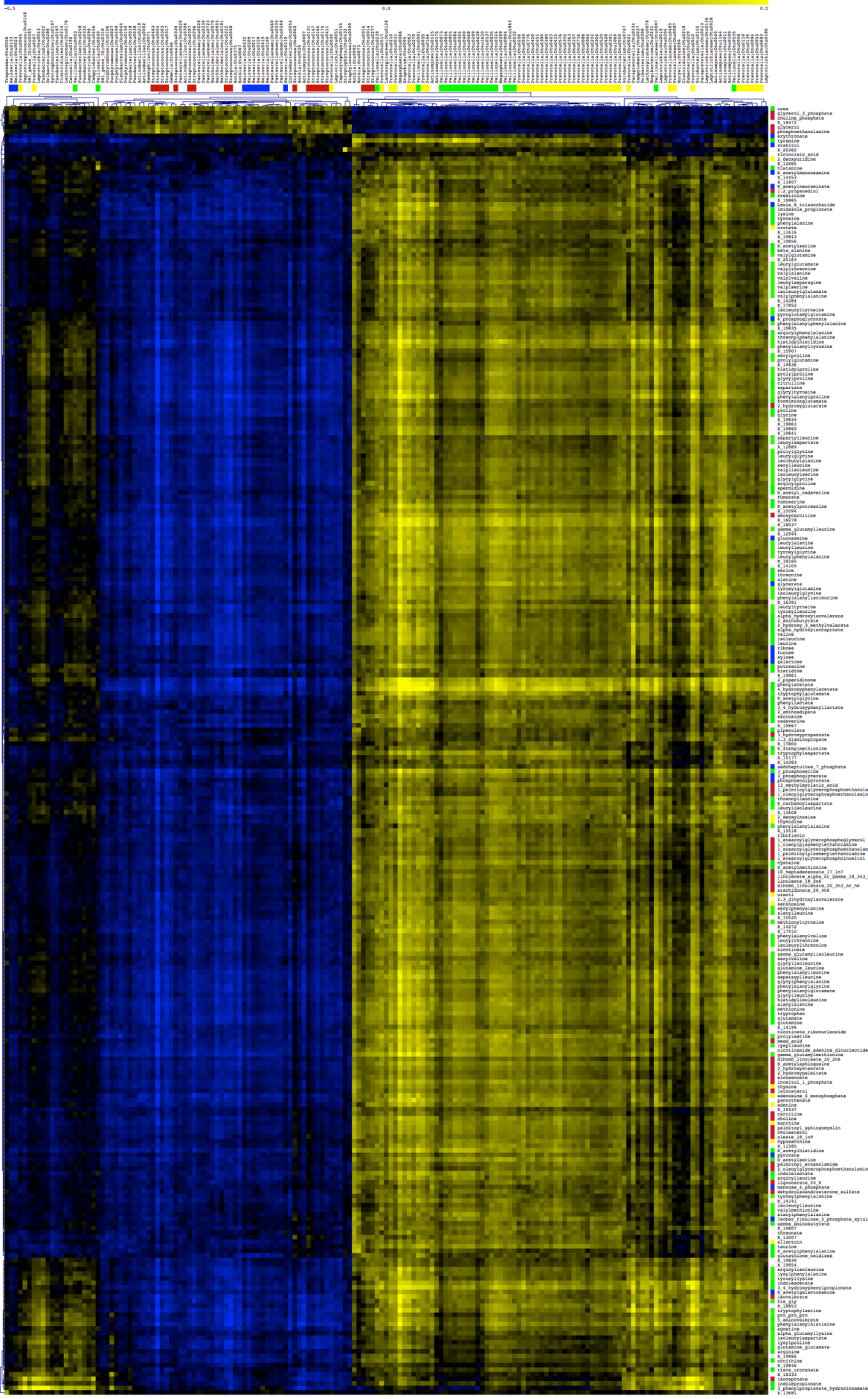
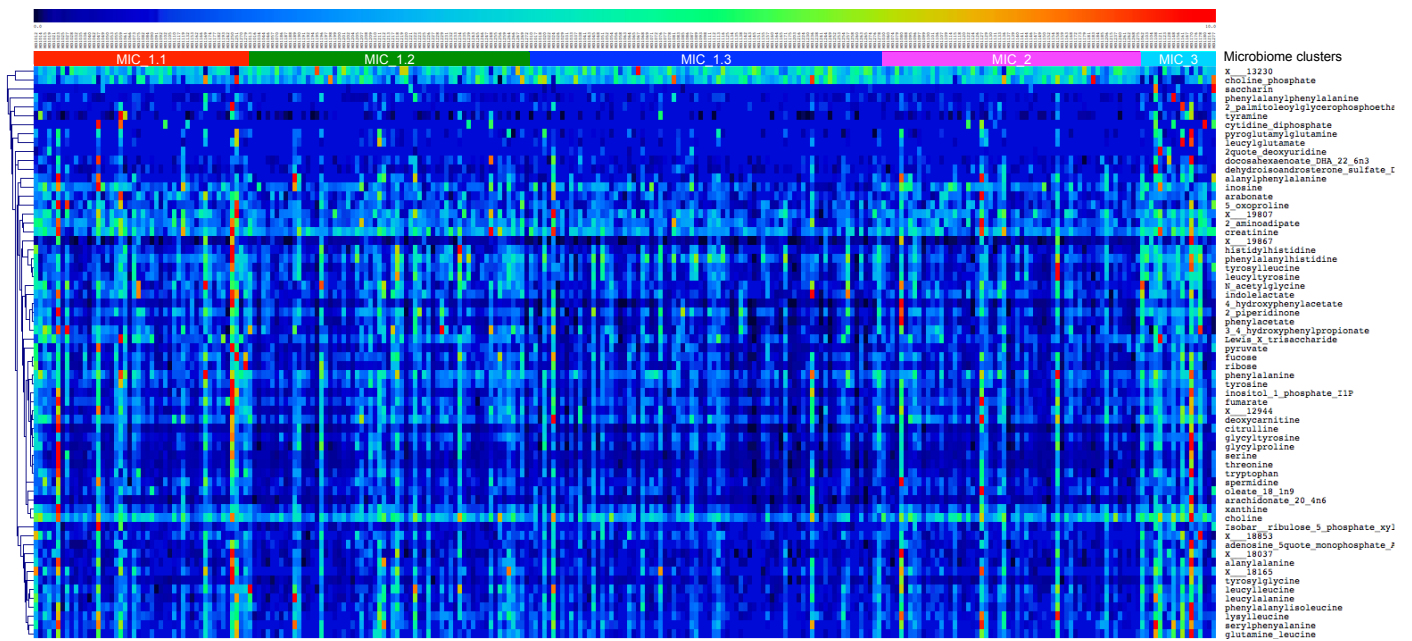


Supplementary Figure S1. Relation between the microbiome and metabolome datasets: Superimposed PCA plots of microbiome and metabolome datasets (Procrustes analysis, $p < 0.0001$, $M^2 = 0.905$): A) labeled by microbiome cluster; B) labeled by metabolome cluster; C) without labels, where grey edges – indicate the microbiome sample; black edges – the metabolome sample.



Supplementary figure S2. Correlations between microbial taxa and metabolites. Average linkage hierarchical clustering. Spearman Rank Correlation matrix of Spearman r values of the significant OTUs (columns) vs significant metabolites (rows). Color scale visualizes r values from low (blue), to zero (black) to high (yellow). OTUs belonging to the same major genera are highlighted in the same color: *Prevotella* – yellow, *Veillonella* – green, *Streptococcus* – red, *Neisseria* – blue. Metabolites belonging to Amino acid and Peptide pathways are highlighted in green, to Carbohydrates – in blue, Lipids – in red and Nucleotides – in yellow.



Supplementary figure S3. Metabolites that significantly discriminated among microbiome sample clusters, using SAM analysis.