less than or equal to 20 mM, bandwidth = 0.135. The clusters observed in these plots were used to define the bin in which the compounds would be grouped.

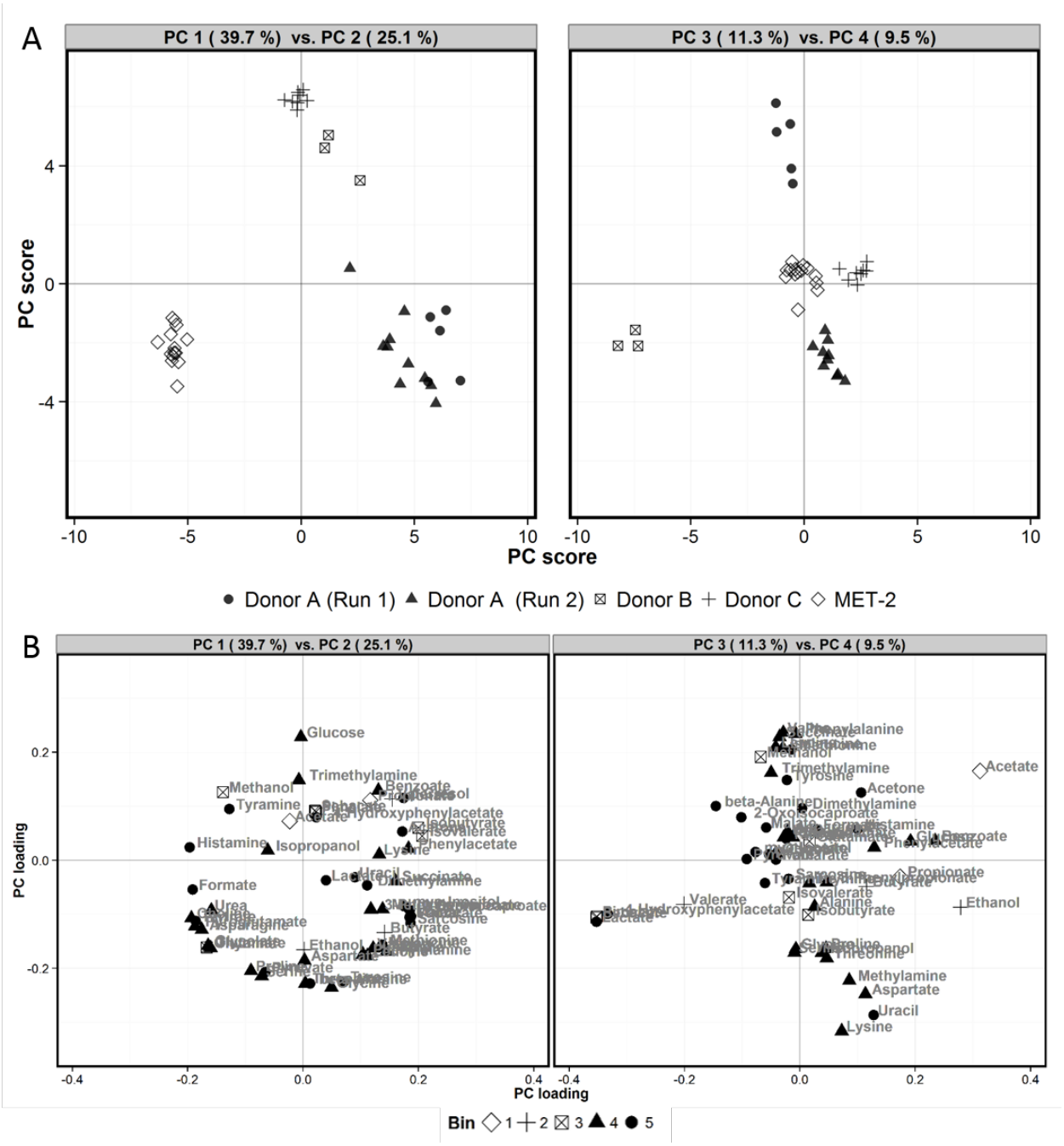

Figure S2. (A) PCA Score plot of metabolite profiles of donor A, B, C and MET-2 cultures. (B) PCA loading plot of metabolite profiles of donor A, B C and MET-2 cultures. Data is mean centered and scaled by unit variance. Bin 1: mean ≥ 20 mM; Bin 2: 10 ≤ mean < 20 mM; Bin 3: 1 ≤ mean < 10 mM; Bin 4: 0.1 ≤ mean < 1 mM; Bin 5: 0 ≤ mean < 0.1 mM