

Supplementary Materials

A) Baseline data

Pearson Correlation (*r*)

	Age	BMI	Energy kcal	Protein	Fat	Carbohydrates	Fibers	Sugars	Sucrose	Starch	Alcohol	Monosaccharides	Disaccharides	Saturated fat	Monounsaturated fat	Polysaturated fat	Total IBS-SSS	Abdominal pain	Diarrhea	Constipation	Bloating and flatulence	Vomiting and nausea	Psychological well-being	Intestinal symptoms influence on daily life
Age	0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
BMI	0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Energy kcal	-0.1	-0.1	0.65	0.87	0.82	0.51	0.38	0.43	0.62	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Protein	-0.1	-0.1	0.65	0.54	0.36	0.25	0.1	0.1	0.40	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Fat	-0.1	-0.1	0.87	0.54	0.49	0.33	0.2	0.22	0.38	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Carbohydrates	-0.1	-0.1	0.82	0.36	0.49	0.51	0.58	0.63	0.70	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Fibers	-0.1	-0.1	0.51	0.25	0.33	0.51	0.23	0.1	0.40	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Sugars	-0.1	-0.1	0.38	0.1	0.2	0.58	0.23	0.70	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Sucrose	-0.1	-0.1	0.43	0.1	0.22	0.63	0.1	0.70	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Starch	-0.1	-0.1	0.62	0.40	0.38	0.70	0.40	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Alcohol	-0.1	-0.1	0.2	0.1	0	0	0.2	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Monosaccharides	-0.1	-0.1	0.35	0.1	0.1	0.51	0.52	0.46	0.2	0.22	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Disaccharides	-0.1	-0.1	0.52	0.1	0.30	0.70	0.2	0.72	0.92	0.22	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Saturated fat	-0.1	-0.1	0.80	0.5	0.91	0.47	0.2	0.18	0.24	0.37	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Monounsaturated fat	-0.1	-0.1	0.80	0.5	0.94	0.43	0.3	0.14	0.20	0.29	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Polysaturated fat	-0.1	-0.1	0.64	0.4	0.73	0.35	0.4	0.12	0.11	0.30	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Total IBS-SSS	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Abdominal pain	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Diarrhea	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Constipation	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Bloating and flatulence	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Vomiting and nausea	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Psychological well-being	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Intestinal symptoms influence on daily life	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1

B) 4-weeks data

Pearson Correlation (*r*)

	Age	BMI	Energy kcal	Protein	Fat	Carbohydrates	Fibers	Sugars	Sucrose	Starch	Alcohol	Monosaccharides	Disaccharides	Saturated fat	Monounsaturated fat	Polysaturated fat	Total IBS-SSS	Abdominal pain	Diarrhea	Constipation	Bloating and flatulence	Vomiting and nausea	Psychological well-being	Intestinal symptoms influence on daily life
Age	0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
BMI	0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Energy kcal	-0.1	-0.1	0.52	0.83	0.57	0.54	0.48	0.39	0.2	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Protein	-0.1	-0.1	0.52	0.42	0.2	0.22	0.1	0.1	0.2	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Fat	-0.1	-0.1	0.83	0.42	0.1	0.29	0.26	0.2	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Carbohydrates	-0.1	-0.1	0.57	0.1	0.1	0.56	0.55	0.52	0.61	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Fibers	-0.1	-0.1	0.54	0.22	0.29	0.56	0.37	0.2	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Sugars	-0.1	-0.1	0.48	0.1	0.26	0.55	0.37	0.73	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Sucrose	-0.1	-0.1	0.39	0.1	0.2	0.52	0.2	0.73	0.28	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Starch	-0.1	-0.1	0.2	-0.2	0.1	0.61	0.1	0.1	0.28	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Alcohol	-0.1	-0.1	0.1	0.1	-0.1	-0.2	-0.1	0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Monosaccharides	-0.1	-0.1	0.35	0.21	0.2	0.28	0.44	0.65	0.30	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Disaccharides	-0.1	-0.1	0.46	-0.2	0.22	0.59	0.32	0.74	0.83	0.35	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Saturated fat	-0.1	-0.1	0.7	0.3	0.8	0	-0.2	0.2	0.2	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Monounsaturated fat	-0.1	-0.1	0.7	0.4	0.9	0	0.3	0.2	0.2	-0.1	-0.1	0.2	0.2	0.6	0.5	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Polysaturated fat	-0.1	-0.1	0.6	0.5	0.6	0.1	0.5	0.1	-0.1	-0.1	-0.1	0.3	-0.2	0.5	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Total IBS-SSS	-0.1	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2
Abdominal pain	-0.1	-0.1	-0.2	-0.1	-0.1	-0.1	-0.2	0.2	0.1	-0.1	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2
Diarrhea	-0.1	-0.1	-0.2	-0.1	-0.1	-0.2	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2	-0.1	-0.2
Constipation	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Bloating and flatulence	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Vomiting and nausea	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Psychological well-being	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
Intestinal symptoms influence on daily life	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1

C) Paired data

Paired data																									
Pearson Correlation (<i>r</i>)																									
	Age	BMI	Energy kcal	Protein	Fat	Carbohydrates	Fibers	Sugars	Sucrose	Starch	Alcohol	Monosaccharides	Disaccharides	Saturated fat	Monounsaturated fat	Polysaturated fat	Total IBS-SSS	Abdominal pain	Diarrhea	Constipation	Bloating and flatulence	Vomiting and nausea	Psychological well-being	Intestinal symptoms ...	
Food diaries (AIVO)	Age																								
	BMI	-0										-0.3	0.1	-0	-0.1	-0.1	0.29	0.23	0.1	0.27	0.24	0.23	0.1	0.24	
	Energy kcal	-0	0.50								0.2	0.2	0.47	0.6	0.7	0.5	0.21	0.1	0.21	0.1	0.2	0	0	0.21	
	Protein	0.1	0.50	0.34							0.1	0.2	0.2	0.3	0.2	0.2	0	0	0.1	0.1	0.1	0	0	0.23	-0.1
	Fat	-0	0.77	0.34	0.1						0	0.2	0.8	0.9	0.5	0.1	0	0	0	0	0	-0.1	-0.1	0.22	0.22
	Carbohydrates	0.1	0.57	0.1	0.1	0.36					0	0.2	0.56	0	0.1	0.1	0.30	0.21	0.28	0.1	0.22	0.1	0.1	0.22	0.22
	Fibers	-0.31	0.31	0.2	0.1	0.36	0.38				0.2	0.47	0.26	0.2	0.2	0.2	-0.1	0.2	0.1	0	0	0	-0.1	-0	0
	Sugars	-0.39	0.1	0.1	0.57	0.38	0.58	0.2			0	0.52	0.67	0.1	0.1	0.28	0.21	0.1	0.1	0	0	0	0	0	0
	Sucrose	0.1	0.42	0.1	0.41	0.2	0.58	0.23	0.1		0	0.70	0.2	0	0.2	0.2	0.2	0.2	0.1	0.1	0	0	0	0	0.2
	Starch	0.23	0.2	-0	0.59	0.2	0.2	0.23	0.1	0.1	-0.1	0.40	-0.2	-0.2	-0.1	0.2	0.1	0.27	0	0.25	0	0.1	0	0	0
	Alcohol	0.1	0.2	0.1	0.1	-0	-0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
	Monosaccharides	-0.3	0.1	0.2	0	0.47	0.52	0.1	-0.1	0.1	0.1	0.22	0.1	-0	-0.1	0.2	0.1	0.36	0.2	0.38	0.25	0.2	0.1	0.33	0.33
	Disaccharides	0.1	0.47	0.2	0.56	0.26	0.67	0.70	0.42	0.1	0.22	0.2	0.1	0	0	0	0	0.36	0.2	0.38	0.25	0.2	0.1	0.33	0.33
	Saturated fat	-0	0.6	0.3	0.8	0	0	0	0	0	0.1	0.2	0.2	0.1	0.5	0.1	0.2	0	0	0	-0.1	-0.1	-0.1	-0.1	-0.1
	Monounsaturated fat	-0.1	0.7	0.2	0.9	0.1	0.2	0.1	0.2	-0.2	0.1	0	0.1	0.5	0.6	0.6	0	0	0.1	0	0	-0.1	-0.1	-0.1	-0.2
Polysaturated fat	-0.1	0.5	0.2	0.5	0.1	0.2	0	-0.1	0.1	-0	-0	0.1	0.6	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	
Questionnaire (VAS-IBS)	Total IBS-SSS	0.29	0.21	0.1	0.30	-0.1	0.28	0.2	0.2	0.1	0.36	0.2	0	-0.1	0	0	0.74	0.38	0.35	0.63	0.32	0	0.71	0.57	
	Abdominal pain	0.23	0.1	-0	0.21	0	0.21	0.1	-0.1	-0.1	0.2	0.2	0	-0.1	0	0	0.74	0.38	0.35	0.63	0.32	0	0.71	0.57	
	Diarrhea	0.1	0.21	0.1	0.28	0.2	0.27	0.1	0.38	0.1	0.38	0.1	0	-0.1	0.38	0.24	0.33	0.47	0.31	0.36	0.2	0.31	0.35	0.31	
	Constipation	0.27	0.1	0.1	0.1	0.1	0.1	0.1	-0.1	-0.2	-0	-0	-0	-0	0.35	0.33	0.1	0.36	0.2	0.2	0.2	0.1	0.35	0.35	
	Bloating and flatulence	0.24	0.2	0.1	0.22	0	0.1	0.25	0.1	0.25	0.1	0.25	0.1	0.1	0.63	0.47	0.36	0.2	0.1	0.1	0.1	0.1	0.52	0.52	
	Vomiting and nausea	0.23	0	0	-0.1	0.1	0	0.1	0	-0.1	-0.2	-0.1	-0.1	-0.1	0.32	0.31	0.2	0.2	0.1	0.1	0.1	0.1	0.52	0.52	
	Psychological well-being	0.1	0	0.23	0.1	0.1	0	0	0.1	0.1	0	0.1	-0.1	-0.1	0	0	0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	
	Intestinal symptoms influence on daily life	0.24	0.21	-0.1	0.22	0.22	-0	0.2	0.2	0.1	-0	0.33	0.2	0.2	0	0.71	0.57	0.31	0.2	0.52	0.35	0.1	0.52	0.52	

baseline data, B) 4-week data, and C) paired data. Significance level $\alpha = .05$. Significant correlations are denoted by bold text and borders. Blue-red colors according to the Pearson correlation coefficient (r), blue color denotes negative correlations and red color denotes positive correlations.

Supplementary Table 1. Metabolomics modeling against food diaries, questionnaire, and clinical data. Orthogonal partial least squares (OPLS) (1+1) models regressing the metabolomics data (n=91, k=322) against each one of the food diaries (AIVO), questionnaires (IBS-SSS, VAS-IBS), and clinical data (age, BMI) descriptors (n=91, k=24). The paired data was calculated as the relative individual change between the baseline data and the 4-week data. The CV-ANOVA p-values refer to OPLS model statistics. Significance levels $\alpha = .05$ (*), $\alpha = .01$ (**), $\alpha = .001$ (***) was used. The OPLS p1-loadings were reported for the metabolic feature with maximum corresponding predictive VIP value. In addition, the maximum absolute correlation (Pearson, r) was reported.

OPLS (1+1) Model	(X=322 metabolic features, N=91)	R2X(cum)	R2Y(cum)	Q2(cum)	p (CV-ANOVA)	Max. VIP (pred.) Metabolite	p-loadings	Max. Correlation Metabolite	Pearson (r)	
Baseline data - Age		0.233	0.685	0.454	1.01E-10	(***)	Inositol, Myo-	0.123	L-Palmitoylcarnitine	0.564
Baseline data - BMI		0.219	0.609	0.209	2.71E-05	(***)	LysoPC(19:0/0:0)	-0.175	Uric acid	0.496
Baseline data - Energy kcal		0.213	0.547	-0.11	1	ns.	Cholic acid	0.181	Deoxycholic acid	0.402
Baseline data - Protein		0.22	0.488	-0.189	1	ns.	Valine	0.175	Tiglylcarnitine	0.363
Baseline data - Fat		0.207	0.522	-0.203	1	ns.	Deoxycholic acid	0.227	Deoxycholic acid	0.479
Baseline data - Carbohydrates		0.215	0.523	-0.133	1	ns.	LysoPC(12:0/0:0)	0.166	Dodecanoic acid	0.322
Baseline data - Fibers		0.192	0.539	0.0385	0.492	ns.	2,4-Dihydroxybenzoic acid	0.228	Dodecanedioic acid	0.399
Baseline data - Sugars		0.226	0.415	-0.104	1	ns.	Palmitoleic acid	0.204	Palmitoleic acid	0.314
Baseline data - Sucrose		0.219	0.413	-0.358	1	ns.	Myristic acid	0.204	Phenylalanylglutamic acid	0.290
Baseline data - Starch		0.227	0.447	-0.239	1	ns.	Octadecenoic acid,-9-(z)-	-0.176	LysoPC(0:0/15:0)	0.328
Baseline data - Alcohol		0.207	0.466	0.0356	0.406	ns.	Inositol, Scyllo-	0.192	3-indolepropionic acid	0.472
Baseline data - Monosaccharides		0.218	0.465	-0.0571	1	ns.	LysoPC(0:0/19:0)	0.165	Tetradecanedioic acid	0.303
Baseline data - Disaccharides		0.215	0.463	-0.356	1	ns.	Myristic acid	0.218	Deoxycholic acid	0.273
Baseline data - Saturated fat		0.212	0.576	-0.0981	1	ns.	Cholic acid	0.250	Deoxycholic acid	0.577
Baseline data - Monounsaturated fat		0.103	0.536	-0.25	1	ns.	Deoxycholic acid	0.220	Deoxycholic acid	0.338
Baseline data - Polyunsaturated fat		0.217	0.425	-0.404	1	ns.	Xanthine	0.182	Xanthine	0.301
Baseline data - Total IBS-SSS		0.134	0.65	-0.0797	1	ns.	Citric acid	-0.236	Citric acid	-0.405
Baseline data - Abdominal pain		0.202	0.519	-0.203	1	ns.	Phenylalanine	-0.176	Homocitrulline	-0.339
Baseline data - Diarrhea		0.106	0.571	-0.0444	1	ns.	Citric acid	-0.223	Citric acid	-0.377
Baseline data - Constipation		0.219	0.478	0.114	0.0320	(*)	2-Hydroxymyristoylcarnitine	-0.176	Propionylcarnitine	-0.380
Baseline data - Bloating and flatulence		0.227	0.362	-0.227	1	ns.	LysoPC(20:2(11Z,14Z)/0:0)	0.159	Docosatetraenoylcarnitine	-0.292
Baseline data - Vomiting and nausea		0.214	0.489	-0.351	1	ns.	Adenosine	0.187	Tartaric acid	0.323

Baseline data - Psychological well-being	0.224	0.437	-0.155	1	ns.	Cytidine	0.159	Cytidine	0.339
Baseline data - Intestinal symptoms influence on daily life	0.191	0.441	-0.258	1	ns.	LysoPC(18:1(9Z)/0:0)	0.200	Tyrosine	-0.293

OPLS (1+1) Model	(X=322 metabolic features, N=91)	R2X(cum)	R2Y(cum)	Q2(cum)	p (CV-ANOVA)	Max. VIP (pred.) Metabolite	p-loadings	Max. Correlation Metabolite	Pearson (r)
4-weeks data - Age		0.228	0.665	0.412	2.19E-09 (***)	gamma-Glutamyltyrosine	0.133	Ornithine	0.571
4-weeks data - BMI		0.167	0.705	0.323	7.58E-07 (***)	L-Glutamic acid	0.199	Glucose	0.495
4-weeks data - Energy kcal		0.229	0.365	-0.251	1 ns.	Oleoylcarnitine	-0.217	Octadecenoic acid,-9-(z)-	-0.275
4-weeks data - Protein		0.213	0.443	-0.015	1 ns.	Valine	0.225	Valine	0.334
4-weeks data - Fat		0.21	0.506	-0.217	1 ns.	12-Hydroxystearic acid	0.189	12-Hydroxystearic acid	0.330
4-weeks data - Carbohydrates		0.15	0.447	-0.0405	1 ns.	LysoPC(0:0/14:0)	0.147	3-Hydroxybutyric acid	-0.380
4-weeks data - Fibers		0.175	0.463	-0.0374	1 ns.	2,4-Dihydroxybenzoic acid	0.199	2,4-Dihydroxybenzoic acid	0.359
4-weeks data - Sugars		0.212	0.393	-0.374	1 ns.	Valine	-0.171	L-threonic acid	0.267
4-weeks data - Sucrose		0.139	0.424	-0.236	1 ns.	Valine	-0.214	L-threonic acid	0.318
4-weeks data - Starch		0.166	0.575	0.149	0.00726 (**)	3-Hydroxydodecanoic acid	-0.144	4-Guanidinobutanoic acid	0.403
4-weeks data - Alcohol		0.206	0.457	-0.258	1 ns.	Palmitoleic acid	-0.213	Malic acid	0.314
4-weeks data - Monosaccharides		0.225	0.417	-0.414	1 ns.	Xanthine	0.224	Xanthine	0.422
4-weeks data - Disaccharides		0.142	0.412	-0.253	1 ns.	Cervonylcarnitine	-0.161	2-Hydroxymyristoylcarnitine	-0.276
4-weeks data - Saturated fat		0.215	0.572	-0.312	1 ns.	2-amino-adipic acid	0.179	Isoleucyl-Leucine	0.394
4-weeks data - Monounsaturated fat		0.212	0.484	-0.15	1 ns.	LysoPE(O-16:0/0:0)	0.201	LysoPE(P-16:0/0:0)	0.360
4-weeks data - Polyunsaturated fat		0.216	0.504	0.106	0.0468462 (*)	LysoPE(O-16:0/0:0)	0.205	LysoPE(O-16:0/0:0)	0.378
4-weeks data - Total IBS-SSS		0.21	0.466	-0.0215	1 ns.	LysoPC(20:0/0:0)	0.181	Propionylcarnitine	-0.302
4-weeks data - Abdominal pain		0.216	0.453	-0.0831	1 ns.	Propionylcarnitine	-0.177	Adipic acid	-0.309
4-weeks data - Diarrhea		0.21	0.466	-0.192	1 ns.	Myristoleic acid	0.201	Abietic acid	0.273
4-weeks data - Constipation		0.191	0.467	0.0945	0.071 ns.	2-Hydroxymyristoylcarnitine	-0.179	2-Hydroxy-lauroylcarnitine	-0.412
4-weeks data - Bloating and flatulence		0.141	0.525	0.0765	0.140 ns.	3-Hydroxyisovaleric acid	-0.172	Eicosanedioic acid	0.397
4-weeks data - Vomiting and nausea		0.216	0.516	-0.0514	1 ns.	Eicosatetraenoic acid, 5,8,11,14-(z,z,z,z,-)	-0.192	Sulfolithocholyglycine	-0.328
4-weeks data - Psychological well-being		0.208	0.473	-0.161	1 ns.	2-Hydroxy-lauroylcarnitine	-0.231	2-Hydroxy-lauroylcarnitine	-0.273

4-weeks data - Intestinal symptoms influence on daily life	0.143	0.525	0.0304	0.478	ns.	LysoPC(20:0/0:0)	0.173	2-Hydroxy-lauroylcarnitine	-0.358
OPLS (1+1) Model	(X=322 metabolic features, N=91)	R2X(cum)	R2Y(cum)	Q2(cum)	p (CV-ANOVA)	Max. VIP (pred.) Metabolite	p-loadings	Max. Correlation Metabolite	Pearson (r)
Paired data - BMI		0.195	0.623	0.15	0.00749073 (**)	3-Hydroxybutyric acid	-0.147	Cholic acid	0.652
Paired data - Energy kcal		0.172	0.571	-0.488	1	ns.	Progesterone	Glyceric acid	0.352
Paired data - Protein		0.108	0.588	-0.154	1	ns.	Sebacic acid	Glycoursodeoxycholic acid	0.325
Paired data - Fat		0.177	0.514	-0.376	1	ns.	LysoPC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	LysoPC(20:0/0:0)	0.305
Paired data - Carbohydrates		0.186	0.541	-0.0833	1	ns.	2-amino-adipic acid	Niacinamide	0.401
Paired data - Fibers		0.149	0.517	-0.164	1	ns.	gamma-Glutamyltryptophan	Pimelic acid	0.329
Paired data - Sugars		0.175	0.563	-0.584	1	ns.	Xanthine	Glucose	0.275
Paired data - Sucrose		0.179	0.592	-0.269	1	ns.	Methylmalonylcarnitine	Ribitol	0.391
Paired data - Starch		0.207	0.489	-0.0235	1	ns.	Valine	LysoPC(0:0/20:3)	0.431
Paired data - Alcohol		0.176	0.566	-0.202	1	ns.	Taurodeoxycholic acid	Lithocholic acid glycine conjugate	-0.376
Paired data - Monosaccharides		0.186	0.621	-0.00088	1	ns.	Butyrylcarnitine	4-Pyridoxic acid	0.582
Paired data - Disaccharides		0.177	0.59	-0.244	1	ns.	Progesterone	4-Hydroxybenzoic acid	0.285
Paired data - Saturated fat		0.172	0.519	-0.478	1	ns.	2-Hydroxycaproic acid	Isoleucyl-Leucine	0.284
Paired data - Monounsaturated fat		0.178	0.561	-0.327	1	ns.	LysoPC(20:0/0:0)	LysoPC(20:0/0:0)	0.375
Paired data - Polyunsaturated fat		0.096	0.626	-0.0851	1	ns.	LysoPE(20:4(5Z,8Z,11Z,14Z)/0:0)	LysoPE(20:4(5Z,8Z,11Z,14Z)/0:0)	-0.313
Paired data - Total IBS-SSS		0.143	0.568	0.0564	0.293	ns.	Progesterone	Sinigrin	0.401
Paired data - Abdominal pain		0.144	0.524	-0.127	1	ns.	Progesterone	Sinigrin	0.459
Paired data - Diarrhea		0.139	0.59	-0.118	1	ns.	4-Hydroxybenzoic acid	4-Hydroxybenzoic acid	0.510
Paired data - Constipation		0.202	0.438	-0.0369	1	ns.	Valine	Urea	-0.351
Paired data - Bloating and flatulence		0.145	0.564	0.00921	0.938	ns.	delta-Hexanolactone	delta-Hexanolactone	-0.370
Paired data - Vomiting and nausea		0.185	0.393	-0.432	1	ns.	Propionylcarnitine	beta-Alanine	0.333
Paired data - Psychological well-being		0.154	0.617	-0.103	1	ns.	Ibuprofen	Ibuprofen	0.741
Paired data - Intestinal symptoms influence on daily life		0.185	0.618	0.0658	0.207	ns.	delta-Hexanolactone	Sinigrin	0.487

Supplementary Table 2. Statistically significant metabolic features linking the Metaboanalyst pathway enrichment and Small Molecule Pathway Database (SMPDB) output with the Human Metabolome Database (HMDB) descriptions [26,27,39]. In total, 105 unique metabolic features were found significantly different between the intervention group and the control group, for the 4-week data and/or the paired data.

Annotated Metabolic features	Analysis	HMDB ID	KEGG ID	Baseline (T0)	Four weeks (T1)	Paired (1+(T1-T0)/T0)	MetaboAnalyst SMPDB pathway association	Pathway	HMDB description nutrient	HMDB description food sources
Dodecanoylcarnitine	LCMS (+)	HMDB000225 0		*	***	***				
Linoleic acid	LCMS (-), GCMS	HMDB000067 3	C01595	ns	***	***	Alpha Linolenic Acid and Linoleic Acid Metabolism	SMP0001 8	omega-6 fatty acid, PUFA essential	plant glyco- sides
Docosapentaenoic acid (22n-3)	LCMS (-)	HMDB000652 8	C16513	ns	***	***	Alpha Linolenic Acid and Linoleic Acid Metabolism	SMP0001 8	omega-3 fatty acid essential	fish oils
Docosahexaenoic acid	GCMS, LCMS (-))	HMDB000218 3	C06429	ns	***	***	Alpha Linolenic Acid and Linoleic Acid Metabolism	SMP0001 8	omega-3 fatty acid	fish oils
Palmitic acid	LCMS (-), GCMS	HMDB000022 0	C00249	ns	***	***	Fatty Acid Biosynthesis	SMP0045 6	saturated fatty acid	palm fruit
3-Hydroxybutyric acid	LCMS (-), GCMS	HMDB000001 1	C01089	ns	***	***	Fatty Acid Biosynthesis	SMP0045 6	ketone body	
(R)-3-Hydroxy-hexadecanoic acid	LCMS (-)	HMDB001073 4		ns	***	***	Fatty Acid Biosynthesis	SMP0045 6	saturated fatty acid	
trans-2-Dodecenoylcarnitine	LCMS (+)	HMDB001332 6		ns	***	***				cow milk macadamia
Palmitoleic acid	GCMS, LCMS (-))	HMDB000322 9	C08362	ns	***	***			monounsaturated fatty acid	oil, sea buck- thorn oil

Oleic acid	LCMS (-)	7	C00712	ns	***	***	monounsaturated fatty acid	olive oil, almond oil
Myristoleoylcarnitine	LCMS (+)	8		ns	***	***		
Myristoleic acid	LCMS (-)	0	C08322	ns	***	***	monounsaturated fatty acid	cow milk, sunflowers, dates
Octadecenoic acid,-9-(z)-	GCMS	3	C01712	ns	***	***	monounsaturated fatty acid	hydrogenated vegetable oils, milk
Eicoseneoylcarnitine	LCMS (+)			ns	***	***		
alpha-Dimorphecolic acid	LCMS (-)	0	C14767	ns	***	***	endogenous fatty acid	
3-Hydroxydodecanoic acid	LCMS (-)	7		ns	***	***	saturated fatty acid	
3-Hydroxycapric acid	LCMS (-)	3		ns	***	***	saturated fatty acid	
3, 5-Tetradecadiencarnitine	LCMS (+)	1		ns	***	***		
2-Hydroxymyristoylcarnitine	LCMS (+)	6		ns	***	***		
2-Hydroxymyristic acid	LCMS (-)	1		ns	***	***		
2-Hydroxylauroylcarnitine	LCMS (+)	4		ns	***	***		
Aconitic acid, cis-	GCMS	2	C00417	ns	**	***		

SMP0005

7

Citric Acid Cycle

Hexose	GCMS	HMDB000012					Transfer of Acetyl Groups	SMP0046	
		2	C00221	ns	**	***	into Mitochondria	6	
Oleoylcarnitine	LCMS (+) GCMS, LCMS (-)	HMDB000506							
		5		ns	**	***			
Citric acid		HMDB000009					Transfer of Acetyl Groups	SMP0046	citrus fruits
		4	C00158	ns	**	***	into Mitochondria	6	
2-amino-adipic acid	GCMS	HMDB000051							
		0	C00956	ns	**	***			
L-Acetylcarnitine	LCMS (+)	HMDB000020					Beta Oxidation of Very	SMP0005	
		1	C02571	ns	*	***	Long Chain Fatty Acids	2	
Urea	GCMS	HMDB000029						SMP0005	
		4	C00086	ns	*	***	Urea Cycle	9	
Decanoylcarnitine	LCMS (+)	HMDB000065							
		1		ns	*	***			
9-Hexadecenoylcarnitine	LCMS (+)	HMDB001320							
		7		ns	*	***			
9,12-Hexadecadienoylcarnitine	LCMS (+)	HMDB001333							
		4		ns	*	***			
1,5-anhydro-d-glucitol	GCMS	HMDB000271							derived mainly from food animal and vegetable fats and oils
		2	C07326	ns	*	***			
Octadecanoic acid	GCMS	HMDB000082					Mitochondrial Beta-Oxidation of Long Chain Saturated FA's	SMP0048	saturated fatty acid
		7	C01530	ns	*	***		2	
L-Octanoylcarnitine	LCMS (+)	HMDB000079					Mitochondrial Beta-Oxidation of Short Chain Saturated FA's	SMP0048	
		1	C02838	ns	ns	***		2	

		HMDB000236							
Tiglylcarnitine	LCMS (+)	6		ns	ns	***			
		HMDB000067							saturated fatty acid
Hexadecanedioic acid	LCMS (-)	2	C19615	ns	ns	***			acid
		HMDB001037							omega-9 fatty acid, PUFA
5,8,11-Eicosatrienoic acid	LCMS (-)	8		ns	ns	***			
		HMDB000055							
3-Methylglutaryl carnitine	LCMS (+)	2		ns	ns	***			
		HMDB002914							
N-gamma-Glutamylglutamine	LCMS (+)	7		ns	ns	***			
									coconut oil, palm kernel oil
	LCMS (-),	HMDB000063					Beta Oxidation of Very	SMP0005	saturated fatty acid
Dodecanoic acid	GCMS	8	C02679	ns	ns	***	Long Chain Fatty Acids	2	acid
		HMDB000079							saturated fatty acid
Sebacic acid	LCMS (-)	2	C08277	ns	ns	***			acid
		HMDB000085							saturated fatty acid
Pimelic acid	LCMS (-)	7	C02656	ns	ns	***			acid
		HMDB000068							
Isovaleryl carnitine	LCMS (+)	8		ns	ns	***			
		HMDB000073							
Isobutyryl-L-carnitine	LCMS (+)	6		ns	ns	***			
		HMDB000062							saturated fatty acid
Dodecanedioic acid	LCMS (-)	3	C02678	ns	ns	***			acid
		HMDB000045							
delta-Hexanolactone	LCMS (-)	3		ns	ns	***			
		HMDB006118							
3-Hydroxyisovaleryl carnitine	LCMS (+)	9		ns	ns	***			

		HMDB000183						
Progesterone	LCMS (+)	0	C00410	*	***	**		steroid hormone
		HMDB001039						
LysoPC(20:3(8Z,11Z,14Z)/0:0)	LCMS (+)	4	C04230	ns	***	**		
							Glycerophospholipid me-	SMP0003
LysoPC(0:0/20:3)	LCMS (+)		C04230	ns	***	**	tabolism	9
		HMDB001312						
Valerylcarnitine	LCMS (+)	8		ns	**	**		cow milk
		HMDB000071						
Hydroxyoctanoic acid	LCMS (-)	1		ns	**	**		
							Mitochondrial Beta-Oxida-	
		HMDB000084					tion of Long Chain Satu-	SMP0048
Stearoylcarnitine	LCMS (+)	8		ns	**	**	rated FA's	2
	LCMS (-),	HMDB000104					Alpha Linolenic Acid and	SMP0001
Arachidonic acid	GCMS	3	C00219	ns	**	**	Linoleic Acid Metabolism	8
								essential fatty acid, PUFA
		HMDB006170						edible vege-
12-Hydroxystearic acid	LCMS (-)	6		ns	*	**		table oils
								(canola oil,
		HMDB000624						castor oil)
gamma-Glutamylalanine	LCMS (+)	8	C03740	ns	*	**	Glutathione Metabolism	SMP0001
								5
		HMDB000008						SMP0004
Cytidine	LCMS (-)	9	C00475	ns	*	**	Pyrimidine Metabolism	6
		HMDB000506						
Tetradecanoylcarnitine	LCMS (+)	6		ns	*	**		
		HMDB000482						
N2,N2-Dimethylguanosine	LCMS (+)	4		ns	*	**		

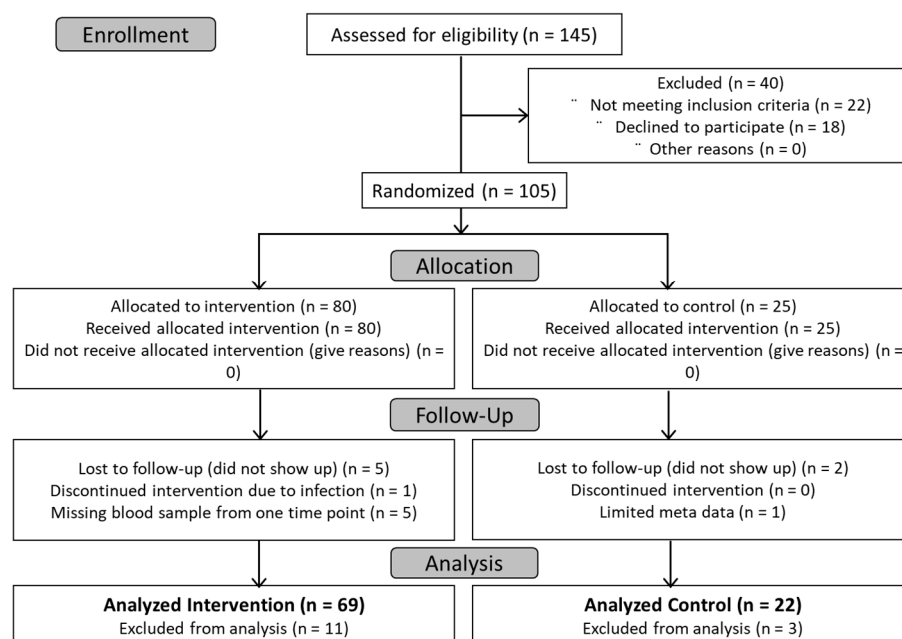
		HMDB001332								
2-Octenoylcarnitine	LCMS (+)	4		ns	ns	**				
		HMDB024058								
cis-4-Decenoylcarnitine	LCMS (+)	5		ns	ns	**				
	LCMS (-),	HMDB000015					Transfer of Acetyl Groups	SMP0046		apples,
Malic acid	GCMS	6	C00149	ns	ns	**	into Mitochondria	6		grapes
		HMDB000075								
Hexanoylcarnitine	LCMS (+)	6		ns	ns	**				
		HMDB003407								black mus-
Sinigrin	LCMS (-)	0	C08427	ns	ns	**				tard, cab-
		HMDB001039								bage, Brus-
LysoPC(20:4(5Z,8Z,11Z,14Z)/0:0)	LCMS (+)	5	C04230	ns	ns	**				sels sprouts
	LCMS (-),	HMDB000080								
Myristic acid	GCMS	6	C06424	ns	***	*	Fatty Acid Biosynthesis	SMP0045	saturated fatty	animal and
	LCMS (+),	HMDB000185						6	acid	vegetable
Acetaminophen	GCMS	9	C06804	ns	**	*				fats
		HMDB001037					Arachidonic Acid Metabo-	SMP0007		drug, pain-
LysoPC(14:0/0:0)	LCMS (+)	9	C04230	ns	**	*	lism	5		killer
		HMDB000088								
Valine	GCMS	3	C00183	ns	**	*			essential amino	
									acids	
LysoPC(0:0/14:0)	LCMS (+)		C04230	ns	**	*	Glycerophospholipid me-	SMP0003		
		HMDB009465					tabolism	9		
Pyroglutamylvaline	LCMS (+)	1		ns	*	*				

Glycine	GCMS	3	C00037	ns	*	*	Glutathione Metabolism	SMP0001 5	non-essential amino acid essential	
alpha-Linolenic acid	LCMS (-)	8	C06427	ns	*	*	Alpha Linolenic Acid and Linoleic Acid Metabolism	SMP0001 8	omega-3 fatty acid	vegetable oils, nuts
L-Palmitoylcarnitine	LCMS (+)	2	C02990	ns	*	*	Fatty acid Metabolism	SMP0005 1		
LysoPC(20:2(11Z,14Z)/0:0)	LCMS (+)	2	C04230	ns	*	*				
LysoPC(0:0/16:1)	LCMS (+)		C04230	ns	*	*	Glycerophospholipid me- tabolism	SMP0003 9		
LysoPC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/ 0:0)	LCMS (+)	4	C04230	ns	ns	*				
Butyrylcarnitine	LCMS (+)	3	C02862	ns	ns	*				
Pyroglutamic acid	GCMS	7	C01879	ns	ns	*	Glutathione Metabolism	SMP0001 5		urinebi- omarker for cheese con- sumption
Cervonylcarnitine	LCMS (+)	0		ns	ns	*				
Eicosapentaenoic acid	LCMS (-)	9	C06428	ns	ns	*	Alpha Linolenic Acid and Linoleic Acid Metabolism	SMP0001 8	important PUFA	fish oils
Abietic acid	LCMS (-)			ns	ns	*				
3-Hydroxyisovaleric acid	LCMS (-)	4		ns	ns	*				prolonged consumption

												of raw egg-whites fish, red meat, beans, dairy products
L-Glutamine	LCMS (+)	1	C00064	ns	ns	*	Urea Cycle	SMP0005 9	non-essential amino acid			
2-Oxovaleric acid	LCMS (-)	5	C06255	ns	ns	*						
Uracil	LCMS (+)	0	C00106	ns	ns	*	Pyrimidine Metabolism	SMP0004 6				
Succinylcarnitine	LCMS (+)	7		ns	ns	*						
Hippuric acid	LCMS (-)	4	C01586	ns	ns	*						tea, wine, fruit juices
Inositol, scyllo-	GCMS	8	C06153	ns	ns	*						coconut palm
3-Hydroxybutyrylcarnitine	LCMS (+)	7		ns	ns	*						
Caprylic acid	LCMS (-)	2	C06423	**	***	ns	Beta Oxidation of Very Long Chain Fatty Acids	SMP0005 2	saturated fatty acid			coconuts additive and gelling agent in jello or gelatins
Adipic acid	GCMS	8	C06104	*	**	ns						
Chenodeoxycholic acid glycine conjugate	LCMS (-)	7	C05466	ns	**	ns	Bile Acid Biosynthesis	SMP0003 5				

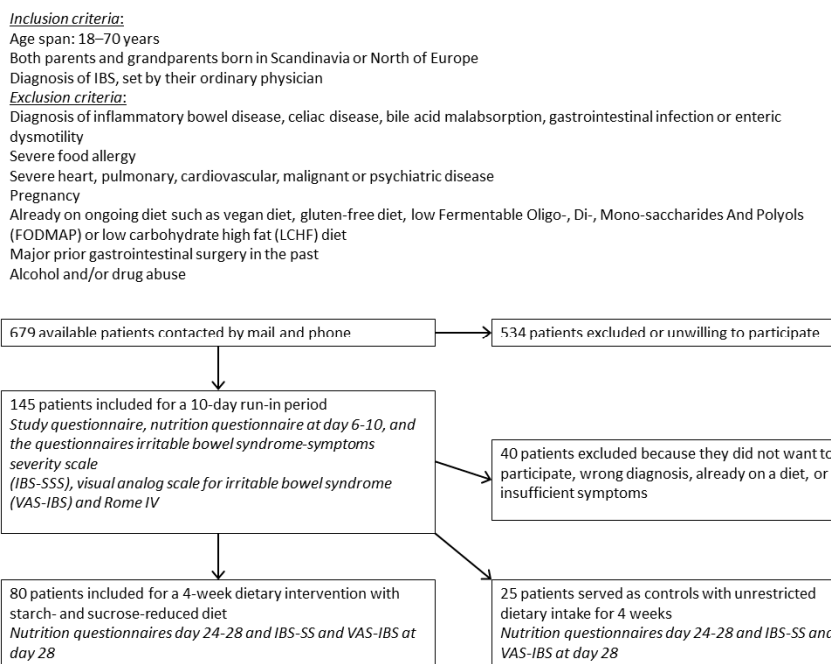
		HMDB000019						SMP0005	
Inosine	LCMS (-)	5	C00294	ns	**	ns	Purine Metabolism	0	
Eicosanedioic acid	LCMS (-)			ns	**	ns			
		HMDB000070							
Glycoursodeoxycholic acid	LCMS (-)	8		ns	*	ns			
		HMDB000025					Starch and Sucrose Metab-	SMP0005	
Sucrose	GCMS	8	C00089	ns	*	ns	olism	8	sugarcane,
Eicosadieneoylcarnitine	LCMS (+)			ns	*	ns			sugar beet
		HMDB000646							
Linoleylcarnitine	LCMS (+)	9		ns	*	ns			
		HMDB001038							
LysoPC(18:3(9Z,12Z,15Z)/0:0)	LCMS (+)	8	C04230	ns	*	ns			
		HMDB000282							
Theobromine	LCMS (+)	5	C07480	ns	*	ns			cacao bean
		HMDB000013							
Guanosine	LCMS (+)	3	C00387	ns	*	ns	Purine Metabolism	0	leeks, gar-
		HMDB000066					Starch and Sucrose Metab-	SMP0005	lic, black-
Fructose	GCMS	0	C02336	ns	*	ns	olism	8	eyed peas
		HMDB001038							honey, tree
LysoPC(16:1(9Z)/0:0)	LCMS (+)	3	C04230	ns	*	ns			fruits, ber-
									ries
LysoPC(0:0/15:0)	LCMS (+)		C04230	ns	*	ns	Glycerophospholipid me-	SMP0003	
							tabolism	9	

CONSORT 2010 Flow Diagram



Supplementary Figure 2. CONSORT 2010 Flow Diagram.

Flow chart over inclusion and exclusion criteria



Supplementary Figure 3. Flow chart over inclusion and exclusion criteria.

Supplementary Table 3. Recommendations for berries, fruit, legumes, and vegetable intake according to starch- and sucrose-reduced diet (SSRD). The dietary recommendations were downloaded from www.sucroseintolerance.com/choosing-your-foods/ [22]. *excess intake can cause bloating/flatulence in all individuals.

Berries and fruits

Well tolerated

Avocado
Blackberries
Blueberries
Boysenberries
Cherries
Cranberries
Currants
Figs
Gooseberries
Grapes
Kiwi fruits
Lemons
Limes
Loganberries
Olives
Papayas
Pears
Pomegranates
Prunes
Raspberries
Rhubarbs
Strawberries

Tolerated by some

Persimmons
Plums
Raisins
Watermelon

Not tolerated

Apples
Apricots
Bananas
Cantaloupe
Dates
Grapefruits
Guava
Honeydew melon
Mangos
Nectarines
Oranges
Passion fruits
Peaches
Pineapples
Tangelos
Tangerines

Vegetables and legumes

Well tolerated

Alfafa sprouts
Artichokes*
Arugulas
Asparagus*
Bamboo shoots
Bok choy
Broccoli*
Brussels sprouts*
Cabbages*
Cauliflower*

Tolerated by some

Edamame soybeans
Jicamas
Leeks
Okra
Pumpkins
Snow peas
Tempeh
Tofu
Yellow wax beans

Not tolerated

Beets
Black beans
Black-eyed peas
Butternut
Carrots
Cassavas
Chickpeas
Corn
Garlic
Green peas

Celery
Chard
Chicories
Chives
Collard greens
Cress
Cucumbers
Eggplants
Endive
Green beans
Kale
Lettuces
Mung bean sprout
Mushrooms
Mustard green
Peppers
Radishes
Spaghetti squash
Spinach
Tomatoes
Turnips
Yellow squash
Zucchini

Lentils
Kidney beans
Lima beans
Navy beans
Onion
Parsnips
Pinto beans
Potatoes
Soybeans
Split peas
Sweet potatoes
Yams