Childhood Obesity Is Associated with Changes in the Serum Metabolite Profile

Simone Wahl[a], Zhonghao Yu[a], Michaela Kleber[b], Paula Singmann[a], Christina Holzapfel[a,c], Ying He[a], Kirstin Mittelstrass[a], Alexey Polonikov[d], Cornelia Prehn[e], Werner Römisch-Margl[f], Jerzy Adamski[e], Karsten Suhre[f], Harald Grallert[a], Thomas Illig[a], Rui Wang-Sattler[a]*, Thomas Reinehr[b]

[a]Research Unit of Molecular Epidemiology, Helmholtz Zentrum München – German Research Center for Environmental Health, Neuherberg, [b]Vestische Kinder- und Jugendklinik Datteln, University of Witten-Herdecke, Datteln, [c]Else Kröner-Fresenius-Center of Nutritional Medicine, Technische Universität München, Freising, Germany, [d]Department of Biology, Medical Genetics and Ecology, Kursk State Medical University, Kursk, Russia, [e]Institute of Experimental Genetics, Genome Analysis Center, [f]Institute of Bioinformatics and Systems Biology, Helmholtz Zentrum München, German Research Center for Environmental Health, Neuherberg, Germany

Supplementary Material

Supplementary Table 1. List of metabolites in the Absolute*IDQ*™ kit p150

Abbreviation	Full biochemical name
Acylcarnitines	
C0	DL-Carnitine
C2	Acetyl-L-carnitine
C3	Propionyl-L-carnitine
C3:1	Propenyl-L-carnitine
C3-DC (C4-OH)[a]	Malonyl-L-carnitine / Hydroxybutyryl-L-carnitine
C3-DC-M (C5-OH)[a]	Methylmalonyl-L-carnitine / Hydroxyvaleryl-L-carnitine
C3-OH	Hydroxypropionyl-L-carnitine
C4	Butyryl-L-carnitine
C4:1	Butenyl-L-carnitine
C4:1-DC (C6)[a]	Fumaryl-L-carnitine / Hexanoyl-L-carnitine
C5	Valeryl-L-carnitine
C5:1	Tiglyl-L-carnitine
C5:1-DC	Glutaconyl-L-carnitine
C5-DC (C6-OH)[a]	Glutaryl-L-carnitine / Hydroxyhexanoyl-L-carnitine
C5-M-DC	Methylglutaryl-L-carnitine
C6:1	Hexenoyl-L-carnitine
C7-DC	Pimelyl-L-carnitine
C8	Octanoyl-L-carnitine
C8:1	Octenoyl-L-carnitine
C9	Nonayl-L-carnitine
C10	Decanoyl-L-carnitine
C10:1	Decenoyl-L-carnitine
C10:2	Decadienyl-L-carnitine
C12	Dodecanoyl-L-carnitine
C12:1	Dodecenoyl-L-carnitine
C12-DC	Dodecanedioyl-L-carnitine
C14	Tetradecanoyl-L-carnitine
C14:1	Tetradecenoyl-L-carnitine
C14:1-OH	Hydroxytetradecenoyl-L-carnitine
C14:2	Tetradecadienyl-L-carnitine
C14:2-OH	Hydroxytetradecadienyl-L-carnitine
C16	Hexadecanoyl-L-carnitine
C16:1	Hexadecenoyl-L-carnitine
C16:1-OH	Hydroxyhexadecenoyl-L-carnitine
C16:2	Hexadecadienyl-L-carnitine
C16:2-OH	Hydroxyhexadecadienyl-L-carnitine
C16-OH	Hydroxyhexadecanoyl-L-carnitine
C18	Octadecanoyl-L-carnitine
C18:1	Octadecenoyl-L-carnitine

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Supplementary Table 1. Continued

Abbreviation	Full biochemical name
Acylcarnitines (continued)	
C18:1-OH	Hydroxyoctadecenoyl-L-carnitine
C18:2	Octadecadienyl-L-carnitine
Amino acids	
Arg	Arginine
Gln	Glutamine
Gly	Glycine
His	Histidine
Met	Methionine
Orn	Ornithine
Phe	Phenylalanine
Pro	Proline
Ser	Serine
Thr	Threonine
Trp	Tryptophan
Tyr	Tyrosine
Val	Valine
xLeu	xLeucine
Diacyl phosphatidylcholines	
PC aa C24:0	Phosphatidylcholine diacyl C24:0
PC aa C26:0	Phosphatidylcholine diacyl C26:0
PC aa C28:1	Phosphatidylcholine diacyl C28:1
PC aa C30:0	Phosphatidylcholine diacyl C30:0
PC aa C30:2	Phosphatidylcholine diacyl C30:2
PC aa C32:0	Phosphatidylcholine diacyl C32:0
PC aa C32:1	Phosphatidylcholine diacyl C32:1
PC aa C32:2	Phosphatidylcholine diacyl C32:2
PC aa C32:3	Phosphatidylcholine diacyl C32:3
PC aa C34:1	Phosphatidylcholine diacyl C34:1
PC aa C34:2	Phosphatidylcholine diacyl C34:2
PC aa C34:3	Phosphatidylcholine diacyl C34:3
PC aa C34:4	Phosphatidylcholine diacyl C34:4
PC aa C36:0	Phosphatidylcholine diacyl C36:0
PC aa C36:1	Phosphatidylcholine diacyl C36:1
PC aa C36:2	Phosphatidylcholine diacyl C36:2
PC aa C36:3	Phosphatidylcholine diacyl C36:3
PC aa C36:4	Phosphatidylcholine diacyl C36:4
PC aa C36:5	Phosphatidylcholine diacyl C36:5
PC aa C36:6	Phosphatidylcholine diacyl C36:6

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Supplementary Table 1. Continued

Abbreviation	Full biochemical name
Diacyl phosphatidylcholines (continued)	
PC aa C38:0	Phosphatidylcholine diacyl C38:0
PC aa C38:1	Phosphatidylcholine diacyl C38:1
PC aa C38:3	Phosphatidylcholine diacyl C38:3
PC aa C38:4	Phosphatidylcholine diacyl C38:4
PC aa C38:5	Phosphatidylcholine diacyl C38:5
PC aa C38:6	Phosphatidylcholine diacyl C38:6
PC aa C40:1	Phosphatidylcholine diacyl C40:1
PC aa C40:2	Phosphatidylcholine diacyl C40:2
PC aa C40:3	Phosphatidylcholine diacyl C40:3
PC aa C40:4	Phosphatidylcholine diacyl C40:4
PC aa C40:5	Phosphatidylcholine diacyl C40:5
PC aa C40:6	Phosphatidylcholine diacyl C40:6
PC aa C42:0	Phosphatidylcholine diacyl C42:0
PC aa C42:1	Phosphatidylcholine diacyl C42:1
PC aa C42:2	Phosphatidylcholine diacyl C42:2
PC aa C42:4	Phosphatidylcholine diacyl C42:4
PC aa C42:5	Phosphatidylcholine diacyl C42:5
PC aa C42:6	Phosphatidylcholine diacyl C42:6
Acyl-alkyl phosphatidylcholines	
PC ae C30:0	Phosphatidylcholine acyl-alkyl C30:0
PC ae C30:1	Phosphatidylcholine acyl-alkyl C30:1
PC ae C30:2	Phosphatidylcholine acyl-alkyl C30:2
PC ae C32:1	Phosphatidylcholine acyl-alkyl C32:1
PC ae C32:2	Phosphatidylcholine acyl-alkyl C32:2
PC ae C34:0	Phosphatidylcholine acyl-alkyl C34:0
PC ae C34:1	Phosphatidylcholine acyl-alkyl C34:1
PC ae C34:2	Phosphatidylcholine acyl-alkyl C34:2
PC ae C34:3	Phosphatidylcholine acyl-alkyl C34:3
PC ae C36:0	Phosphatidylcholine acyl-alkyl C36:0
PC ae C36:1	Phosphatidylcholine acyl-alkyl C36:1
PC ae C36:2	Phosphatidylcholine acyl-alkyl C36:2
PC ae C36:3	Phosphatidylcholine acyl-alkyl C36:3
PC ae C36:4	Phosphatidylcholine acyl-alkyl C36:4
PC ae C36:5	Phosphatidylcholine acyl-alkyl C36:5
PC ae C38:0	Phosphatidylcholine acyl-alkyl C38:0
PC ae C38:1	Phosphatidylcholine acyl-alkyl C38:1
PC ae C38:2	Phosphatidylcholine acyl-alkyl C38:2
PC ae C38:3	Phosphatidylcholine acyl-alkyl C38:3
PC ae C38:4	Phosphatidylcholine acyl-alkyl C38:4

Supplementary Table 1.continued on next page

Supplementary Table 1. Continued

Abbreviation	Full biochemical name
Acyl-alkyl phosphatidylcholines (continued)	
PC ae C38:5	Phosphatidylcholine acyl-alkyl C38:5
PC ae C38:6	Phosphatidylcholine acyl-alkyl C38:6
PC ae C40:0	Phosphatidylcholine acyl-alkyl C40:0
PC ae C40:1	Phosphatidylcholine acyl-alkyl C40:1
PC ae C40:2	Phosphatidylcholine acyl-alkyl C40:2
PC ae C40:3	Phosphatidylcholine acyl-alkyl C40:3
PC ae C40:4	Phosphatidylcholine acyl-alkyl C40:4
PC ae C40:5	Phosphatidylcholine acyl-alkyl C40:5
PC ae C40:6	Phosphatidylcholine acyl-alkyl C40:6
PC ae C42:0	Phosphatidylcholine acyl-alkyl C42:0
PC ae C42:1	Phosphatidylcholine acyl-alkyl C42:1
PC ae C42:2	Phosphatidylcholine acyl-alkyl C42:2
PC ae C42:3	Phosphatidylcholine acyl-alkyl C42:3
PC ae C42:4	Phosphatidylcholine acyl-alkyl C42:4
PC ae C42:5	Phosphatidylcholine acyl-alkyl C42:5
PC ae C44:3	Phosphatidylcholine acyl-alkyl C44:3
PC ae C44:4	Phosphatidylcholine acyl-alkyl C44:4
PC ae C44:5	Phosphatidylcholine acyl-alkyl C44:5
PC ae C44:6	Phosphatidylcholine acyl-alkyl C44:6
Lysophosphatidylcholines	
LPC a C14:0	Lysophosphatidylcholine acyl C14:0
LPC a C16:0	Lysophosphatidylcholine acyl C16:0
LPC a C16:1	Lysophosphatidylcholine acyl C16:1
LPC a C17:0	Lysophosphatidylcholine acyl C17:0
LPC a C18:0	Lysophosphatidylcholine acyl C18:0
LPC a C18:1	Lysophosphatidylcholine acyl C18:1
LPC a C18:2	Lysophosphatidylcholine acyl C18:2
LPC a C20:3	Lysophosphatidylcholine acyl C20:3
LPC a C20:4	Lysophosphatidylcholine acyl C20:4
LPC a C24:0	Lysophosphatidylcholine acyl C24:0
LPC a C26:0	Lysophosphatidylcholine acyl C26:0
LPC a C26:1	Lysophosphatidylcholine acyl C26:1
LPC a C28:0	Lysophosphatidylcholine acyl C28:0
LPC a C28:1	Lysophosphatidylcholine acyl C28:1
LPC a C6:0	Lysophosphatidylcholine acyl C6:0
Sphingomyelins	
SM (OH) C14:1	Hydroxysphingomyelin C14:1
SM (OH) C16:0	Hydroxysphingomyelin C16:0

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Supplementary Table 1. Continued

Abbreviation	Full biochemical name
Sphingomyelins (continued)	
SM (OH) C22:1	Hydroxysphingomyelin C22:1
SM (OH) C22:2	Hydroxysphingomyelin C22:2
SM (OH) C24:1	Hydroxysphingomyelin C24:1
SM C16:0	Sphingomyelin C16:0
SM C16:1	Sphingomyelin C16:1
SM C18:0	Sphingomyelin C18:0
SM C18:1	Sphingomyelin C18:1
SM C20:2	Sphingomyelin C20:2
SM C22:3	Sphingomyelin C22:3
SM C24:0	Sphingomyelin C24:0
SM C24:1	Sphingomyelin C24:1
SM C26:0	Sphingomyelin C26:0
SM C26:1	Sphingomyelin C26:1
Sugars	
H1	Hexose

[a]The analytical technique applied in this study is not capable of differentiating these analytes.

Supplementary Table 2. Comparison of metabolite concentration in obese and normal-weight children

Metabolite[a]	Normal-weight (n = 40)[b]	Obese (n = 80)[b]	Δ Obese – normal-weight[c]	OR (95 % CI)[d]	p value
Acylcarnitines					
C0	35.82 ± 5.62	35.09 ± 8.51	-2.0%	0.83 (0.54, 1.24)	3.8E-01
C2	5.90 ± 2.26	6.80 ± 3.02	15.3%	1.51 (1.00, 2.37)	6.0E-02
C3	0.378 ± 0.09	0.358 ± 0.125	-5.5%	0.75 (0.48, 1.12)	1.8E-01
C3-DC-M (C5-OH)	0.023 ± 0.006	0.023 ± 0.008	1.4%	0.97 (0.65, 1.45)	8.8E-01
C4	0.067 ± 0.015	0.073 ± 0.041	9.0%	0.99 (0.67, 1.48)	9.6E-01
C4:1-DC (C6)	0.053 ± 0.009	0.055 ± 0.021	3.6%	0.98 (0.66, 1.45)	9.0E-01
C5	0.09 ± 0.029	0.093 ± 0.036	2.7%	1.03 (0.70, 1.52)	8.6E-01
C7-DC	0.027 ± 0.012	0.033 ± 0.011	22.8%	2.07 (1.35, 3.31)	1.3E-03
C8	0.121 ± 0.042	0.15 ± 0.055	23.4%	2.27 (1.45, 3.78)	7.5E-04
C8:1	0.101 ± 0.043	0.111 ± 0.061	10.0%	1.08 (0.73, 1.60)	7.1E-01
C9	0.033 ± 0.009	0.031 ± 0.011	-4.5%	0.78 (0.52, 1.15)	2.2E-01
C10	0.193 ± 0.077	0.245 ± 0.093	26.5%	2.18 (1.41, 3.54)	7.8E-04
C10:1	0.128 ± 0.045	0.154 ± 0.046	20.6%	2.07 (1.35, 3.34)	1.5E-03
C10:2	0.045 ± 0.013	0.044 ± 0.011	-3.4%	0.89 (0.60, 1.33)	5.6E-01
C12	0.070 ± 0.029	0.083 ± 0.032	19.3%	1.92 (1.26, 3.07)	3.8E-03
C12:1	0.098 ± 0.031	0.13 ± 0.043	32.3%	3.62 (2.09, 6.98)	2.6E-05
C14	0.040 ± 0.010	0.045 ± 0.016	11.8%	1.40 (0.94, 2.14)	1.1E-01
C14:1	0.110 ± 0.036	0.127 ± 0.045	15.1%	1.63 (1.08, 2.56)	2.5E-02
C14:1-OH	0.011 ± 0.003	0.013 ± 0.004	14.4%	1.61 (1.08, 2.46)	2.2E-02
C14:2	0.023 ± 0.012	0.031 ± 0.014	35.2%	2.34 (1.50, 3.89)	4.3E-04
C16	0.093 ± 0.024	0.099 ± 0.029	6.5%	1.23 (0.84, 1.83)	2.9E-01
C16:1	0.035 ± 0.007	0.043 ± 0.012	20.8%	2.74 (1.64, 4.98)	3.3E-04
C18	0.043 ± 0.010	0.038 ± 0.012	-10.3%	0.64 (0.41, 0.96)	3.5E-02
C18:1	0.093 ± 0.033	0.109 ± 0.038	16.9%	1.86 (1.21, 3.03)	7.8E-03
C18:2	0.034 ± 0.014	0.042 ± 0.016	24.4%	2.02 (1.31, 3.27)	2.3E-03
Amino acids					
Arginine	127.02 ± 26.21	112.92 ± 21.28	-11.1%	0.49 (0.28, 0.78)	5.2E-03
Glutamine	638.62 ± 109.94	509.43 ± 114.91	-20.2%	0.20 (0.09, 0.38)	7.0E-06
Glycine	275.32 ± 76.69	233.9 ± 48.06	-15.0%	0.47 (0.28, 0.74)	2.3E-03
Histidine	103.52 ± 19.19	88.39 ± 19.98	-14.6%	0.37 (0.19, 0.62)	6.9E-04
Methionine	35.09 ± 8.76	27.55 ± 6.81	-21.5%	0.28 (0.15, 0.49)	3.4E-05
Ornithine	61.11 ± 16.64	57.72 ± 16.92	-5.5%	0.77 (0.50, 1.15)	2.1E-01
Phenylalanine	68.78 ± 18.40	63.43 ± 15.92	-7.8%	0.67 (0.41, 1.02)	7.6E-02
Proline	258.91 ± 91.00	180.88 ± 63.23	-30.1%	0.27 (0.14, 0.46)	1.3E-05
Serine	114.69 ± 26.61	97.83 ± 29.46	-14.7%	0.45 (0.26, 0.73)	2.3E-03
Threonine	92.21 ± 25.56	79.15 ± 29.44	-14.2%	0.56 (0.34, 0.86)	1.2E-02
Tryptophan	84.13 ± 12.21	80.39 ± 16.49	-4.4%	0.72 (0.45, 1.10)	1.5E-01
Tyrosine	83.14 ± 20.15	87.12 ± 20.90	4.8%	1.15 (0.78, 1.69)	4.9E-01
Valine	267.72 ± 55.3	262.91 ± 69.01	-1.8%	0.85 (0.55, 1.26)	4.3E-01
xLeucine	234.4 ± 54.86	204.48 ± 52.26	-12.8%	0.48 (0.28, 0.78)	5.4E-03

Supplementary Table 2. Continued

Metabolite[a]	Normal-weight (n = 40)[b]	Obese (n = 80)[b]	Δ Obese – normal-weight[c]	OR (95 % CI)[d]	p value
Diacyl phosphatidylcholines					
PC aa C28:1	2.28 ± 0.72	2.45 ± 0.68	7.3%	1.24 (0.84, 1.85)	2.7E-01
PC aa C30:0	3.45 ± 1.45	3.47 ± 1.28	0.4%	0.99 (0.67, 1.45)	9.5E-01
PC aa C32:0	13.97 ± 3.83	11.54 ± 3.11	-17.4%	0.41 (0.23, 0.66)	8.3E-04
PC aa C32:1	14.01 ± 6.20	16.07 ± 7.35	14.7%	1.24 (0.84, 1.86)	2.7E-01
PC aa C32:2	2.98 ± 1.34	3.51 ± 1.70	17.9%	1.25 (0.85, 1.86)	2.5E-01
PC aa C32:3	0.45 ± 0.16	0.48 ± 0.15	5.9%	1.19 (0.8, 1.76)	3.9E-01
PC aa C34:1	208.33 ± 58.26	189.63 ± 57.04	-9.0%	0.68 (0.42, 1.03)	8.0E-02
PC aa C34:2	370.43 ± 79.87	318.12 ± 85.74	-14.1%	0.46 (0.27, 0.74)	2.6E-03
PC aa C34:3	14.95 ± 4.30	14.66 ± 4.95	-2.0%	0.88 (0.58, 1.3)	5.3E-01
PC aa C34:4	1.39 ± 0.62	1.57 ± 0.62	12.8%	1.35 (0.91, 2.01)	1.3E-01
PC aa C36:0	2.25 ± 0.84	2.25 ± 0.78	-0.1%	0.98 (0.66, 1.45)	9.2E-01
PC aa C36:1	48.17 ± 14.69	43.21 ± 15.01	-10.3%	0.64 (0.4, 0.98)	4.9E-02
PC aa C36:2	245.48 ± 58.36	213.15 ± 63.01	-13.2%	0.53 (0.32, 0.82)	7.6E-03
PC aa C36:3	132.30 ± 34.26	120.33 ± 38.03	-9.0%	0.67 (0.42, 1.02)	7.6E-02
PC aa C36:4	165.61 ± 42.75	148.85 ± 42.60	-10.1%	0.64 (0.4, 0.97)	4.5E-02
PC aa C36:5	14.71 ± 6.58	15.72 ± 7.37	6.8%	1.13 (0.75, 1.69)	5.6E-01
PC aa C36:6	0.60 ± 0.31	0.65 ± 0.27	7.7%	1.25 (0.84, 1.87)	2.7E-01
PC aa C38:0	2.77 ± 0.98	2.44 ± 0.87	-12.0%	0.63 (0.41, 0.94)	2.9E-02
PC aa C38:3	43.48 ± 14.68	49.80 ± 18.21	14.5%	1.35 (0.92, 2.02)	1.3E-01
PC aa C38:4	99.92 ± 30.52	95.89 ± 30.76	-4.0%	0.84 (0.56, 1.24)	4.0E-01
PC aa C38:5	45.53 ± 12.70	44.12 ± 14.78	-3.1%	0.84 (0.55, 1.24)	4.0E-01
PC aa C38:6	61.06 ± 22.90	56.18 ± 21.18	-8.0%	0.75 (0.49, 1.11)	1.5E-01
PC aa C40:2	0.30 ± 0.07	0.30 ± 0.13	-1.4%	0.84 (0.56, 1.23)	3.7E-01
PC aa C40:3	0.55 ± 0.14	0.52 ± 0.17	-4.3%	0.79 (0.52, 1.17)	2.5E-01
PC aa C40:4	3.59 ± 1.00	4.06 ± 1.46	13.1%	1.27 (0.86, 1.89)	2.3E-01
PC aa C40:5	8.58 ± 2.30	10.05 ± 4.04	17.2%	1.33 (0.9, 1.99)	1.6E-01
PC aa C40:6	19.92 ± 8.05	21.74 ± 9.31	9.1%	1.15 (0.78, 1.72)	4.7E-01
PC aa C42:0	0.51 ± 0.20	0.48 ± 0.16	-6.1%	0.86 (0.56, 1.28)	4.7E-01
PC aa C42:1	0.26 ± 0.09	0.25 ± 0.09	-3.9%	0.84 (0.57, 1.24)	3.8E-01
PC aa C42:2	0.18 ± 0.05	0.17 ± 0.07	-7.9%	0.68 (0.44, 1.01)	6.2E-02
PC aa C42:4	0.17 ± 0.04	0.18 ± 0.06	2.8%	0.98 (0.67, 1.45)	9.4E-01
PC aa C42:5	0.37 ± 0.11	0.35 ± 0.13	-4.4%	0.79 (0.52, 1.17)	2.5E-01
Acyl-alkyl phosphatidylcholines					
PC ae C30:0	0.41 ± 0.15	0.40 ± 0.14	-4.2%	0.89 (0.60, 1.30)	5.4E-01
PC ae C30:2	0.13 ± 0.04	0.13 ± 0.05	0.7%	1.00 (0.68, 1.48)	1.0E+00
PC ae C32:1	2.85 ± 0.97	2.44 ± 0.63	-14.6%	0.57 (0.35, 0.88)	1.6E-02
PC ae C32:2	0.68 ± 0.22	0.61 ± 0.17	-9.9%	0.68 (0.44, 1.02)	7.6E-02
PC ae C34:0	1.34 ± 0.47	1.16 ± 0.33	-13.3%	0.60 (0.38, 0.92)	2.4E-02
PC ae C34:1	10.26 ± 3.20	8.26 ± 2.07	-19.5%	0.34 (0.18, 0.59)	3.0E-04
PC ae C34:2	12.70 ± 4.07	9.32 ± 2.69	-26.6%	0.29 (0.15, 0.50)	4.1E-05

Supplementary Table 2. Continued

Metabolite[a]	Normal-weight (n = 40)[b]	Obese (n = 80)[b]	Δ Obese – normal-weight[c]	OR (95 % CI)[d]	p value
Acyl-alkyl phosphatidylcholines (continued)					
PC ae C34:3	9.22 ± 3.31	6.95 ± 2.02	-24.6%	0.39 (0.23, 0.62)	2.3E-04
PC ae C36:0	0.90 ± 0.25	0.82 ± 0.40	-8.6%	0.67 (0.44, 1.00)	5.4E-02
PC ae C36:1	6.36 ± 1.87	5.83 ± 1.76	-8.3%	0.69 (0.44, 1.04)	8.6E-02
PC ae C36:2	13.63 ± 3.69	10.25 ± 2.55	-24.8%	0.24 (0.12, 0.43)	1.1E-05
PC ae C36:3	8.51 ± 2.52	6.61 ± 1.86	-22.2%	0.33 (0.17, 0.56)	2.0E-04
PC ae C36:4	19.65 ± 7.28	16.85 ± 5.39	-14.3%	0.65 (0.41, 0.98)	5.1E-02
PC ae C36:5	11.4 ± 4.50	10.13 ± 3.08	-11.2%	0.77 (0.50, 1.16)	2.3E-01
PC ae C38:0	1.56 ± 0.56	1.56 ± 0.54	-0.4%	0.97 (0.65, 1.44)	8.9E-01
PC ae C38:2	1.96 ± 0.51	1.55 ± 0.48	-21.0%	0.36 (0.20, 0.59)	1.8E-04
PC ae C38:3	3.34 ± 0.90	3.30 ± 0.88	-1.3%	0.92 (0.61, 1.35)	6.6E-01
PC ae C38:4	13.97 ± 3.75	12.05 ± 2.97	-13.7%	0.50 (0.30, 0.79)	5.1E-03
PC ae C38:5	18.51 ± 5.50	15.37 ± 4.28	-17.0%	0.47 (0.28, 0.74)	2.2E-03
PC ae C38:6	6.75 ± 2.53	6.02 ± 1.99	-10.7%	0.69 (0.45, 1.02)	7.1E-02
PC ae C40:1	1.13 ± 0.36	0.95 ± 0.28	-15.9%	0.53 (0.33, 0.82)	7.5E-03
PC ae C40:2	1.38 ± 0.40	1.48 ± 0.43	7.3%	1.19 (0.81, 1.79)	3.8E-01
PC ae C40:3	0.97 ± 0.23	1.00 ± 0.29	3.7%	1.05 (0.71, 1.55)	7.9E-01
PC ae C40:4	2.33 ± 0.61	2.16 ± 0.54	-7.6%	0.68 (0.43, 1.02)	7.2E-02
PC ae C40:5	3.23 ± 0.77	2.93 ± 0.77	-9.2%	0.62 (0.39, 0.94)	3.2E-02
PC ae C40:6	4.21 ± 1.37	3.59 ± 1.04	-14.8%	0.52 (0.32, 0.80)	5.2E-03
PC ae C42:1	0.34 ± 0.08	0.33 ± 0.12	-3.1%	0.84 (0.56, 1.24)	3.8E-01
PC ae C42:2	0.55 ± 0.16	0.54 ± 0.17	-3.1%	0.83 (0.54, 1.22)	3.5E-01
PC ae C42:3	0.64 ± 0.18	0.60 ± 0.18	-5.5%	0.75 (0.49, 1.13)	1.8E-01
PC ae C42:4	0.90 ± 0.30	0.82 ± 0.26	-8.2%	0.72 (0.46, 1.08)	1.3E-01
PC ae C42:5	2.15 ± 0.63	2.00 ± 0.52	-6.7%	0.78 (0.51, 1.17)	2.5E-01
PC ae C44:3	0.11 ± 0.03	0.10 ± 0.04	-3.8%	0.80 (0.53, 1.18)	2.7E-01
PC ae C44:4	0.38 ± 0.13	0.37 ± 0.11	-3.8%	0.89 (0.58, 1.32)	5.7E-01
PC ae C44:5	1.86 ± 0.60	1.71 ± 0.53	-8.2%	0.82 (0.51, 1.23)	3.6E-01
PC ae C44:6	1.19 ± 0.40	1.09 ± 0.35	-8.3%	0.79 (0.51, 1.19)	2.8E-01
Lysophosphatidylcholines					
LPC a C14:0	1.90 ± 0.55	2.53 ± 1.64	32.7%	1.55 (1.02, 2.49)	5.1E-02
LPC a C16:0	64.74 ± 14.40	73.75 ± 22.40	13.9%	1.49 (1.01, 2.28)	5.2E-02
LPC a C16:1	1.99 ± 0.63	2.52 ± 1.05	26.9%	1.99 (1.29, 3.25)	3.4E-03
LPC a C17:0	1.00 ± 0.28	1.01 ± 0.34	1.4%	1.03 (0.70, 1.53)	8.7E-01
LPC a C18:0	18.73 ± 4.68	22.3 ± 6.35	19.1%	1.75 (1.17, 2.72)	9.0E-03
LPC a C18:1	17.13 ± 4.59	12.73 ± 3.96	-25.7%	0.29 (0.15, 0.49)	1.8E-05
LPC a C18:2	36.37 ± 11.44	18.09 ± 5.07	-50.3%	0.05 (0.01, 0.13)	5.7E-08
LPC a C20:3	2.20 ± 0.73	1.79 ± 0.61	-18.8%	0.54 (0.33, 0.83)	8.2E-03
LPC a C20:4	5.82 ± 1.77	4.40 ± 1.21	-24.4%	0.36 (0.20, 0.58)	1.2E-04

Supplementary Table 2. Continued

Metabolite[a]	Normal-weight (n = 40)[b]	Obese (n = 80)[b]	Δ Obese – normal-weight[c]	OR (95 % CI)[d]	p value
Sphingomyelins					
SM (OH) C14:1	4.27 ± 1.17	4.25 ± 1.22	-0.5%	0.91 (0.61, 1.34)	6.3E-01
SM (OH) C16:1	2.42 ± 0.73	2.49 ± 0.69	2.8%	1.04 (0.70, 1.54)	8.3E-01
SM (OH) C22:1	9.27 ± 2.66	10.39 ± 3.01	12.1%	1.44 (0.96, 2.20)	8.1E-02
SM (OH) C22:2	7.93 ± 2.13	8.56 ± 2.36	7.9%	1.23 (0.83, 1.84)	2.9E-01
SM (OH) C24:1	0.90 ± 0.28	1.02 ± 0.34	14.3%	1.48 (0.99, 2.28)	6.4E-02
SM C16:0	89.92 ± 23.88	82.61 ± 22.06	-8.1%	0.66 (0.43, 0.99)	5.1E-02
SM C16:1	11.81 ± 3.07	13.04 ± 3.84	10.4%	1.33 (0.90, 2.01)	1.6E-01
SM C18:0	18.74 ± 6.95	20.05 ± 5.50	7.0%	1.29 (0.87, 1.95)	2.1E-01
SM C18:1	8.75 ± 2.98	9.91 ± 2.97	13.3%	1.49 (1.00, 2.29)	5.7E-02
SM C20:2	0.61 ± 0.21	0.65 ± 0.20	7.3%	1.25 (0.85, 1.86)	2.6E-01
SM C24:0	16.70 ± 5.50	18.55 ± 5.92	11.1%	1.42 (0.95, 2.19)	1.0E-01
SM C24:1	39.90 ± 13.05	40.29 ± 11.69	1.0%	1.03 (0.70, 1.52)	9.0E-01
SM C26:0	0.16 ± 0.06	0.18 ± 0.08	15.2%	1.42 (0.95, 2.18)	9.6E-02
SM C26:1	0.24 ± 0.09	0.27 ± 0.13	9.6%	1.12 (0.76, 1.66)	5.7E-01
Sugars					
Hexose	5366.80 ± 913.55	4652.07 ± 1066.45	-13.3%	0.40 (0.22, 0.66)	9.3E-04

[a]Cx:y, acyl-group with chain length x and y double bonds; PC aa, diacyl phosphatidylcholine; PC ae, acyl-alkyl phosphatidylcholine; LPC a, lysophosphatidylcholine with an acyl chain; SM, sphingomyelin; SM (OH), hydroxysphingomyelin.

[b]All values are mean ± SD of serum metabolite concentration in µmol/l.

[c]Percentage (%) difference in values between obese and normal-weight children.

[d]Odds Ratio (OR) of logistic regression analysis with respective 95 % confidence interval (CI); age, sex and pubertal stage were included as covariates.

Supplementary Table 3. 69 metabolite concentration ratios differing significantly between obese and normal-weight children with a high p gain

Metabolite ratio[a]	OR (95 % CI)[b]	p value	p gain
Lysophosphatidylcholine/lysophosphatidylcholine ratios			
LPC a C16:0 / LPC a C20:3	5.98 (3.30, 12.21)	6.3E-08	1.3E+05
LPC a C18:0 / LPC a C20:3	9.58 (4.52, 24.61)	1.3E-07	6.1E+04
LPC a C16:1 / LPC a C20:3	12.21 (5.38, 35.45)	1.4E-07	2.5E+04
LPC a C16:0 / LPC a C20:4	6.47 (3.45, 13.81)	1.0E-07	1.1E+03
LPC a C18:0 / LPC a C20:4	8.41 (4.12, 20.10)	1.1E-07	1.1E+03
Lysophosphatidylcholine/phosphatidylcholine ratios			
LPC a C18:0 / PC aa C36:2	8.30 (4.15, 19.59)	6.5E-08	1.2E+05
LPC a C18:0 / PC ae C40:1	6.25 (3.32, 13.36)	2.1E-07	3.6E+04
LPC a C18:0 / PC aa C36:1	5.66 (3.08, 11.99)	4.4E-07	2.0E+04
LPC a C18:0 / PC aa C36:3	5.43 (2.97, 11.29)	5.3E-07	1.7E+04
LPC a C18:0 / PC aa C34:2	6.74 (3.49, 15.15)	2.8E-07	9.3E+03
LPC a C16:1 / PC ae C40:1	4.40 (2.55, 8.37)	8.5E-07	4.0E+03
PC aa C38:3 / LPC a C20:3	4.05 (2.34, 7.68)	3.2E-06	2.5E+03
LPC a C16:1 / PC aa C34:2	5.34 (2.88, 11.13)	1.0E-06	2.5E+03
LPC a C16:0 / PC aa C32:0	5.30 (2.95, 10.73)	3.3E-07	2.5E+03
LPC a C18:0 / PC ae C38:4	4.67 (2.61, 9.44)	2.1E-06	2.4E+03
LPC a C18:0 / PC aa C32:0	7.19 (3.63, 16.76)	3.4E-07	2.4E+03
LPC a C16:0 / PC aa C36:2	3.75 (2.24, 6.88)	3.3E-06	2.3E+03
LPC a C16:1 / PC aa C32:0	7.59 (3.75, 18.12)	3.7E-07	2.3E+03
LPC a C18:0 / PC aa C34:1	3.85 (2.27, 7.20)	4.0E-06	2.3E+03
LPC a C16:1 / PC aa C36:2	4.68 (2.62, 9.32)	1.6E-06	2.2E+03
LPC a C18:0 / PC ae C34:0	3.79 (2.25, 7.09)	4.3E-06	2.1E+03
LPC a C16:1 / PC aa C36:3	4.92 (2.70, 10.06)	1.7E-06	2.0E+03
LPC a C16:1 / PC aa C34:1	4.45 (2.53, 8.74)	1.9E-06	1.8E+03
LPC a C16:0 / PC aa C34:2	4.38 (2.51, 8.52)	1.8E-06	1.4E+03
LPC a C16:0 / PC ae C40:1	3.32 (2.05, 5.78)	5.3E-06	1.4E+03
LPC a C18:0 / PC ae C34:1	7.12 (3.65, 16.39)	2.2E-07	1.4E+03
LPC a C18:0 / PC ae C36:3	9.13 (4.35, 23.27)	1.7E-07	1.2E+03
LPC a C18:0 / PC ae C38:2	11.83 (5.20, 33.91)	1.8E-07	1.0E+03
Phosphatidylcholine/phosphatidylcholine ratios			
PC aa C38:3 / PC aa C36:3	7.61 (3.85, 17.50)	1.2E-07	6.6E+05
PC aa C38:3 / PC aa C36:1	4.31 (2.53, 8.11)	7.0E-07	7.0E+04
PC aa C40:6 / PC aa C38:6	4.69 (2.55, 9.75)	5.4E-06	2.8E+04
PC aa C40:5 / PC aa C36:1	4.10 (2.39, 7.78)	2.4E-06	2.1E+04
PC aa C28:1 / PC ae C36:1	3.43 (2.10, 6.09)	5.0E-06	1.7E+04
PC aa C28:1 / PC ae C34:0	4.27 (2.47, 8.18)	1.7E-06	1.4E+04
PC aa C38:3 / PC aa C36:2	4.93 (2.77, 9.87)	7.1E-07	1.1E+04
PC aa C40:4 / PC aa C36:1	3.52 (2.13, 6.31)	4.6E-06	1.1E+04

Supplementary Table 3. Continued

Metabolite ratio[a]	OR (95 % CI)[b]	*p*-value	*p*-gain
Phosphatidylcholine/phosphatidylcholine ratios (continued)			
PC aa C40:4 / PC aa C36:2	4.34 (2.45, 8.57)	3.7E-06	2.0E+03
PC ae C40:2 / PC ae C40:6	3.89 (2.29, 7.29)	3.3E-06	1.5E+03
PC aa C32:3 / PC aa C32:0	4.29 (2.53, 7.99)	5.5E-07	1.5E+03
PC aa C32:3 / PC ae C34:1	7.27 (3.67, 16.79)	2.6E-07	1.2E+03
PC aa C32:3 / PC ae C38:2	6.55 (3.46, 14.31)	1.7E-07	1.1E+03
PC aa C38:3 / PC aa C34:2	4.42 (2.51, 8.69)	2.4E-06	1.1E+03
Sphingomyelin/phosphatidylcholine ratios			
SM (OH) C22:1 / PC ae C38:4	5.13 (2.86, 10.31)	4.8E-07	1.1E+04
SM C24:0 / PC aa C36:2	4.18 (2.44, 7.83)	1.3E-06	6.0E+03
SM C16:1 / PC ae C38:4	5.60 (2.99, 11.95)	8.9E-07	5.7E+03
SM C16:1 / PC ae C32:1	3.72 (2.22, 6.75)	3.2E-06	4.9E+03
SM C16:1 / PC aa C32:0	8.13 (3.99, 19.73)	2.1E-07	4.0E+03
SM C18:1 / PC ae C38:4	5.84 (3.03, 12.99)	1.6E-06	3.2E+03
SM C24:0 / PC ae C38:4	5.36 (2.88, 11.52)	1.7E-06	3.1E+03
SM C16:1 / PC aa C36:2	3.89 (2.31, 7.24)	2.5E-06	3.1E+03
SM C24:0 / PC aa C34:2	4.36 (2.52, 8.27)	1.0E-06	2.5E+03
SM (OH) C22:2 / PC ae C38:4	3.75 (2.25, 6.77)	2.2E-06	2.3E+03
SM C16:1 / PC aa C34:2	4.32 (2.50, 8.31)	1.4E-06	1.9E+03
SM (OH) C22:1 / PC ae C40:6	4.77 (2.62, 9.77)	2.8E-06	1.8E+03
SM (OH) C22:1 / PC aa C34:2	4.05 (2.38, 7.53)	1.6E-06	1.6E+03
SM C18:1 / PC aa C32:0	5.29 (2.92, 10.87)	5.5E-07	1.5E+03
SM (OH) C22:1 / PC aa C36:2	3.63 (2.16, 6.62)	5.3E-06	1.4E+03
SM C18:1 / PC ae C40:6	5.82 (2.95, 13.4)	4.4E-06	1.2E+03
SM (OH) C24:1 / PC ae C40:6	3.90 (2.28, 7.35)	4.6E-06	1.1E+03
SM C24:0 / PC aa C32:0	7.00 (3.48, 16.41)	7.6E-07	1.1E+03
SM (OH) C22:2 / PC ae C40:6	4.14 (2.36, 8.08)	4.9E-06	1.1E+03
Sphingomyelin/sphingomyelin ratios			
SM C16:1 / SM C16:0	10.31 (4.82, 26.68)	6.5E-08	7.9E+05
SM C24:0 / SM C16:0	7.30 (3.71, 16.87)	2.1E-07	2.4E+05
SM C18:1 / SM C16:0	5.77 (3.07, 12.44)	7.2E-07	7.1E+04
SM (OH) C22:1 / SM C16:0	4.85 (2.65, 9.99)	2.7E-06	1.9E+04
Other metabolite ratios			
Acylcarnitine C18:1 / Acylcarnitine C18	5.02 (2.80, 10.18)	7.7E-07	1.0E+04
LPC a C18:0 / Arginine	3.84 (2.27, 7.13)	3.4E-06	1.5E+03
Acylcarnitine C16:1 / PC aa C32:0	5.23 (2.93, 10.48)	2.9E-07	1.1E+03
Valine / xLeucine	4.58 (2.53, 9.47)	5.1E-06	1.1E+03

[a]Cx:y, acyl-group with chain length x and y double bonds; LPC a, lysophosphatidylcholine with acyl chain; PC aa, diacyl phosphatidylcholine; PC ae, acyl-alkyl phosphatidylcholine; SM, sphingomyelin; SM (OH), hydroxysphingomyelin.

[b]Odds Ratio (OR) of logistic regression analysis with respective 95 % confidence interval (CI); age, sex and pubertal stage were included as covariates; only metabolite pairs whose concentration ratios differed significantly after adjustment for multiple testing ($p \leq 6.0E-06$) with a *p*-gain $\geq 1.0E+03$ were included in the table.