

Supplementary Table 1: Metabolites found at significantly different levels in children who became obese by age 3-5

Major Metabolic Pathway	Metabolite	Odds Ratio	p-value
Amino acid	glycine	1.56	0.0668
	serine	1.42	0.0884
	beta-alanine	1.42	0.0739
	glutamate	1.82	0.0487
	N-acetyltyrosine	0.74	0.0735
	kynurenamate	0.73	0.0292
	tryptophan	0.92	0.0584
	indolepropionate	0.5	0.0169
	cysteine	1.24	0.0605
	S-methylcysteine	1.26	0.0787
	cystine	1.49	0.0112
	N-acetylmethionine	0.87	0.074
	2-hydroxybutyrate (AHB)	0.76	0.0518
	ornithine	1.71	0.0573
	2-aminobutyrate	0.83	0.0576
Peptide	pro-hydroxy-pro	0.89	0.0596
	gamma-glutamylvaline	0.88	0.0514
Carbohydrate	mannitol	0.4	0.0617
	3-phosphoglycerate	1.43	0.041
	arabinose	1.12	0.0869
Energy	citrate	1.15	0.0893
Lipid	linoleate (18:2n6)	1.39	0.0491
	linolenate [alpha or gamma; (18:3n3 or 6)]	1.47	0.0602
	pelargonate (9:0)	0.83	0.0474
	caprate (10:0)	1.33	0.0205
	laurate (12:0)	1.64	0.0064
	myristate (14:0)	1.32	0.0508
	palmitate (16:0)	1.22	0.0315
	10-heptadecenoate (17:1n7)	1.56	0.0634
	stearate (18:0)	1.16	0.0454
	oleate (18:1n9)	1.53	0.0428

	10-nonadecenoate (19:1n9)	1.57	0.0686
	eicosenoate (20:1n9 or 11)	1.51	0.0682
	3-hydroxydecanoate	1.31	0.0677
	2-hydroxypalmitate	1.14	0.0228
	2-aminoctanoate	0.83	0.0905
	Carnitine	1.11	0.087
	Acetylcarnitine	1.2	0.0737
	hexanoylcarnitine	1.24	0.0559
	octanoylcarnitine	1.35	0.0568
	decanoylcarnitine	1.31	0.0295
	Lauroylcarnitine	1.45	0.0454
	Oleoylcarnitine	1.4	0.0149
	glycochenodeoxycholate	1.49	0.0217
	Ethanolamine	2.1	0.0216
	phosphoethanolamine	1.47	0.0448
	2-oleylglycerophosphoethanolamine*	1.36	0.0463
	5alpha-pregnan-3alpha,20beta-diol disulfate 1*	1.43	0.0624
	pregnenolone sulfate	0.83	0.0877
Cofactors and vitamins	Threonate	0.88	0.0434
	Pantothenate	0.58	0.0534
	pyridoxate	0.59	0.0064
	gamma-tocopherol	1.47	0.0354
Xenobiotics	catechol sulfate	0.56	0.0248
	benzoate	0.85	0.024
	glycolate (hydroxyacetate)	0.88	0.0927
	glycerol 2-phosphate	1.63	0.087
	2-piperidinone	1.38	0.0553
	4-acetaminophen sulfate	2.26	0.0441
	4-acetamidophenol	2.95	0.02
	2-hydroxyacetaminophen sulfate*	3.47	0.0152
	2-methoxyacetaminophen sulfate*	3.49	0.0357
	3-(cystein-S-yl)acetaminophen*	2.11	0.0721
	2-methoxyacetaminophen glucuronide*	2.7	0.0472
	3-(N-acetyl-L-cystein-S-yl) acetaminophen*	2.15	0.0243
	cinnamoylglycine	0.56	0.0012

3,7-dimethylurate	0.31	0.0247
3-methylxanthine	0.42	0.0489

**These values are not adjusted for confounding.