

Modelling Longitudinal Metabonomics and Microbiota Interactions in C57BL/6 mice fed a high fat diet

Running title: Longitudinal integration of Metabonomics and Microbiota

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Supporting Information

Supporting Information Available: 5 Supplementary Figures and 2 Supplementary Tables.

Table S1: Summary of model parameters for group comparison

Model / Diet comparison	Factors	R²X	R²Y	Q²Y
LF HF	1+2+0	0.529	0.699	0.644
LF HF_S	1+3+0	0.566	0.568	0.473
HF HF_S	1+1+0	0.442	0.685	0.645
HF HF + GOS	1+2+0	0.533	0.743	0.699
HF HF + BMOS	1+2+0	0.557	0.736	0.689
HF HF + FOS_IN	1+1+0	0.514	0.683	0.656
HF_S HF + BMOS	1+2+0	0.566	0.605	0.524

Table S2: Summary of metabolites associated with body weight with the different feeding models

Model / Metabolites	HF HF_S	HF HF+GOS	HF HF + GOS	HF HF + FOS_IN	HF HF+BMOS	HF_S HF + BMOS
α -keto-methylvalerate	De					
α -ketoisovalerate	De					
Acyl-carnitine		In	In			
Carnitine	In	In	In	In	De	De
Creatine		In	In	In		
Creatinine	In	In	In	In	In	In
Guanidoacetate	In			In		
Hippurate	In			In	In	
Indoxyl-sulfate		In	In	In	In	In
Isobutyrate	De					
Leucine	De					
Nicotinate	In	In	In	In	In	In
Nicotinurate	In	In	In	In	In	In
Oxaloacetate		In	In	In	In	In
Phenylacetylglutamine		In	In	In	In	In
Sucrose		In	In			De
Taurine				De		
Tartarate	In	In	In	In	In	In
TMA					De	De
TMAO					De	De

Key: In, Increase; De, Decrease;

Figure S1: Body weight variations observed with the different nutritional intervention. Data are reported as body weight average at each weekly visit. Key: LF: low fat, HF: high fat, Dx: Visit time in days before or after diet switch (D0).

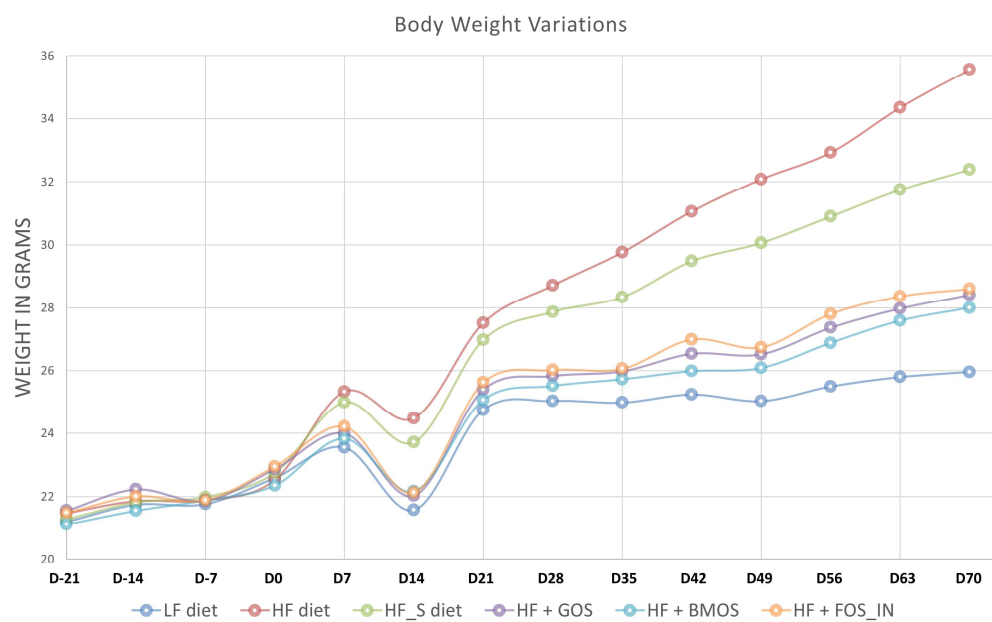


Figure S2: PLS Model comparison for HF|HF_S with HF|HF + prebiotics diets. Metabolite associated variables on the diagonal had similar importance in explaining body weight variance in the two models. A threshold value of 0.2 was applied to select the most influential variables. This selection corresponds mostly to values of VIP for the variable on any of both models ≥ 1.0 .

Figure S1

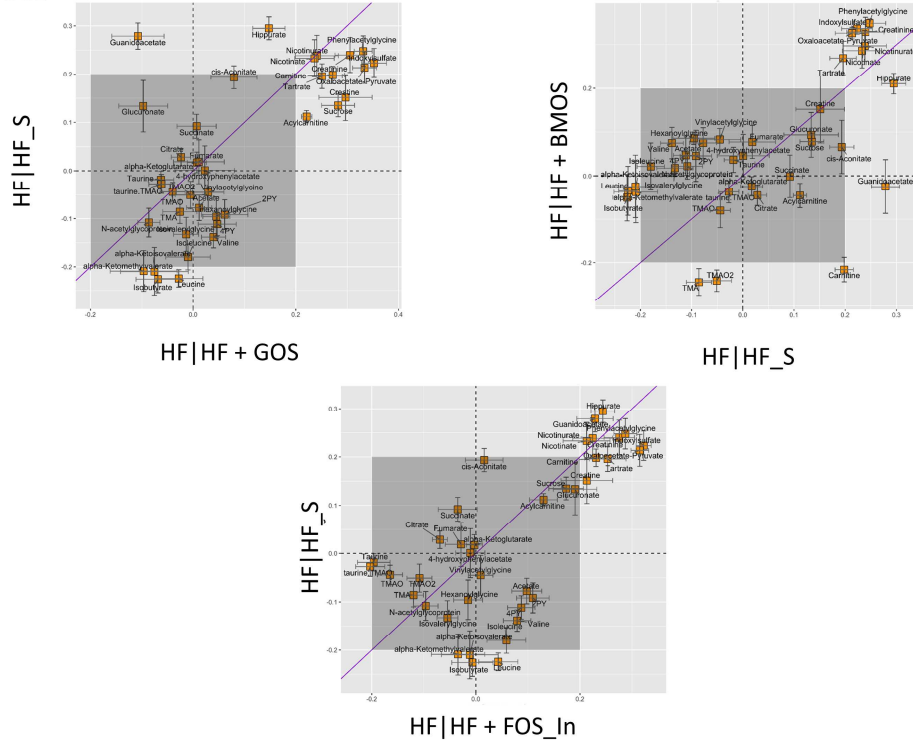


Figure S4: PLS Model comparison for HF|HF + BMOS with HF_S|HF + BMOS, and HF|HF + BMOS with HF|HF + FOS_IN. Metabolite associated variables on the diagonal had similar importance in explaining body weight variance in the two models. A threshold value of 0.2 was applied to select the most influential variables. This selection corresponds mostly to values of VIP for the variable on any of both models ≥ 1.0 .

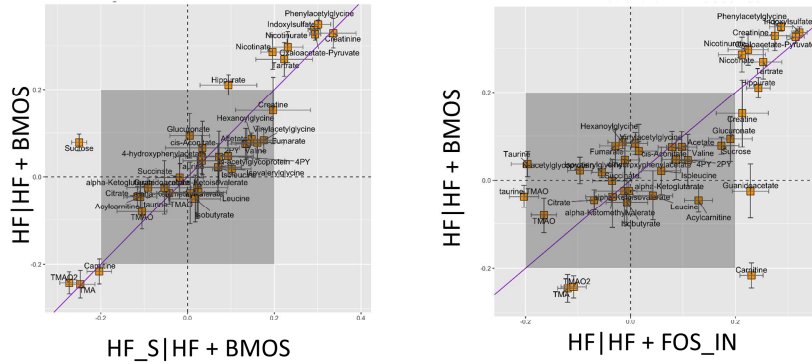


Figure S5: Curves of number of variables (A metabolites and B microbiota species) for increasing similarity score thresholds. No single pair of variables have high similarity score thresholds for at least one of the groups (>0.7) and the lowest similarity score for all variables is 0.2, below which all the variables are selected for at least one dietary group. The blue vertical lines depict the thresholds chosen which give a reasonable number of variables to visually inspect and compare via heatmaps.

