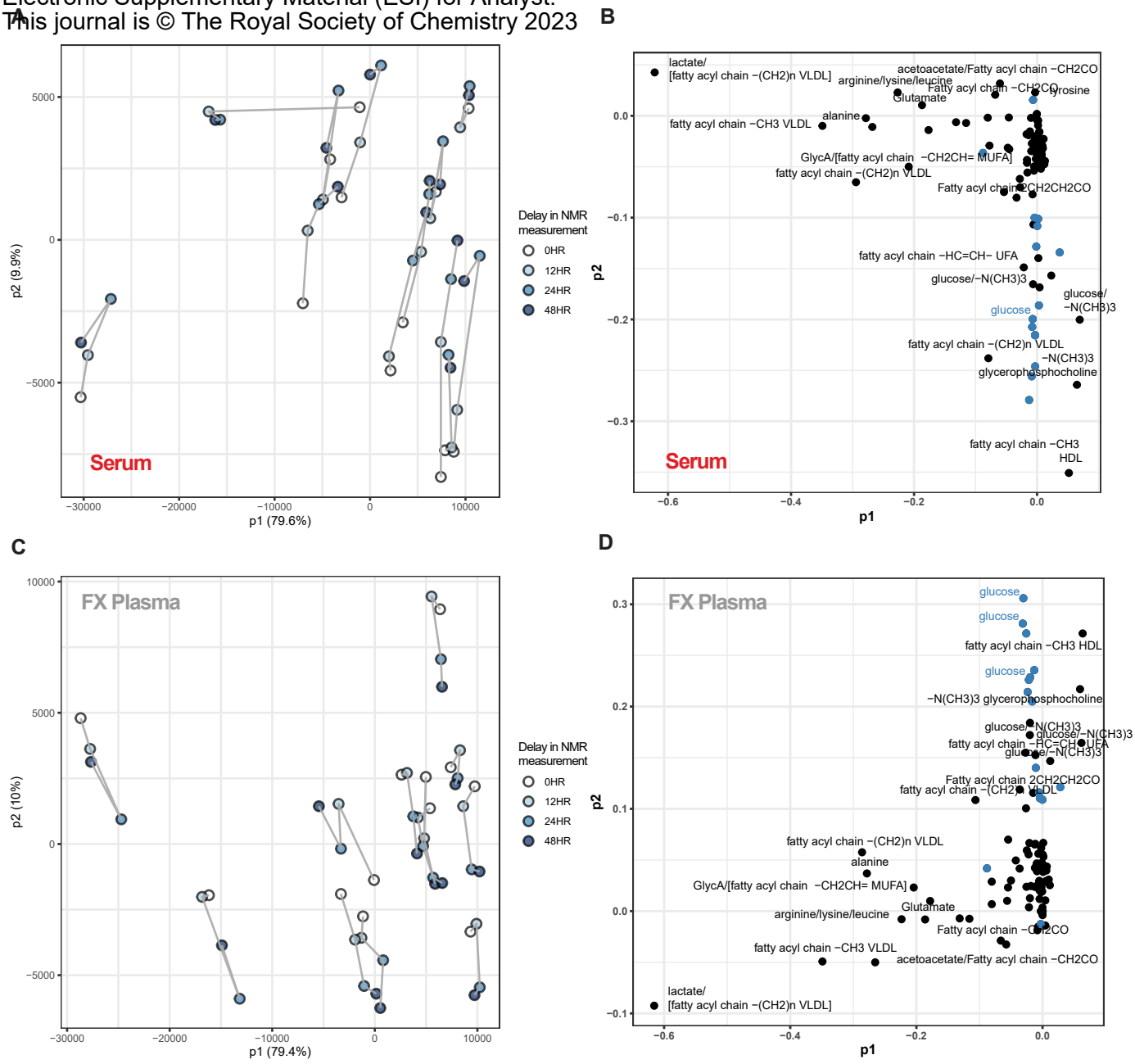

Figure S1 Variation in the metabolome due to delayed sample measurement is small compared to interindividual variation in the healthy control cohort. (A, C) PCA scores plot demonstrating the effect of delayed NMR measurement on LH plasma samples. Each line connects samples from the same individual. (B, D) Loadings plot illustrating the metabolites that contribute to the variation observed in principal component 1 and 2.

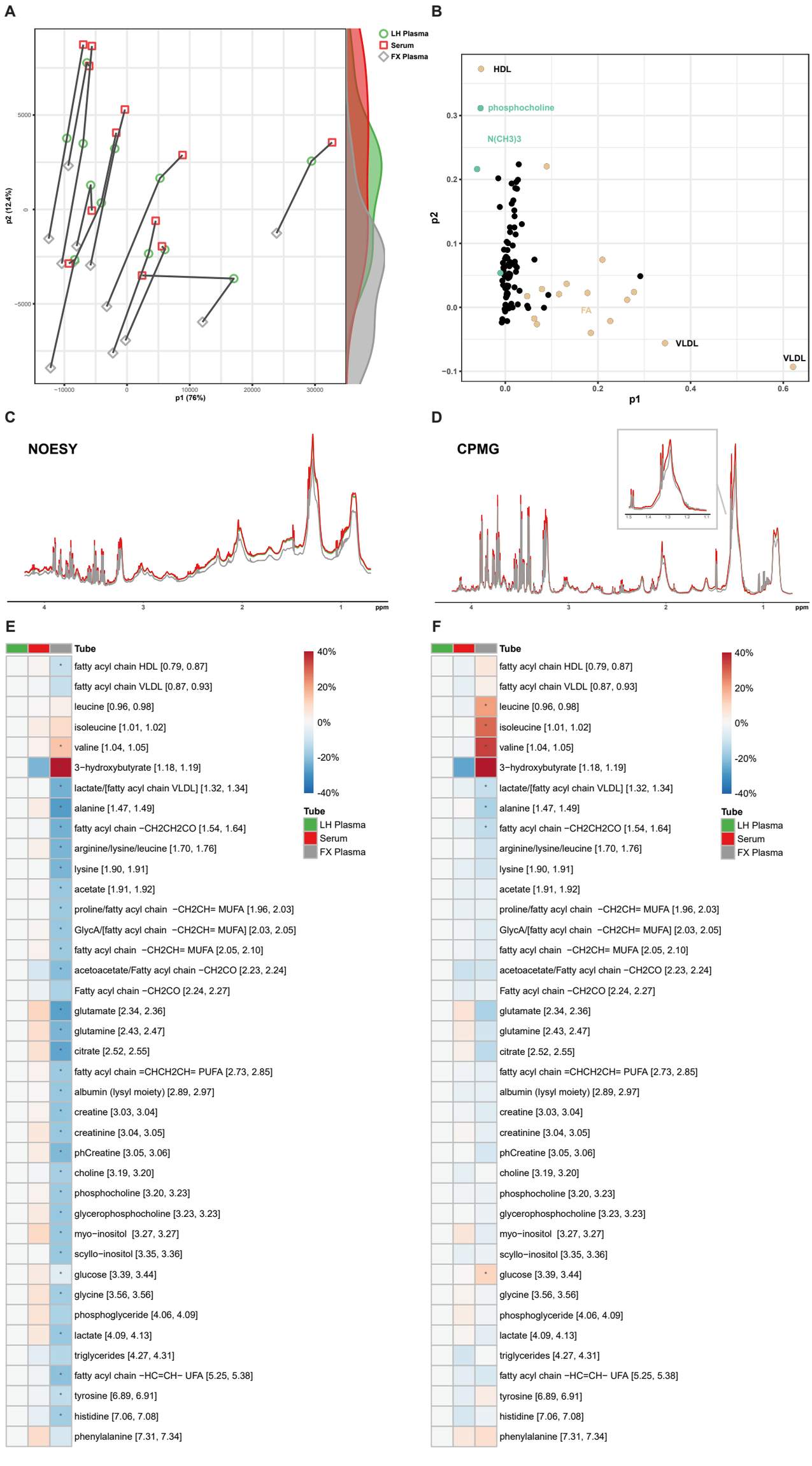

Figure S2 Differences in the metabolome exist by blood collection tube under optimal processing conditions. (A) PCA scores plot showing the effect of different blood tubes on samples under optimal processing conditions. (C, D) Mean NOSEY/CPMG spectra of LH plasma (Green), serum (red) and FX Plasma (Grey). (E, F) Heatmap displaying percentage changes in metabolite levels three types of plasma/serum. The numbers in square brackets represent the corresponding spectral region boundaries in parts per million (ppm). Percentage changes calculated from absolute (E) / sum-normalised (F) integral values and compared to LH Plasma. Significant differences in means of metabolites were represented by * (q<0.05).

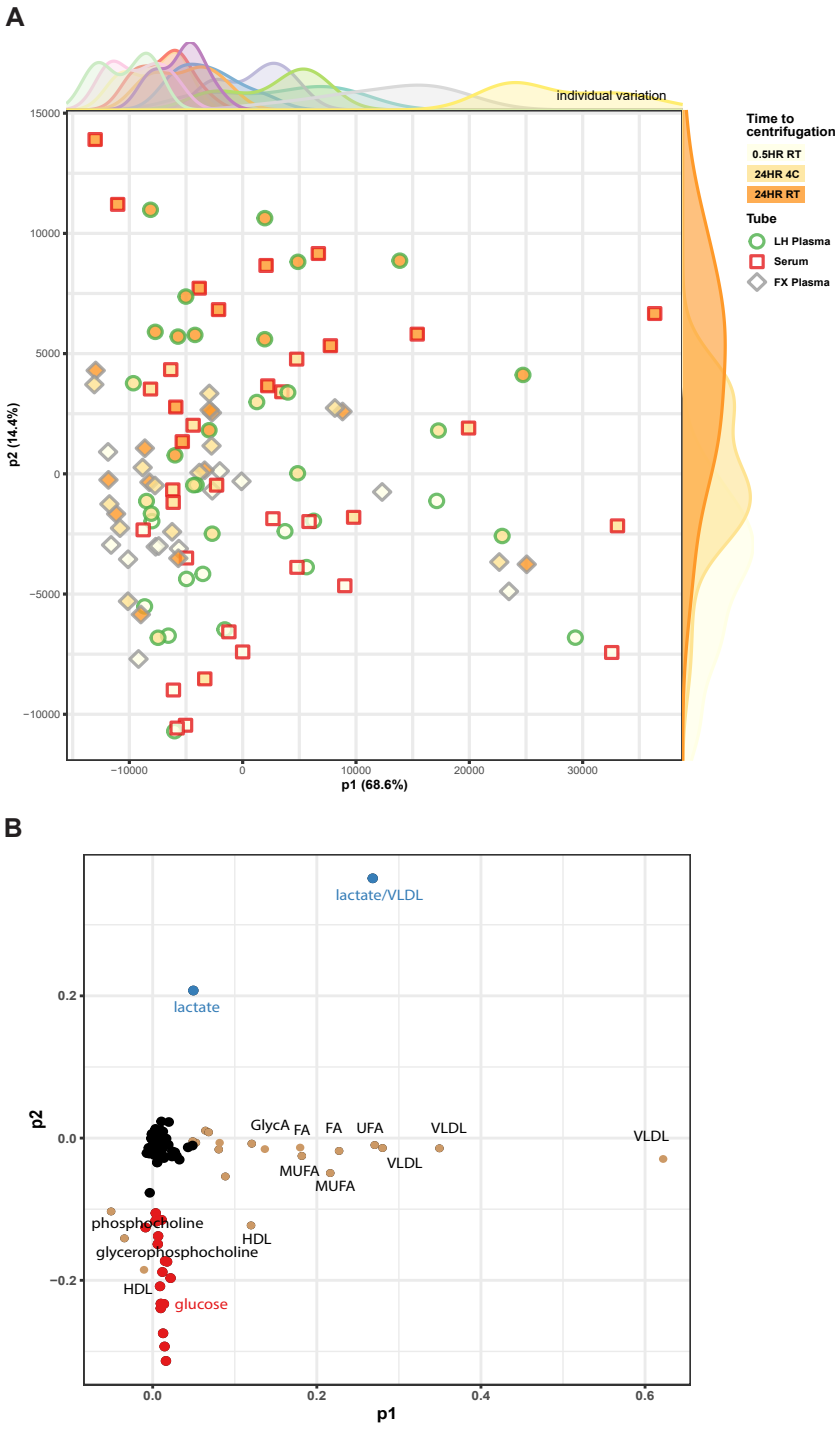

Figure S3 (A) PCA scores plot demonstrating the influence of different pre-processing conditions on samples, specifically observed in PC2, whereas PC1 showing individual variation in metabolome. (B) Loadings plot of the PCA highlighting glucose and lactate as contributors to the variation observed in PC2.

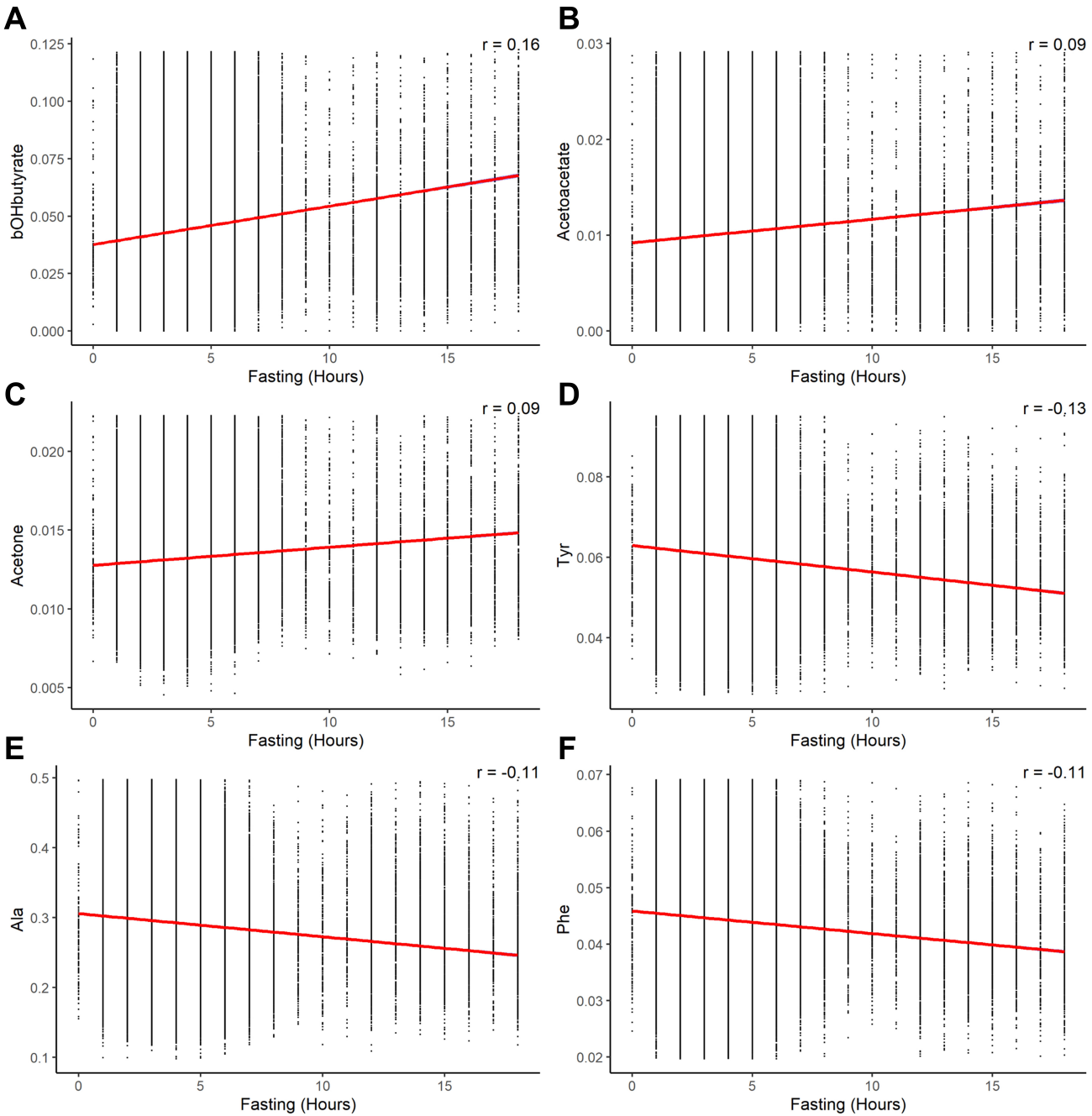

Figure S4 Levels of certain metabolites, primarily ketone bodies, were correlated with fasting time.