



Supplementary Figure 1 Combined urinary spectra from young adults born prematurely. Overlay of all acquired urinary spectroscopic data including closer view of spectral regions containing alcohol peaks.

	Comparison of Nutritional Groups			Correlation of Metabolic Data with Clinical Data		
	(1) PTF vs. (BBM+TF)	(2) PTF vs. TF	(3) PTF vs. BBM	Birth weight	Birth weight z score	Gestational age
Combined						
R ² Y	0.25	0.31	0.25	0.49	0.24	0.30
Q ² Y	-0.19	-0.24	-0.26	-0.18	-0.22	-0.13
Male						
R ² Y	0.38	0.43	0.39	0.73	0.36	0.44
Q ² Y	-0.28	-0.26	-0.25	-0.10	-0.20	-0.22
Female						
R ² Y	0.28	0.45	0.33	0.66	0.39	0.45
Q ² Y	-0.23	-0.28	-0.12	-0.15	-0.18	-0.18

Supplementary Table 1 Re-modelled O-PLS-DA R²Y and Q²Y values for dietary group comparison and correlation of metabolic data with clinical data (modelled sex-specifically and combined) following removal of spectral regions corresponding to alcohol and exclusion of outlier samples identified in the initial PCA (n=178).