

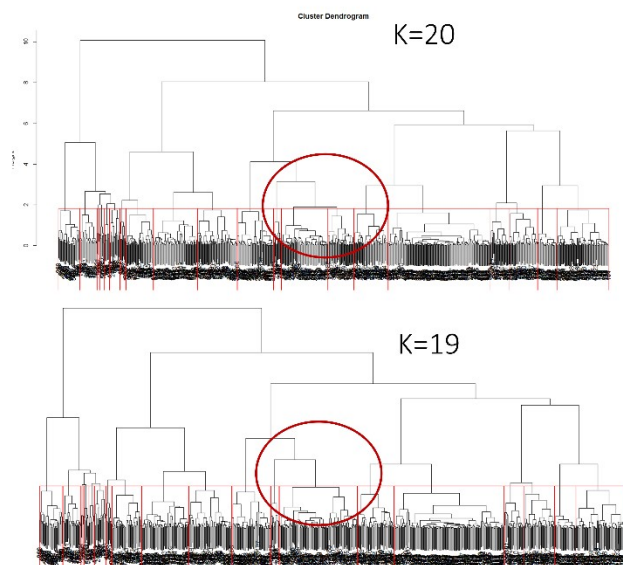
**Supplemental Figure 1**

for **Metabolomics Analysis of Time-Series Human Small Intestine Lumen Samples Collected *in vivo***

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**Supplemental Figure 1.** The smallest optimal number of clusters was determined by reducing the number of clusters (k) by one from 26 original clusters. Dendrograms are generated from correlation of intensities from metabolites annotated in this study. These dendrograms show two groups (Food cluster 1 and bile cluster 2) being combined between k=20 and k=19 (cluster highlighted with red circle).

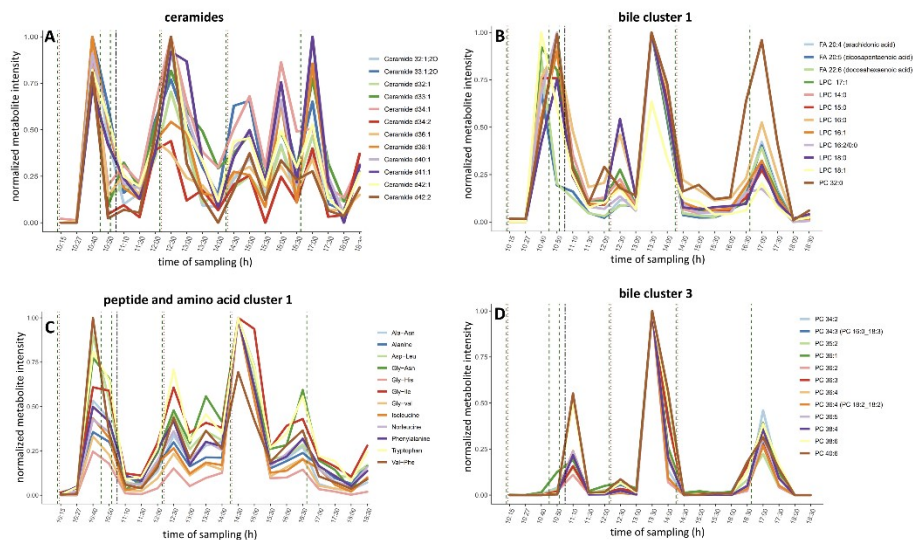
**Supplemental Figure 2**

for **Metabolomics Analysis of Time-Series Human Small Intestine Lumen Samples Collected *in vivo***

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**Supplemental Figure 2.** Four groups of metabolites. Each graph shows the intensity profile of metabolites across the testing period. Vertical lines represent meals (green dashed lines), coffee consumption (brown dotted lines) and acetaminophen consumption (black dashed line). Intensities are normalized to the highest intensity for each metabolite. Panel A contains ceramide lipids. Panel B contains bile related metabolites showing mostly lysophosphatidylcholines (LPCs). Panel C includes metabolites clustered in the di- and tripeptide and amino acid cluster 1. Panel D contains metabolites of bile cluster 3 showing exclusively phosphatidylcholines (PC).