

Supplementary materials

for

Changes in Serum Metabolome Following Low-Energy Diet-Induced Weight Loss in Women with Overweight and Prediabetes: A PREVIEW-New Zealand Sub-Study

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Table S1 - Observed ¹H and ¹³C NMR chemical shifts (d) for quantified metabolites (referenced to DSS at 0.00 ppm) in pooled serum samples.

Metabolite	¹ H chemical shift (ppm)	¹³ C chemical shift (ppm)
2-Hydroxybutyrate	0.88	11.3
	1.66	29.8
	1.70	29.3
	3.99	76.2
3-Hydroxybutyrate	1.19	24.5
	2.30	49.2
	2.39	49.3
	4.14	68.5
Acetate	1.91	25.9
Acetone	2.22	32.9
Alanine	1.46	19.1

	3.76	53.4
Betaine	3.25	54.9
	3.89	68.8
Carnitine	2.42	45.6
	3.22	56.7
	3.44	73.1
	4.55	66.4
Choline	3.19 ¹	56.6 ¹
	3.51	70.3
	4.07	58.8
Creatine	3.02	39.7
	3.92	56.6
Creatinine	3.03	33.0
	4.05	59.1
Dimethyl sulfone	3.14	– ²
Dimethylamine	2.70	36.9
Ethanol	1.17	19.6
	3.64	60.3
Formate	8.44	
Glycerol	3.56	65.3
	3.64	65.3
	3.78	74.9
Histidine	3.04	31.5
	3.18	31.6
	3.90	57.8
	7.01	120.8
	7.72	139.2
Isobutyrate	1.07	21.8
	2.38	39.9
Isoleucine	0.92	13.8
	1.00	17.3
	1.24	27.2
	1.46	27.2
	1.95	38.8
	3.64	62.5
Lactate	1.31	22.8
	4.10	71.8
Leucine	0.94	23.7
	0.95	24.8
	1.66	42.8
	1.67	37.6
	1.70	42.8
	3.70	56.4
Lysine	1.43	23.9
	1.48	23.9
	1.70	29.3
	1.86	33.2
	3.02	42.1
	3.68	57.3
Mannose (α + β)³	3.36	78.8
	3.57	69.7

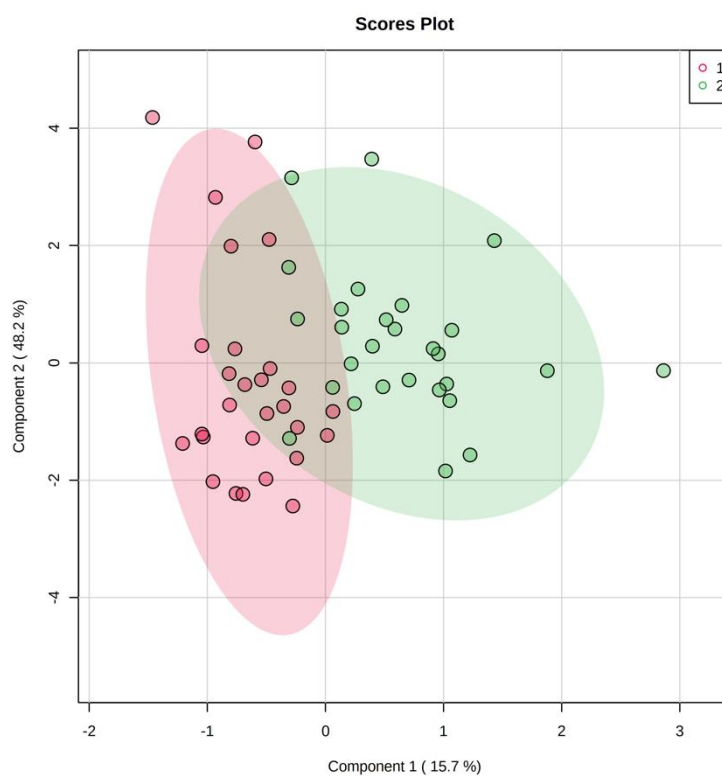
	3.65	69.7
	3.76	59.5
	3.84	73.1
	3.88	59.3
	3.91	59.0
	3.92	73.6
	5.17	96.8
Methanol	3.35	51.7
Methionine	2.10	18.0
	2.16	32.4
	2.62	31.6
	3.78	56.9
Methylamine	2.60	27.0
O-Acetylcarnitine	2.13	23.3
	2.51	43.1
	2.60	43.0
	3.18 ¹	56.5 ¹
	3.58	71.0
	3.85	71.4
	5.59	69.9
O-Phosphocholine	3.21	56.0
	3.58	68.7
	4.16	61.0
Phenylalanine	3.08	38.9
	3.23	39.0
	3.91	59.1
	7.31	132.1
	7.35	130.3
	7.41	131.8
Pyruvate	2.36	29.3
Threonine	1.30	22.1
	3.54	64.4
	4.19	69.4
Trimethylamine N-oxide	3.25	62.3
Tryptophan	3.28	29.1
	3.45	29.3
	4.00	58.0
	7.20	122.2
	7.27	124.8
	7.30	128.0
	7.53	114.8
	7.72	121.2
Tyrosine	3.00	38.4
	3.15	38.9
	3.88	59.3
	6.86	118.7
	7.17	133.5
Valine	0.97	19.3
	1.02	20.7
	2.25	32.0
	3.57	63.4

¹Cross peaks from choline and *O*-acetylcarnitine overlap.

²No cross peak was detected in the HSQC.

³Not all cross peaks for the α and β forms of mannose were detected. For instance, the cross peak from the anomeric proton in β -mannose was obscured by the large water peak.

(a)



(b)

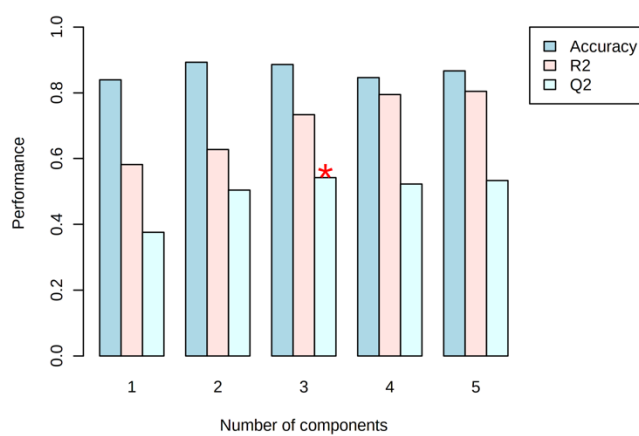


Figure S1 - (a) Scores Plot of PLS-DA of all paired samples and (b) results of cross validation. Red symbols - CD1, Green symbols - CD2