

ESM Table 1. Time in bed, according to group, as estimated by ActivPal inclinometer. Values are mean \pm SD. *P* values are from paired t-tests.

Group	5-d high-fat diet	Exercise/no exercise	<i>p</i> value
Control	8.2 \pm 1.4	8.4 \pm 1.3	0.62
EXam	7.7 \pm 1.3	7.3 \pm 1.0	0.20
EXpm	8.3 \pm 0.8	8.9 \pm 1.2	0.22

ESM Table 2. Fasting and postprandial circulating markers of metabolic health and blood pressure before and after five days of high fat diet. Data are observed means \pm SD. *P* values from paired samples t-tests.

	Habitual diet (<i>n</i> =24)	High fat diet (<i>n</i> =24)	<i>p</i> value
Fasting			
Glucose (mmol/l)	4.9 \pm 0.4	4.8 \pm 0.3	0.07
Insulin (pmol/l)	69 \pm 44	71 \pm 47	0.77
HOMA-IR	2.21 \pm 1.5	2.16 \pm 1.6	0.96
Cholesterol (mmol/l)	4.8 \pm 0.8	4.8 \pm 0.8	0.60
Triacylglycerol (mmol/l)	1.54 \pm 0.7	1.25 \pm 0.6	0.03
HDL (mmol/l)	1.04 \pm 0.2	1.05 \pm 0.1	0.63
LDL (mmol/l)	3.0 \pm 0.7	3.2 \pm 0.7	0.049
Systolic blood pressure (mmHg)	130 \pm 9	126 \pm 10	0.06
Diastolic blood pressure (mmHg)	84 \pm 6	82 \pm 5	0.06
Postprandial			
Glucose (mmol/l)	5.1 \pm 1.0	5.1 \pm 0.5	0.92
Insulin (pmol/l)	432 \pm 420	328 \pm 243	0.15
Cholesterol (mmol/l)	4.8 \pm 0.8	5.0 \pm 0.8	0.08
Triacylglycerol (mmol/l)	2.4 \pm 1.2	2.3 \pm 1.0	0.52
HDL (mmol/l)	1.0 \pm 0.2	1.1 \pm 0.1	0.06
LDL (mmol/l)	2.7 \pm 0.8	2.9 \pm 0.7	0.18

ESM Table 3. Metabolites significantly changed in morning samples after 5 d high-fat diet.

	change	<i>p</i> value	<i>q</i> value
(N(1) + N(8))-acetylsermidine	15%	0.0022	0.0090
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)	17%	0.0099	0.0294
1-(1-enyl-palmitoyl)-GPC (P-16:0)	-12%	0.0011	0.0053
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)	29%	<0.0001	<0.0001
1.2-dilinoleoyl-GPC (18:2/18:2)	-20%	<0.0001	0.0003
1.2-dilinoleoyl-GPE (18:2/18:2)	-13%	0.0037	0.0137
1.2-dipalmitoyl-GPE (16:0/16:0)	-29%	0.0006	0.0031
1.3-dimethylurate	38%	0.0098	0.0293
1.5-anhydroglucitol (1.5-AG)	-3%	0.0093	0.0280
1.7-dimethylurate	32%	0.0014	0.0065
10-nonadecenoate (19:1n9)	42%	0.0043	0.0152
10-undecenoate (11:1n1)	48%	0.0040	0.0145
12.13-DiHOME	697%	<0.0001	0.0001
1-arachidonoyl-GPE (20:4n6)	-7%	0.0173	0.0463
1-carboxyethylisoleucine	-38%	<0.0001	0.0001
1-carboxyethylleucine	-13%	0.0147	0.0407
1-carboxyethylphenylalanine	-35%	<0.0001	0.0001
1-carboxyethylvaline	-22%	0.0001	0.0006
1-lignoceroyl-GPC (24:0)	-27%	0.0002	0.0015
1-linolenoyl-GPC (18:3)	-45%	<0.0001	0.0003
1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)	-9%	0.0023	0.0095
1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)	-37%	0.0001	0.0006
1-linoleoyl-GPC (18:2)	-11%	0.0010	0.0046
1-linoleoyl-GPE (18:2)	-24%	0.0007	0.0035
1-linoleoyl-GPI (18:2)	-19%	0.0119	0.0344
1-methylhistidine	-7%	0.0078	0.0246
1-methylurate	-17%	0.0044	0.0153
1-methylxanthine	8%	0.0120	0.0344
1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)	-15%	0.0020	0.0084
1-oleoyl-GPC (18:1)	-12%	0.0002	0.0013
1-oleoyl-GPE (18:1)	-21%	0.0017	0.0076
1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)	65%	0.0014	0.0064
1-palmitoleoyl-GPC (16:1)	-26%	<0.0001	<0.0001
1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)	-27%	0.0007	0.0034
1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	-22%	0.0004	0.0022
1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	-30%	0.0001	0.0008
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	-8%	0.0027	0.0103
1-palmitoyl-2-oleoyl-GPE (16:0/18:1)	-23%	0.0001	0.0008
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)	-28%	<0.0001	0.0003
1-palmitoyl-GPC (16:0)	-15%	0.0001	0.0009
1-palmitoyl-GPE (16:0)	-21%	0.0001	0.0008
1-ribosyl-imidazoleacetate	-23%	0.0007	0.0034
1-stearoyl-2-linoleoyl-GPE (18:0/18:2)	-14%	0.0122	0.0346

1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	-18%	0.0003	0.0019
1-stearoyl-GPC (18:0)	-13%	<0.0001	0.0004
1-stearoyl-GPE (18:0)	-20%	<0.0001	0.0002
2,3-dihydroxy-5-methylthio-4-pentenoate (DMTPA)	-7%	<0.0001	0.0003
2,3-dihydroxyisovalerate	-39%	<0.0001	0.0003
21-hydroxypregnenolone disulfate	12%	0.0168	0.0455
2-acetamidophenol sulfate	-35%	0.0001	0.0006
2-aminoadipate	20%	0.0002	0.0011
2-aminobutyrate	75%	<0.0001	<0.0001
2-aminophenol sulfate	-59%	<0.0001	0.0004
2-hydroxy-3-methylvalerate	14%	0.0128	0.0362
2-hydroxybutyrate/2-hydroxyisobutyrate	93%	<0.0001	<0.0001
2-hydroxyglutarate	-20%	<0.0001	<0.0001
2-linoleoylglycerol (18:2)	-31%	0.0085	0.0263
2-methylbutyrylcarnitine (C5)	40%	<0.0001	<0.0001
2-methylcitrate/homocitrate	39%	<0.0001	0.0001
2-oxoarginine	-25%	<0.0001	0.0001
2-palmitoleoyl-GPC (16:1)	-23%	0.0064	0.0209
3-(3-hydroxyphenyl)propionate	31%	0.0063	0.0206
3-(4-hydroxyphenyl)lactate	-9%	0.0040	0.0144
3,7-dimethylurate	361%	0.0106	0.0314
3-acetylphenol sulfate	600%	0.0088	0.0271
3-aminoisobutyrate	25%	0.0007	0.0036
3-carboxy-4-methyl-5-pentyl-2-furanpropionate (3-CMPFP)	50%	<0.0001	<0.0001
3-hydroxy-2-ethylpropionate	63%	<0.0001	<0.0001
3-hydroxyadipate	180%	0.0020	0.0082
beta-hydroxybutyrate (β OHB)	224%	<0.0001	0.0001
3-hydroxybutyrylglycine	125%	<0.0001	0.0002
3-hydroxybutyrylcarnitine (1)	455%	<0.0001	<0.0001
3-hydroxybutyrylcarnitine (2)	73%	<0.0001	<0.0001
3-hydroxydecanoate	99%	<0.0001	<0.0001
3-hydroxyhexanoate	86%	<0.0001	<0.0001
3-hydroxyhippurate	-36%	0.0024	0.0098
3-hydroxyisobutyrate	60%	0.0002	0.0011
3-hydroxylaurate	95%	<0.0001	<0.0001
3-hydroxyoctanoate	81%	<0.0001	<0.0001
3-hydroxypyridine sulfate	-12%	0.0037	0.0136
3-hydroxysebacate	234%	<0.0001	<0.0001
3-methoxycatechol sulfate (2)	-31%	0.0005	0.0029
3-methyl catechol sulfate (1)	17%	0.0178	0.0474
3-methyl-2-oxobutyrate	19%	0.0004	0.0021
3-methyl-2-oxovalerate	17%	0.0016	0.0071
3-methylglutaconate	15%	0.0022	0.0092
3-methylhistidine	-36%	0.0004	0.0023
3-methylxanthine	271%	0.0174	0.0463

3-ureidopropionate	18%	0.0024	0.0096
4-acetylphenol sulfate	-44%	<0.0001	0.0004
4-allylphenol sulfate	-51%	0.0026	0.0103
4-ethylphenylsulfate	-27%	0.0057	0.0190
4-guanidinobutanoate	-33%	0.0001	0.0005
4-hydroxyhippurate	-27%	0.0018	0.0076
4-hydroxyphenylpyruvate	-17%	<0.0001	0.0001
4-methoxyphenol sulfate	-73%	0.0001	0.0008
4-methyl-2-oxopentanoate	18%	0.0014	0.0065
4-methylhexanoylglutamine	320%	<0.0001	<0.0001
4-vinylphenol sulfate	-66%	0.0050	0.0171
5-acetylamino-6-amino-3-methyluracil	13%	0.0026	0.0102
5alpha-androstan-3beta.17beta-diol disulfate	-11%	0.0004	0.0023
5alpha-androstan-3beta.17beta-diol monosulfate (2)	-10%	0.0032	0.0122
5alpha-pregnan-3beta.20alpha-diol disulfate	30%	0.0030	0.0114
5alpha-pregnan-3beta.20alpha-diol monosulfate (2)	42%	0.0120	0.0344
5-dodecenoate (12:1n7)	72%	0.0001	0.0004
5-dodecenoylcarnitine (C12:1)	101%	0.0001	0.0007
7-methylurate	188%	0.0120	0.0344
7-methylxanthine	245%	0.0086	0.0264
acetoacetate	340%	<0.0001	0.0004
acetylcarnitine (C2)	54%	<0.0001	<0.0001
acisoga	41%	0.0008	0.0039
adipoylcarnitine (C6-DC)	80%	<0.0001	0.0001
alanine	-10%	0.0173	0.0463
alpha-hydroxyisocaproate	19%	0.0030	0.0115
alpha-hydroxyisovalerate	16%	0.0043	0.0153
alpha-ketobutyrate	177%	0.0002	0.0012
alpha-ketoglutamamate	-9%	0.0099	0.0294
androstenediol (3beta.17beta) disulfate (1)	-14%	<0.0001	<0.0001
androstenediol (3beta.17beta) monosulfate (2)	-11%	<0.0001	0.0004
arabitol/xylitol	-21%	0.0001	0.0006
arabonate/xylonate	-13%	0.0050	0.0170
argininate	-15%	0.0016	0.0071
arginine	-4%	0.0071	0.0226
aspartate	15%	0.0069	0.0221
behenoyl dihydrosphingomyelin (d18:0/22:0)	31%	<0.0001	0.0002
benzoylcarnitine	84%	<0.0001	0.0001
beta-hydroxyisovalerate	42%	<0.0001	<0.0001
betaine	8%	0.0007	0.0035
caffeine	36%	0.0015	0.0069
caproate (6:0)	20%	0.0025	0.0100
carboxyethyl-GABA	-18%	0.0078	0.0245
carotene diol (1)	27%	0.0046	0.0159
ceramide (d18:1/17:0. d17:1/18:0)	72%	<0.0001	<0.0001

ceramide (d18:1/20:0. d16:1/22:0. d20:1/18:0)	-7%	0.0159	0.0433
chenodeoxycholate	-22%	0.0121	0.0346
cis-4-decenoate (10:1n6)	38%	0.0008	0.0038
cis-4-decenoylcarnitine (C10:1)	43%	0.0182	0.0481
citrate	28%	0.0003	0.0018
creatine	10%	0.0095	0.0285
decanoylcarnitine (C10)	121%	<0.0001	<0.0001
diacylglycerol (14:0/18:1. 16:0/16:1) [1]	-33%	0.0045	0.0157
diacylglycerol (14:0/18:1. 16:0/16:1) [2]	-21%	0.0145	0.0405
diacylglycerol (16:1/18:2 [2]. 16:0/18:3 [1])	-33%	0.0007	0.0034
dihomo-linolenoylcarnitine (C20:3n3 or 6)	-10%	0.0071	0.0226
dihydroorotate	8%	0.0079	0.0248
dimethylglycine	13%	0.0001	0.0009
docosahexaenoylcarnitine (C22:6)	77%	<0.0001	<0.0001
dodecadienoate (12:2)	46%	0.0029	0.0112
dodecenedioate (C12:1-DC)	108%	<0.0001	<0.0001
dopamine 3-O-sulfate	-21%	0.0011	0.0051
dopamine 4-sulfate	-15%	0.0052	0.0174
eicosanedioate (C20-DC)	-36%	0.0003	0.0018
eicosapentaenoylcholine	5%	0.0019	0.0081
erythritol	944%	0.0001	0.0006
Fibrinopeptide A (7-16)	39%	0.0130	0.0366
galactonate	47%	0.0073	0.0232
gamma-CEHC	-29%	0.0001	0.0004
gamma-glutamyl-2-aminobutyrate	109%	<0.0001	<0.0001
gamma-glutamylglycine	-10%	0.0067	0.0216
gamma-glutamylhistidine	-9%	0.0013	0.0059
gamma-glutamylleucine	11%	0.0148	0.0407
gamma-glutamylthreonine	-11%	0.0158	0.0430
gamma-glutamyltryptophan	-9%	0.0016	0.0072
gamma-glutamyltyrosine	-11%	0.0042	0.0149
gamma-glutamylvaline	18%	0.0114	0.0332
gamma-tocopherol/beta-tocopherol	-48%	<0.0001	<0.0001
glucose	-2%	0.0189	0.0493
glutamine	-4%	0.0134	0.0374
glycerol	45%	0.0003	0.0018
glycerol 3-phosphate	-7%	0.0038	0.0141
glycerophosphorylcholine (GPC)	-14%	0.0007	0.0035
glycine	-7%	0.0066	0.0214
glycine conjugate of C10H14O2 (1)	-64%	<0.0001	0.0004
glyco-beta-muricholate	207%	0.0039	0.0141
glycosyl ceramide (d18:1/23:1. d17:1/24:1)	31%	0.0001	0.0004
glycosyl ceramide (d18:2/24:1. d18:1/24:2)	10%	0.0049	0.0168
glycosyl-N-nervonoyl-sphingosine (d18:1/24:1)	17%	0.0189	0.0493
glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	21%	<0.0001	0.0001

glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	11%	0.0020	0.0082
glycosyl-N-tricosanoyl-sphingadienine (d18:2/23:0)	30%	<0.0001	<0.0001
guaiacol sulfate	-14%	0.0116	0.0339
guanidinoacetate	-11%	0.0002	0.0011
guanidinosuccinate	34%	<0.0001	<0.0001
heptenedioate (C7:1-DC)	206%	<0.0001	0.0003
hexadecanedioate (C16-DC)	30%	0.0004	0.0023
hexanoylcarnitine (C6)	75%	<0.0001	<0.0001
hexanoylglutamine	154%	<0.0001	0.0001
hexanoylglycine	125%	0.0146	0.0405
homoarginine	16%	0.0005	0.0025
hydroxypalmitoyl sphingomyelin (d18:1/16:0(OH))	9%	0.0091	0.0277
indole-3-carboxylate	36%	0.0017	0.0074
indoleacetate	20%	0.0045	0.0158
indoleacetylcarnitine	62%	0.0001	0.0009
isoleucine	7%	0.0053	0.0175
isovalerylcarnitine (C5)	28%	0.0006	0.0031
lactate	-13%	0.0019	0.0081
laurylcarnitine (C12)	118%	<0.0001	<0.0001
leucine	7%	0.0092	0.0278
linolenoylcarnitine (C18:3)	-22%	0.0009	0.0042
linoleoyl-arachidonoyl-glycerol (18:2/20:4) [2]	-24%	0.0168	0.0455
linoleoyl-linolenoyl-glycerol (18:2/18:3) [1]	-52%	0.0007	0.0035
linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]	-13%	0.0062	0.0205
malate	10%	0.0131	0.0370
mannitol/sorbitol	-26%	0.0182	0.0481
mannose	26%	<0.0001	<0.0001
margaroylcarnitine (C17)	65%	<0.0001	<0.0001
methionine	-7%	0.0052	0.0174
myristoleoylcarnitine (C14:1)	120%	<0.0001	<0.0001
myristoyl dihydrosphingomyelin (d18:0/14:0)	54%	<0.0001	<0.0001
myristoylcarnitine (C14)	68%	<0.0001	<0.0001
myristoylcholine	-21%	0.0002	0.0011
N1-methylinosine	10%	0.0085	0.0263
N6.N6-dimethyllysine	-5%	0.0172	0.0462
N-acetyl-3-methylhistidine	-35%	0.0001	0.0008
N-acetylglycine	70%	<0.0001	0.0001
N-acetylmethionine	-12%	<0.0001	0.0001
N-acetylphenylalanine	-10%	0.0007	0.0034
N-acetylproline	-16%	0.0042	0.0149
N-acetylputrescine	-7%	0.0111	0.0327
N-acetyltaurine	-7%	0.0154	0.0422
N-acetyltryptophan	-22%	<0.0001	0.0002
N-acetyltyrosine	-15%	0.0007	0.0036
N-behenoyl-sphingadienine (d18:2/22:0)	-11%	0.0019	0.0080

nonanoylcarnitine (C9)	125%	<0.0001	<0.0001
N-stearoyl-sphingadienine (d18:2/18:0)	441%	0.0004	0.0021
N-stearoyl-sphinganine (d18:0/18:0)	135%	<0.0001	0.0003
N-stearoyl-sphingosine (d18:1/18:0)	31%	0.0001	0.0004
octadecadienedioate (C18:2-DC)	127%	0.0007	0.0036
octadecanedioate (C18-DC)	99%	<0.0001	<0.0001
octadecanedioylcarnitine (C18-DC)	81%	<0.0001	<0.0001
octadecenedioylcarnitine (C18:1-DC)	55%	<0.0001	0.0003
octanoylcarnitine (C8)	110%	<0.0001	0.0002
oleate/vaccenate (18:1)	34%	0.0036	0.0136
oleoylcarnitine (C18:1)	22%	0.0004	0.0021
oleoylcholine	-11%	0.0041	0.0147
orotidine	-19%	0.0048	0.0166
palmitoleate (16:1n7)	19%	0.0091	0.0277
palmitoleoylcarnitine (C16:1)	48%	<0.0001	<0.0001
palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]	-29%	0.0008	0.0039
palmitoleoylcholine	-23%	0.0001	0.0008
palmitoyl dihydrosphingomyelin (d18:0/16:0)	25%	<0.0001	<0.0001
palmitoyl sphingomyelin (d18:1/16:0)	9%	<0.0001	0.0002
palmitoyl-arachidonoyl-glycerol (16:0/20:4) [1]	-11%	0.0133	0.0374
palmitoylcarnitine (C16)	16%	0.0016	0.0071
pantothenate	11%	0.0008	0.0039
paraxanthine	-15%	0.0002	0.0010
phenylacetylcarnitine	73%	0.0030	0.0114
phenyllactate (PLA)	-7%	0.0019	0.0080
phytanate	194%	<0.0001	<0.0001
picolinate	24%	0.0003	0.0017
pipecolate	30%	0.0110	0.0324
pregnenediol-3-glucuronide	53%	0.0025	0.0100
pristanate	634%	<0.0001	0.0003
pro-hydroxy-pro	15%	0.0051	0.0172
proline	-14%	<0.0001	0.0001
propionylcarnitine (C3)	20%	0.0023	0.0095
pyrraline	-50%	<0.0001	<0.0001
pyruvate	-23%	0.0002	0.0013
ribitol	-13%	0.0003	0.0019
ribonate	-10%	0.0032	0.0119
serine	11%	0.0009	0.0043
S-methylcysteine	113%	<0.0001	<0.0001
S-methylcysteine sulfoxide	228%	<0.0001	<0.0001
S-methylmethionine	384%	0.0028	0.0107
sphingomyelin (d17:1/14:0. d16:1/15:0)	17%	0.0037	0.0136
sphingomyelin (d17:1/16:0. d18:1/15:0. d16:1/17:0)	16%	<0.0001	<0.0001
sphingomyelin (d17:2/16:0. d18:2/15:0)	13%	0.0014	0.0065
sphingomyelin (d18:0/18:0. d19:0/17:0)	98%	<0.0001	<0.0001

sphingomyelin (d18:0/20:0. d16:0/22:0)	51%	<0.0001	<0.0001
sphingomyelin (d18:1/14:0. d16:1/16:0)	15%	<0.0001	0.0002
sphingomyelin (d18:1/17:0. d17:1/18:0. d19:1/16:0)	32%	<0.0001	<0.0001
sphingomyelin (d18:1/18:1. d18:2/18:0)	26%	<0.0001	<0.0001
sphingomyelin (d18:1/19:0. d19:1/18:0)	22%	0.0007	0.0035
sphingomyelin (d18:1/20:1. d18:2/20:0)	10%	0.0051	0.0172
sphingomyelin (d18:1/20:2. d18:2/20:1. d16:1/22:2)	30%	0.0003	0.0018
sphingomyelin (d18:1/21:0. d17:1/22:0. d16:1/23:0)	14%	<0.0001	0.0003
sphingomyelin (d18:1/22:2. d18:2/22:1. d16:1/24:2)	26%	<0.0001	0.0002
sphingomyelin (d18:1/25:0. d19:0/24:1. d20:1/23:0. d19:1/24:0)	36%	<0.0001	<0.0001
sphingomyelin (d18:2/16:0. d18:1/16:1)	7%	0.0062	0.0204
sphingomyelin (d18:2/18:1)	51%	<0.0001	<0.0001
sphingomyelin (d18:2/21:0. d16:2/23:0)	30%	<0.0001	<0.0001
sphingomyelin (d18:2/23:0. d18:1/23:1. d17:1/24:1)	19%	<0.0001	<0.0001
sphingomyelin (d18:2/23:1)	30%	<0.0001	<0.0001
sphingomyelin (d18:2/24:2)	13%	0.0026	0.0102
stearoyl sphingomyelin (d18:1/18:0)	33%	<0.0001	<0.0001
stearoylcarnitine (C18)	50%	<0.0001	<0.0001
suberoylcarnitine (C8-DC)	220%	0.0021	0.0085
succinylcarnitine (C4-DC)	-16%	0.0001	0.0004
tetradecadienoate (14:2)	58%	0.0001	0.0006
theobromine	484%	0.0150	0.0413
theophylline	32%	0.0002	0.0010
threonine	-13%	<0.0001	0.0003
tiglylcarnitine (C5:1-DC)	54%	<0.0001	<0.0001
tricosanoyl sphingomyelin (d18:1/23:0)	19%	<0.0001	<0.0001
trimethylamine N-oxide	71%	0.0001	0.0004
tryptophan	-5%	0.0065	0.0213
tyrosine	-11%	<0.0001	0.0002
urea	19%	0.0003	0.0018
uridine	23%	<0.0001	0.0001
ursodeoxycholate	-9%	0.0067	0.0216
valine	7%	0.0082	0.0257
vanillactate	-8%	0.0113	0.0332
xanthine	23%	0.0185	0.0486

ESM Table 4. Metabolites significantly changed in evening samples after 5 d high-fat diet.

	change	p value	q value
(N(1) + N(8))-acetylsermidine	-8%	0.0081	0.0206
1-(1-enyl-oleoyl)-GPE (P-18:1)	26%	0.0142	0.0339
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)	34%	0.0002	0.0011
1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)	24%	0.0190	0.0430
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)	6%	0.0110	0.0271
1-(1-enyl-palmitoyl)-GPC (P-16:0)	-16%	0.0001	0.0003
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)	50%	<0.0001	<0.0001
1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)	30%	0.0002	0.0008
1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	33%	0.0001	0.0006
1,2-dilinoleoyl-GPC (18:2/18:2)	-11%	0.0049	0.0139
1,2-dipalmitoyl-GPC (16:0/16:0)	11%	0.0002	0.0007
1,5-anhydroglucitol (1,5-AG)	-3%	0.0044	0.0127
10-nonadecenoate (19:1n9)	49%	<0.0001	0.0002
10-undecenoate (11:1n1)	51%	0.0012	0.0042
12,13-DiHOME	831%	<0.0001	<0.0001
13-HODE + 9-HODE	149%	<0.0001	0.0001
1-arachidonoyl-GPC (20:4n6)	8%	0.0002	0.0011
1-arachidonoyl-GPE (20:4n6)	17%	0.0003	0.0012
1-arachidonoylglycerol (20:4)	84%	0.0009	0.0031
1-docosahexaenoylglycerol (22:6)	133%	0.0002	0.0007
1-lignoceroyl-GPC (24:0)	-30%	<0.0001	<0.0001
1-linolenoyl-GPC (18:3)	-22%	0.0010	0.0036
1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)	-33%	0.0002	0.0011
1-methylhistidine	-14%	0.0009	0.0033
1-methylnicotinamide	74%	0.0047	0.0136
1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)	29%	0.0100	0.0249
1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	54%	0.0036	0.0107
1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)	-17%	0.0017	0.0055
1-palmitoleoyl-GPC (16:1)	-18%	0.0001	0.0005
1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	9%	0.0062	0.0167
1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)	-12%	0.0183	0.0419
1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)	-5%	0.0051	0.0143
1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)	9%	0.0021	0.0067
1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	-23%	<0.0001	0.0003
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)	-15%	0.0015	0.0052
1-palmitoyl-GPC (16:0)	-7%	0.0042	0.0123
1-palmitoyl-GPE (16:0)	-15%	0.0001	0.0007
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	10%	0.0017	0.0056
1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	19%	0.0191	0.0430
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)	7%	0.0139	0.0333
1-stearoyl-2-oleoyl-GPI (18:0/18:1)	25%	0.0132	0.0317
1-stearoyl-GPC (18:0)	-4%	0.0213	0.0469

1-stearoyl-GPE (18:0)	-12%	0.0003	0.0014
2,3-dihydroxy-5-methylthio-4-pentenoate (DMTPA)	12%	0.0171	0.0400
2,3-dihydroxyisovalerate	-84%	0.0001	0.0005
2-aminoadipate	50%	0.0003	0.0012
2-aminobutyrate	104%	<0.0001	<0.0001
2-aminophenol sulfate	-55%	0.0035	0.0105
2-hydroxy-3-methylvalerate	50%	<0.0001	0.0002
2-hydroxybutyrate/2-hydroxyisobutyrate	135%	<0.0001	<0.0001
2-hydroxyglutarate	-18%	<0.0001	<0.0001
2-hydroxyhippurate (salicylurate)	-51%	0.0050	0.0142
2-hydroxynervonate	31%	0.0004	0.0017
2-keto-3-deoxy-gluconate	30%	0.0045	0.0130
2-linoleoylglycerol (18:2)	-37%	0.0011	0.0038
2-methylbutyrylcarnitine (C5)	71%	<0.0001	<0.0001
2-methylcitrate/homocitrate	30%	<0.0001	0.0001
2-oxoarginine	28%	0.0058	0.0160
3-(3-hydroxyphenyl)propionate	-53%	0.0063	0.0170
3-(4-hydroxyphenyl)lactate	28%	<0.0001	<0.0001
3,4-methyleneheptanoate	3%	0.0012	0.0042
3-acetylphenol sulfate	-38%	0.0053	0.0146
3-carboxy-4-methyl-5-pentyl-2-furanpropionate (3-CMPFP)	58%	<0.0001	<0.0001
3-ethylphenylsulfate	1062%	<0.0001	<0.0001
3-formylindole	-7%	0.0179	0.0411
3-hydroxy-2-ethylpropionate	118%	<0.0001	<0.0001
3-hydroxy-3-methylglutarate	-19%	0.0094	0.0237
3-hydroxyadipate	202%	0.0001	0.0006
beta-hydroxybutyrate (β OHB)	522%	<0.0001	<0.0001
3-hydroxybutyrylglycine	366%	<0.0001	<0.0001
3-hydroxybutyrylcarnitine (1)	569%	<0.0001	<0.0001
3-hydroxybutyrylcarnitine (2)	107%	<0.0001	<0.0001
3-hydroxydecanoate	134%	<0.0001	<0.0001
3-hydroxyhexanoate	148%	<0.0001	<0.0001
3-hydroxyhippurate	-54%	0.0024	0.0077
3-hydroxyisobutyrate	120%	<0.0001	<0.0001
3-hydroxylaurate	142%	<0.0001	<0.0001
3-hydroxyoctanoate	97%	<0.0001	<0.0001
3-hydroxyoleate	340%	<0.0001	<0.0001
3-hydroxypyridine sulfate	-33%	0.0114	0.0279
3-hydroxysebacate	470%	<0.0001	<0.0001
3-methoxycatechol sulfate (2)	-53%	0.0001	0.0004
3-methoxytyramine sulfate	-31%	0.0004	0.0018
3-methoxytyrosine	-12%	0.0044	0.0127
3-methyl catechol sulfate (1)	4%	0.0162	0.0380
3-methyl-2-oxobutyrate	35%	<0.0001	<0.0001
3-methyl-2-oxovalerate	24%	0.0001	0.0004

3-methylglutaconate	66%	<0.0001	<0.0001
3-ureidopropionate	-8%	0.0117	0.0285
4-acetylphenol sulfate	-65%	<0.0001	<0.0001
4-allylphenol sulfate	-54%	0.0070	0.0183
4-cholesten-3-one	-15%	0.0042	0.0123
4-guanidinobutanoate	-15%	0.0176	0.0406
4-hydroxyhippurate	-42%	<0.0001	0.0002
4-methoxyphenol sulfate	-80%	0.0007	0.0025
4-methyl-2-oxopentanoate	25%	<0.0001	0.0001
4-methylguaiaicol sulfate	40%	0.0089	0.0225
4-methylhexanoylglutamine	459%	<0.0001	<0.0001
4-vinylphenol sulfate	-71%	0.0001	0.0007
5-(galactosylhydroxy)-L-lysine	-10%	0.0070	0.0183
5.6-dihydrouridine	-8%	0.0002	0.0007
5-acetylamino-6-amino-3-methyluracil	-9%	0.0190	0.0430
5alpha-androstan-3alpha.17beta-diol monosulfate (2)	17%	0.0172	0.0401
5alpha-androstan-3beta.17beta-diol disulfate	-13%	0.0011	0.0038
5alpha-pregnan-3beta.20alpha-diol monosulfate (2)	65%	0.0068	0.0182
5-dodecenoate (12:1n7)	574%	<0.0001	<0.0001
5-dodecenoylcarnitine (C12:1)	109%	0.0078	0.0201
5-hydroxyhexanoate	100%	0.0014	0.0048
6-bromotryptophan	-8%	0.0080	0.0205
6-oxopiperidine-2-carboxylate	29%	0.0203	0.0453
9-hydroxystearate	136%	<0.0001	0.0001
acetoacetate	376%	<0.0001	0.0001
acetylcarnitine (C2)	59%	<0.0001	<0.0001
adenosine	103%	0.0052	0.0144
adipate (C6-DC)	416%	<0.0001	0.0002
adipoylcarnitine (C6-DC)	187%	<0.0001	<0.0001
allantoin	-20%	0.0038	0.0114
alliin	-60%	0.0001	0.0003
alpha-hydroxycaproate	165%	0.0053	0.0146
alpha-hydroxyisocaproate	36%	0.0004	0.0017
alpha-hydroxyisovalerate	31%	0.0006	0.0024
alpha-ketobutyrate	262%	<0.0001	0.0002
androstenediol (3beta.17beta) disulfate (1)	-14%	<0.0001	0.0001
androstenediol (3beta.17beta) monosulfate (2)	-14%	<0.0001	0.0001
arabinose	102%	0.0005	0.0020
arabitol/xylitol	-27%	<0.0001	<0.0001
arabonate/xylonate	-26%	0.0006	0.0024
arachidonoylcarnitine (C20:4)	-9%	0.0059	0.0160
argininate	39%	<0.0001	0.0002
behenoyl dihydrosphingomyelin (d18:0/22:0)	46%	<0.0001	<0.0001
benzoylcarnitine	60%	0.0019	0.0060
beta-alanine	79%	0.0004	0.0018

beta-citrylglutamate	22%	0.0004	0.0017
beta-hydroxyisovalerate	83%	<0.0001	<0.0001
caprate (10:0)	636%	<0.0001	<0.0001
caproate (6:0)	56%	0.0002	0.0007
caprylate (8:0)	719%	<0.0001	0.0001
carboxyethyl-GABA	-12%	0.0053	0.0146
carotene diol (1)	41%	<0.0001	0.0001
carotene diol (2)	35%	0.0031	0.0095
carotene diol (3)	33%	0.0068	0.0182
ceramide (d16:1/24:1. d18:1/22:1)	19%	0.0210	0.0466
ceramide (d18:1/14:0. d16:1/16:0)	32%	<0.0001	<0.0001
ceramide (d18:1/17:0. d17:1/18:0)	99%	<0.0001	<0.0001
chenodeoxycholate	185%	0.0008	0.0030
cholate	994%	0.0017	0.0055
choline phosphate	37%	0.0001	0.0005
cis-4-decenoate (10:1n6)	103%	0.0069	0.0183
citrulline	-10%	0.0017	0.0055
cystathionine	72%	0.0019	0.0061
decanoylcarnitine (C10)	186%	<0.0001	<0.0001
diacylglycerol (16:1/18:2 [2]. 16:0/18:3 [1])	-26%	0.0003	0.0012
dihomo-linolenoylcarnitine (C20:3n3 or 6)	-15%	<0.0001	0.0003
dihomo-linolenoyl-choline	-13%	0.0044	0.0127
dihomo-linoleoylcarnitine (C20:2)	-10%	0.0034	0.0103
dimethyl sulfone	-12%	0.0074	0.0194
dimethylglycine	36%	<0.0001	<0.0001
docosahexaenoate (DHA; 22:6n3)	43%	0.0004	0.0018
docosahexaenoylcarnitine (C22:6)	32%	0.0078	0.0201
docosapentaenoate (n6 DPA; 22:5n6)	50%	<0.0001	0.0002
dodecadienoate (12:2)	125%	<0.0001	0.0001
dodecanedioate (C12-DC)	1384%	<0.0001	0.0001
dodecenedioate (C12:1-DC)	210%	<0.0001	0.0001
eicosanedioate (C20-DC)	-33%	0.0001	0.0006
eicosapentaenoylcholine	-11%	0.0027	0.0084
erythritol	1943%	0.0009	0.0032
ethylmalonate	28%	0.0038	0.0114
eugenol sulfate	-70%	0.0051	0.0144
Fibrinopeptide A. des-ala(1)	10%	0.0029	0.0089
Fibrinopeptide B (1-13)	9%	0.0077	0.0200
formiminoglutamate	93%	0.0003	0.0013
fructose	-28%	0.0077	0.0200
gamma-CEHC	-37%	<0.0001	0.0001
gamma-glutamyl-2-aminobutyrate	153%	<0.0001	<0.0001
gamma-glutamylglutamate	23%	0.0046	0.0131
gamma-glutamylglycine	-17%	<0.0001	0.0001
gamma-glutamylhistidine	-7%	0.0112	0.0276

gamma-glutamylisoleucine	35%	<0.0001	<0.0001
gamma-glutamylleucine	39%	<0.0001	<0.0001
gamma-glutamyltryptophan	19%	0.0026	0.0081
gamma-glutamyltyrosine	25%	0.0099	0.0247
gamma-glutamylvaline	55%	<0.0001	<0.0001
gamma-tocopherol/beta-tocopherol	-45%	<0.0001	<0.0001
gentisate	-50%	<0.0001	<0.0001
gluconate	-22%	0.0076	0.0198
glutaryl carnitine (C5-DC)	8%	0.0012	0.0041
glycerol	98%	<0.0001	<0.0001
glycerophosphoinositol	-21%	0.0048	0.0137
glycerophosphorylcholine (GPC)	-11%	0.0004	0.0016
glycine	-13%	0.0001	0.0003
glycine conjugate of C10H14O2 (1)	-76%	<0.0001	<0.0001
glyco-beta-muricholate	124%	<0.0001	0.0001
glycochenodeoxycholate 3-sulfate	77%	0.0001	0.0003
glycodeoxycholate 3-sulfate	75%	0.0006	0.0022
glycosyl ceramide (d18:1/23:1. d17:1/24:1)	35%	<0.0001	<0.0001
glycosyl ceramide (d18:2/24:1. d18:1/24:2)	14%	0.0001	0.0003
glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	16%	0.0002	0.0008
glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	18%	<0.0001	0.0002
glycosyl-N-tricosanoyl-sphingadinenine (d18:2/23:0)	42%	<0.0001	<0.0001
guaiaicol sulfate	-38%	0.0026	0.0081
guanidinoacetate	-20%	0.0006	0.0022
guanidinosuccinate	31%	<0.0001	<0.0001
heptenedioate (C7:1-DC)	118%	0.0211	0.0467
hexadecanedioate (C16-DC)	83%	0.0001	0.0003
hexanoyl carnitine (C6)	118%	<0.0001	<0.0001
hexanoylglutamine	410%	<0.0001	<0.0001
hexanoylglycine	332%	<0.0001	<0.0001
hippurate	-23%	0.0071	0.0188
hydantoin-5-propionate	138%	<0.0001	0.0002
hydroquinone sulfate	-30%	0.0117	0.0285
hydroxyasparagine	-9%	<0.0001	0.0001
hyocholate	245%	0.0003	0.0013
indoleacetylcarnitine	39%	<0.0001	0.0002
indolepropionate	-37%	0.0014	0.0047
isobutyrylcarnitine (C4)	76%	<0.0001	0.0001
isocitrate	-20%	0.0002	0.0010
isoleucine	22%	<0.0001	0.0001
isovalerylcarnitine (C5)	55%	0.0002	0.0008
kynurenate	16%	0.0005	0.0020
lactate	-20%	0.0001	0.0005
lactosyl-N-behenoyl-sphingosine (d18:1/22:0)	13%	0.0006	0.0021
lactosyl-N-nervonoyl-sphingosine (d18:1/24:1)	9%	0.0136	0.0325

lanthionine	-24%	0.0093	0.0235
laurate (12:0)	678%	<0.0001	<0.0001
laurylcarnitine (C12)	248%	<0.0001	<0.0001
leucine	24%	<0.0001	0.0001
lignoceroyl sphingomyelin (d18:1/24:0)	13%	0.0003	0.0012
linoleate (18:2n6)	62%	<0.0001	0.0001
linolenoylcarnitine (C18:3)	-24%	0.0003	0.0012
linoleoyl-arachidonoyl-glycerol (18:2/20:4) [1]	-5%	0.0162	0.0381
linoleoyl-arachidonoyl-glycerol (18:2/20:4) [2]	-5%	0.0177	0.0407
linoleoylcarnitine (C18:2)	-10%	0.0040	0.0118
linoleoyl-linolenoyl-glycerol (18:2/18:3) [1]	-48%	0.0012	0.0041
linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]	-26%	0.0018	0.0059
mannitol/sorbitol	-41%	0.0053	0.0146
mannose	67%	<0.0001	<0.0001
margaroylcarnitine (C17)	66%	<0.0001	<0.0001
myristoleoylcarnitine (C14:1)	93%	<0.0001	0.0001
myristoyl dihydrosphingomyelin (d18:0/14:0)	90%	<0.0001	<0.0001
myristoylcarnitine (C14)	135%	<0.0001	<0.0001
N1-methyladenosine	-8%	0.0001	0.0003
N6.N6.N6-trimethyllysine	-25%	0.0017	0.0055
N6.N6-dimethyllysine	-17%	0.0001	0.0003
N6-carbamoylthreonyladenosine	-9%	0.0121	0.0293
N6-carboxymethyllysine	1613%	0.0004	0.0015
N-acetyl-1-methylhistidine	-55%	<0.0001	<0.0001
N-acetyl-2-aminooctanoate	-36%	0.0015	0.0051
N-acetyl-3-methylhistidine	-63%	<0.0001	0.0002
N-acetylarginine	-13%	0.0217	0.0475
N-acetylaspargine	-16%	0.0028	0.0085
N-acetylcarnosine	-6%	0.0161	0.0380
N-acetylglutamate	42%	<0.0001	<0.0001
N-acetylglycine	60%	<0.0001	<0.0001
N-acetylhistidine	10%	0.0010	0.0035
N-acetyl-isoptreanine	-18%	<0.0001	<0.0001
N-acetylneuramate	11%	0.0005	0.0020
N-acetylphenylalanine	-28%	<0.0001	0.0001
N-acetylproline	-34%	<0.0001	0.0001
N-acetylputrescine	-11%	0.0032	0.0097
N-acetyltaurine	-14%	0.0080	0.0204
N-acetylthreonine	-6%	0.0212	0.0468
N-acetyltryptophan	-41%	<0.0001	<0.0001
N-acetyltyrosine	-20%	0.0024	0.0077
N-behenoyl-sphingadienine (d18:2/22:0)	-12%	0.0013	0.0044
N-carbamoylalanine	-19%	0.0061	0.0165
N-delta-acetylornithine	-20%	0.0051	0.0144
nervonoylcarnitine (C24:1)	27%	0.0209	0.0466

N-oleoyltaurine	128%	0.0089	0.0225
nonanoylcarnitine (C9)	166%	<0.0001	<0.0001
N-palmitoylglycine	11%	0.0203	0.0453
N-palmitoyl-heptadecaspingosine (d17:1/16:0)	31%	<0.0001	0.0001
N-palmitoyl-sphingadienine (d18:2/16:0)	14%	0.0110	0.0271
N-palmitoyl-sphinganine (d18:0/16:0)	81%	<0.0001	<0.0001
N-palmitoyl-sphingosine (d18:1/16:0)	26%	<0.0001	<0.0001
N-stearoyl-sphingadienine (d18:2/18:0)	542%	0.0001	0.0007
N-stearoyl-sphinganine (d18:0/18:0)	243%	<0.0001	<0.0001
N-stearoyl-sphingosine (d18:1/18:0)	49%	<0.0001	<0.0001
o-cresol sulfate	-16%	0.0025	0.0078
octadecanedioate (C18-DC)	128%	<0.0001	0.0002
octadecanedioylcarnitine (C18-DC)	90%	<0.0001	<0.0001
octadecenedioylcarnitine (C18:1-DC)	52%	0.0005	0.0018
octanoylcarnitine (C8)	143%	<0.0001	<0.0001
oleate/vaccenate (18:1)	66%	<0.0001	0.0001
oleoyl-arachidonoyl-glycerol (18:1/20:4) [1]	-8%	0.0216	0.0475
oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	-13%	0.0014	0.0047
oleoyl-linoleoyl-glycerol (18:1/18:2) [2]	-12%	0.0044	0.0127
oxalate (ethanedioate)	-8%	0.0149	0.0353
palmitate (16:0)	41%	<0.0001	<0.0001
palmitoleate (16:1n7)	24%	0.0007	0.0027
palmitoleoylcarnitine (C16:1)	35%	0.0066	0.0177
palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]	-29%	0.0005	0.0019
palmitoleoylcholine	-16%	0.0042	0.0123
palmitoyl dihydrosphingomyelin (d18:0/16:0)	38%	<0.0001	<0.0001
palmitoyl sphingomyelin (d18:1/16:0)	12%	<0.0001	<0.0001
palmitoylcarnitine (C16)	20%	0.0007	0.0025
paraxanthine	13%	0.0036	0.0108
pentadecanoylcholine	40%	0.0029	0.0088
perfluorooctanoate (PFOA)	4%	0.0117	0.0285
phenylacetylcarnitine	91%	0.0188	0.0429
phosphate	7%	0.0001	0.0004
phytanate	450%	<0.0001	<0.0001
picolinate	53%	<0.0001	0.0001
pristanate	590%	<0.0001	<0.0001
propionylcarnitine (C3)	39%	0.0001	0.0004
pseudouridine	-7%	0.0002	0.0007
pyruvate	-27%	0.0008	0.0029
retinol (Vitamin A)	5%	0.0199	0.0448
ribonate	-17%	0.0024	0.0076
ribulonate/xylulonate	-12%	0.0074	0.0194
S-allylcysteine	-63%	0.0005	0.0020
sarcosine	48%	0.0001	0.0005
sebacate (C10-DC)	172%	0.0003	0.0013

serine	11%	0.0017	0.0055
S-methylcysteine sulfoxide	104%	<0.0001	<0.0001
S-methylmethionine	-80%	0.0003	0.0013
sphingomyelin (d17:1/14:0. d16:1/15:0)	31%	<0.0001	<0.0001
sphingomyelin (d17:1/16:0. d18:1/15:0. d16:1/17:0)	21%	<0.0001	<0.0001
sphingomyelin (d17:2/16:0. d18:2/15:0)	24%	<0.0001	<0.0001
sphingomyelin (d18:0/18:0. d19:0/17:0)	136%	<0.0001	<0.0001
sphingomyelin (d18:0/20:0. d16:0/22:0)	71%	<0.0001	<0.0001
sphingomyelin (d18:1/14:0. d16:1/16:0)	22%	<0.0001	<0.0001
sphingomyelin (d18:1/17:0. d17:1/18:0. d19:1/16:0)	37%	<0.0001	<0.0001
sphingomyelin (d18:1/18:1. d18:2/18:0)	29%	<0.0001	<0.0001
sphingomyelin (d18:1/19:0. d19:1/18:0)	28%	<0.0001	<0.0001
sphingomyelin (d18:1/20:2. d18:2/20:1. d16:1/22:2)	77%	0.0008	0.0029
sphingomyelin (d18:1/21:0. d17:1/22:0. d16:1/23:0)	18%	<0.0001	0.0002
sphingomyelin (d18:1/22:2. d18:2/22:1. d16:1/24:2)	20%	0.0003	0.0011
sphingomyelin (d18:1/25:0. d19:0/24:1. d20:1/23:0. d19:1/24:0)	46%	<0.0001	<0.0001
sphingomyelin (d18:2/14:0. d18:1/14:1)	18%	<0.0001	0.0001
sphingomyelin (d18:2/16:0. d18:1/16:1)	9%	0.0007	0.0027
sphingomyelin (d18:2/18:1)	61%	<0.0001	<0.0001
sphingomyelin (d18:2/21:0. d16:2/23:0)	40%	<0.0001	<0.0001
sphingomyelin (d18:2/23:0. d18:1/23:1. d17:1/24:1)	22%	<0.0001	<0.0001
sphingomyelin (d18:2/23:1)	36%	<0.0001	<0.0001
sphingomyelin (d18:2/24:2)	12%	0.0149	0.0353
stachydrine	-27%	0.0107	0.0265
stearate (18:0)	35%	<0.0001	0.0001
stearidonate (18:4n3)	46%	0.0007	0.0027
stearoyl sphingomyelin (d18:1/18:0)	31%	<0.0001	<0.0001
stearoylcarnitine (C18)	25%	0.0007	0.0027
suberate (C8-DC)	251%	<0.0001	<0.0001
suberoylcarnitine (C8-DC)	720%	<0.0001	<0.0001
succinylcarnitine (C4-DC)	-10%	0.0163	0.0381
sucrose	327%	0.0024	0.0077
sulfate	23%	<0.0001	<0.0001
tartronate (hydroxymalonate)	-14%	0.0053	0.0146
tauro-beta-muricholate	364%	0.0004	0.0015
taurochenodeoxycholate	87%	0.0108	0.0267
tetradecadienoate (14:2)	118%	<0.0001	<0.0001
tetradecanedioate (C14-DC)	197%	<0.0001	<0.0001
theophylline	38%	0.0016	0.0052
threonate	-6%	0.0180	0.0412
thymol sulfate	64%	0.0174	0.0403
tiglylcarnitine (C5:1-DC)	153%	<0.0001	<0.0001
tricosanoyl sphingomyelin (d18:1/23:0)	25%	<0.0001	<0.0001
trigonelline (N-methylnicotinate)	-31%	0.0135	0.0325
tyrosine	14%	0.0012	0.0040

urea	51%	<0.0001	<0.0001
valine	33%	<0.0001	<0.0001
vanillactate	-21%	0.0002	0.0010
xanthurenate	37%	0.0191	0.0430

ESM Table 5. Cardiorespiratory fitness and body composition at baseline and after the intervention period. Values are observed means \pm SD. Estimates with 95% CI and *p* values for the effect compared to the control group, from linear mixed models.

	Baseline (Visit 1)	At study completion (Visit 3)	Estimate	95% CI	<i>p</i> value
	Mean \pm SD	Mean \pm SD			
VO₂peak (ml kg⁻¹ min⁻¹)					
Control	29.0 \pm 4.3	28.5 \pm 3.9			
EXam	28.5 \pm 6.1	29.7 \pm 6.2	1.3	0.5 to 2.0	0.003
EXpm	31.2 \pm 4.4	33.4 \pm 5.0	1.4	0.6 to 2.2	0.001
Peak power output (W)					
Control	193 \pm 33	191 \pm 34			
EXam	209 \pm 65	220 \pm 65	6.8	0.5 to 13.1	0.04
EXpm	208 \pm 26	234 \pm 29	14.4	8.1 to 20.7	<0.001
Body mass (kg)					
Control	94.5 \pm 10.4	95.4 \pm 9.8			
EXam	103.1 \pm 16.1	102.1 \pm 15.9	1.6	-1.9 to 5.2	0.36
EXpm	99.3 \pm 8.1	98.6 \pm 8.3	1.8	-1.8 to 5.3	0.32
Waist circumference (cm)					
Control	107.6 \pm 5.9	105.9 \pm 5.4			
EXam	110.7 \pm 10.5	110.7 \pm 10.2	1.2	-0.4 to 2.8	0.13
EXpm	109.1 \pm 8.3	106.8 \pm 8.7	-0.2	-1.6 to 1.3	0.84
Waist-hip ratio					
Control	0.99 \pm 0.07	0.98 \pm 0.07			
EXam	0.97 \pm 0.05	0.97 \pm 0.04	0.01	-0.01 to 0.02	0.37
EXpm	0.97 \pm 0.06	0.95 \pm 0.06	0.00	-0.01 to 0.1	0.55
Fat mass (kg)					
Control	31.3 \pm 3.0	31.1 \pm 3.2			
EXam	36.1 \pm 7.0	35.2 \pm 7.0	-0.29	-0.68 to 0.10	0.14
EXpm	32.9 \pm 5.3	32.7 \pm 5.4	-0.01	-0.39 to 0.38	0.98
Fat free mass (kg)					
Control	65.4 \pm 9.0	64.7 \pm 9.0			
EXam	67.2 \pm 10.1	66.7 \pm 9.6	0.13	-0.34 to 0.61	0.57
EXpm	66.7 \pm 3.9	66.0 \pm 3.8	0.07	-0.41 to 0.55	0.77
Visceral fat mass (g)					
Control	1969 \pm 495	1906 \pm 475			
EXam	2013 \pm 1424	1826 \pm 1382	-61	-122 to 0.4	0.05
EXpm	1479 \pm 573	1356 \pm 508	-0.34	-96 to 27	0.26

ESM Table 6. Fasting and postprandial circulating markers of metabolic health and blood pressure after five days of high-fat diet (HFD) and at study completion, according to group. Values are observed means \pm SD. Estimates with 95% CI and *p* values for the interaction between time and group, from linear mixed models. Data were log or square root transformed when they had non-normal distribution (insulin, triacylglycerol, HOMA-IR, morning LDL). Estimates and 95% CIs for log-transformed variables are reported (in brackets). EXam = morning exercise, EXpm = evening exercise.

	After 5 d high-fat diet	At study completion	Estimate	95% CI	<i>p</i> value
MORNING (fasting)					
Glucose (mmol/l)					
Control	4.8 \pm 0.2	4.7 \pm 0.3			
EXam	4.9 \pm 0.5	4.8 \pm 0.3	0.01	-0.09 to 0.12	0.85
EXpm	4.6 \pm 0.2	4.4 \pm 0.2	-0.12	-0.23 to -0.02	0.02
Insulin (pmol/l)					
Control	70 \pm 35	59 \pm 33			
EXam	74 \pm 52	36 \pm 19	(-0.46)	(-1.21 to 0.30)	0.22
EXpm	40 \pm 24	24 \pm 10	(-0.94)	(-1.69 to -0.19)	0.02
HOMA-IR					
Control	2.67 \pm 1.7	1.58 \pm 1.3			
EXam	2.33 \pm 1.2	1.48 \pm 0.8	(-0.09)	(-0.24 to 0.05)	0.20
EXpm	1.63 \pm 1.2	1.15 \pm 0.6	(-0.18)	(-0.33 to -0.04)	0.01
Cholesterol (mmol/l)					
Control	5.1 \pm 0.8	4.9 \pm 0.8			
EXam	5.1 \pm 0.6	4.6 \pm 0.4	-0.14	-0.35 to 0.07	0.19
EXpm	4.3 \pm 0.6	3.7 \pm 0.5	-0.38	-0.59 to -0.18	<0.001
HDL (mmol/l)					
Control	1.01 \pm 0.2	0.99 \pm 0.2			
EXam	1.02 \pm 0.1	1.00 \pm 0.1	0.02	-0.03 to 0.07	0.36
EXpm	1.10 \pm 0.2	1.01 \pm 0.1	-0.02	-0.07 to 0.03	0.37
LDL (mmol/l)					
Control	3.4 \pm 0.7	3.3 \pm 0.7			
EXam	3.3 \pm 0.8	3.1 \pm 0.4	(-0.01)	(-0.04 to 0.02)	0.61
EXpm	2.9 \pm 0.5	2.4 \pm 0.5	(-0.05)	(-0.08 to -0.02)	0.001
Triacylglycerol (mmol/l)					
Control	1.48 \pm 0.6	1.35 \pm 0.6			
EXam	1.44 \pm 0.8	0.97 \pm 0.3	(-0.04)	(-0.10 to 0.01)	0.09
EXpm	0.83 \pm 0.1	0.68 \pm 0.1	(-0.09)	(-0.14 to -0.03)	0.002
Systolic blood pressure (mm Hg)					
Control	129 \pm 9	129 \pm 11			
EXam	125 \pm 11	124 \pm 4	-1.1	-4.3 to 2.1	0.50
EXpm	122 \pm 10	127 \pm 6	-0.9	-4.5 to 2.0	0.42
Diastolic blood pressure (mm Hg)					
Control	84 \pm 4	87 \pm 9			
EXam	80 \pm 5	80 \pm 2	-1.6	-3.6 to 0.4	0.12
EXpm	82 \pm 6	83 \pm 4	-1.4	-3.4 to 0.6	0.17
EVENING (postprandial)					
Glucose (mmol/l)					
Control	5.2 \pm 0.4	5.1 \pm 0.5			
EXam	4.9 \pm 0.4	4.7 \pm 0.5	-0.11	-0.26 to 0.03	0.12
EXpm	5.2 \pm 0.8	4.6 \pm 0.3	-0.12	-0.26 to 0.03	0.11
Insulin (pmol/l)					
Control	432 \pm 252	283 \pm 145			
EXam	189 \pm 130	129 \pm 65	(-2.13)	(-3.67 to -0.60)	0.008
EXpm	230 \pm 161	139 \pm 99	(-1.89)	(-3.42 to 0.35)	0.02

Cholesterol (mmol/l)					
Control	5.4 ± 0.8	5.1 ± 0.7			
EXam	5.3 ± 0.8	4.7 ± 0.6	-0.15	-0.37 to 0.07	0.18
EXpm	4.5 ± 0.7	3.9 ± 0.5	-0.37	-0.59 to -0.15	0.002
Triacylglycerol (mmol/l)					
Control	2.97 ± 1.2	2.29 ± 0.6			
EXam	2.09 ± 0.7	1.78 ± 0.9	(-0.05)	(-0.11 to 0.01)	0.10
EXpm	1.73 ± 0.7	1.20 ± 0.3	(-0.09)	(-0.15 to -0.04)	0.003
HDL (mmol/l)					
Control	1.02 ± 0.1	1.01 ± 0.1			
EXam	1.05 ± 0.1	1.01 ± 0.1	0.00	-0.04 to 0.05	0.90
EXpm	1.12 ± 0.2	1.07 ± 0.2	0.01	-0.04 to 0.05	0.73
LDL (mmol/l)					
Control	3.1 ± 0.9	3.0 ± 0.8			
EXam	3.2 ± 0.7	2.9 ± 0.4	-0.10	-0.30 to 0.11	0.36
EXpm	2.6 ± 0.5	2.3 ± 0.4	-0.25	-0.45 to -0.04	0.02
Systolic blood pressure (mm Hg)					
Control	132 ± 5	132 ± 9			
EXam	133 ± 9	129 ± 8	-0.9	-3.4 to 1.6	0.47
EXpm	131 ± 6	132 ± 4	-0.1	-2.6 to 2.4	0.94
Diastolic blood pressure (mm Hg)					
Control	86 ± 7	88 ± 6			
EXam	84 ± 6	83 ± 6	-1.6	-3.6 to 0.4	0.11
EXpm	86 ± 6	84 ± 5	-1.3	-3.3 to 0.7	0.19

ESM Table 7. Fasting and postprandial circulating markers of metabolic health and blood pressure after five days of high-fat diet (HFD) and at study completion, according to group. Values are observed means \pm SD. Estimates with 95% CI and *p* values for the effect of evening exercise (EXpm) compared to morning exercise (EXAm), from linear mixed models. Data were log or square root transformed when they had non-normal distribution (insulin, triacylglycerol, HOMA-IR, morning LDL). Estimates and 95% CIs for log-transformed variables are reported (in brackets).

	After 5 d high-fat diet	At study completion	Estimate	95% CI	<i>p</i> value
MORNING (fasting)					
Glucose (mmol/l)					
EXAm	4.9 \pm 0.5	4.8 \pm 0.3			
EXpm	4.6 \pm 0.2	4.4 \pm 0.2	-0.15	-0.24 to -0.03	0.02
Insulin (pmol/l)					
EXAm	74 \pm 52	36 \pm 19			
EXpm	40 \pm 24	24 \pm 10	(-0.48)	(-1.23 to -0.27)	0.20
HOMA-IR					
EXAm	2.33 \pm 1.2	1.48 \pm 0.8			
EXpm	1.63 \pm 1.2	1.15 \pm 0.6	(-0.09)	(-0.24 to 0.06)	0.22
Cholesterol (mmol/l)					
EXAm	5.1 \pm 0.6	4.6 \pm 0.4			
EXpm	4.3 \pm 0.6	3.7 \pm 0.5	-0.25	-0.46 to -0.04	0.02
HDL (mmol/l)					
EXAm	1.02 \pm 0.1	1.00 \pm 0.1			
EXpm	1.10 \pm 0.2	1.01 \pm 0.1	-0.04	-0.09 to 0.00	0.08
LDL (mmol/l)					
EXAm	3.3 \pm 0.8	3.1 \pm 0.4			
EXpm	2.9 \pm 0.5	2.4 \pm 0.5	(-0.04)	(-0.07 to -0.01)	0.006
Triacylglycerol (mmol/l)					
EXAm	1.44 \pm 0.8	0.97 \pm 0.3			
EXpm	0.83 \pm 0.1	0.68 \pm 0.1	(-0.04)	(-0.09 to 0.01)	0.12
Systolic blood pressure (mm Hg)					
EXAm	125 \pm 11	124 \pm 4			
EXpm	122 \pm 10	127 \pm 6	-0.2	-3.5 to 2.0	0.89
Diastolic blood pressure (mm Hg)					
EXAm	80 \pm 5	80 \pm 2			
EXpm	82 \pm 6	83 \pm 4	-0.2	-1.9 to 2.2	0.17
EVENING (postprandial)					
Glucose (mmol/l)					
EXAm	4.9 \pm 0.4	4.7 \pm 0.5			
EXpm	5.2 \pm 0.8	4.6 \pm 0.3	-0.003	-0.15 to 0.14	0.96
Insulin (pmol/l)					
EXAm	189 \pm 130	129 \pm 65			
EXpm	230 \pm 161	139 \pm 99	(0.25)	(-1.29 to 1.78)	0.74
Cholesterol (mmol/l)					
EXAm	5.3 \pm 0.8	4.7 \pm 0.6			
EXpm	4.5 \pm 0.7	3.9 \pm 0.5	-0.21	-0.44 to 0.01	0.06
Triacylglycerol (mmol/l)					
EXAm	2.09 \pm 0.7	1.78 \pm 0.9			
EXpm	1.73 \pm 0.7	1.20 \pm 0.3	(-0.05)	(-0.10 to 0.01)	0.12
HDL (mmol/l)					
EXAm	1.05 \pm 0.1	1.01 \pm 0.1			
EXpm	1.12 \pm 0.2	1.07 \pm 0.2	0.004	-0.04 to 0.05	0.84
LDL (mmol/l)					
EXAm	3.2 \pm 0.7	2.9 \pm 0.4			

EXpm	2.6 ± 0.5	2.3 ± 0.4	-0.15	-0.36 to 0.06	0.15
Systolic blood pressure (mm Hg)					
EXam	133 ± 9	129 ± 8			
EXpm	131 ± 6	132 ± 4	0.8	-1.7 to 3.3	0.52
Diastolic blood pressure (mm Hg)					
EXam	84 ± 6	83 ± 6			
EXpm	86 ± 6	84 ± 5	-0.3	-1.7 to 2.3	0.77

ESM Table 8. Metabolites differently changed in morning samples after evening exercise compared to no exercise, using linear mixed model.

	Change (%) after morning exercise (EXAm)	Change (%) after evening exercise (EXpm)	Change (%) after no exercise (CON)	<i>q</i> value between-group difference between EXpm and CON
androsterone sulfate	12.2	33.4	-9.9	<0.0001
epiandrosterone sulfate	10.9	40.5	-6.2	<0.0001
5alpha-androstan-3alpha,17beta-diol monosulfate (1)	8.8	38.4	-15.0	<0.0001
andro steroid monosulfate C19H28O6S (1)	46.8	64.4	-4.5	<0.0001
16a-hydroxy DHEA 3-sulfate	34.8	64.2	-1.6	<0.0001
carnitine	-6.8	-10.5	3.6	<0.0001
1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)	-6.7	-17.5	3.3	0.001
5alpha-androstan-3beta,17beta-diol monosulfate (2)	17.8	45.9	-16.4	0.001
androstenediol (3beta,17beta) disulfate (2)	11.3	19.2	-0.6	0.002
1-stearoyl-2-oleoyl-GPC (18:0/18:1)	-10.2	-16.7	-1.8	0.002
1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)	-20.0	-38.2	-1.8	0.002
tryptophan	-5.6	-6.4	3.1	0.003
dehydroisoandrosterone sulfate (DHEA-S)	-1.4	18.0	-4.7	0.004
alpha-hydroxyisovalerate	56.8	64.5	-6.3	0.004
gamma-glutamylglycine	1.4	-9.2	16.7	0.005
1-linoleoylglycerol (18:2)	-20.2	11.2	-29.0	0.007
pyroglutamine	-8.8	-17.4	4.0	0.007
N-acetylthreonine	-7.6	-9.7	3.3	0.007
2-hydroxy-3-methylvalerate	19.4	62.5	-5.8	0.007
hippurate	-11.3	156.1	44.8	0.007
acetoacetate	130.8	222.4	24.9	0.007
3-hydroxybutyrylglycine	157.4	176.5	11.8	0.008
1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)	-11.5	-18.7	-4.0	0.008
androstenediol (3alpha, 17alpha) monosulfate (3)	-4.3	11.0	-4.5	0.008
gamma-glutamylserine	12.9	-4.5	19.1	0.008
suberate (C8-DC)	171.4	291.1	35.6	0.010
2-hydroxybutyrate/2-hydroxyisobutyrate	47.0	71.4	-3.8	0.010
azelate (C9-DC)	109.7	341.9	128.8	0.010
sphingomyelin (d17:1/14:0, d16:1/15:0)	-19.1	-20.9	1.3	0.012
androstenediol (3beta,17beta) monosulfate (1)	-1.1	18.9	-11.0	0.012
beta-hydroxybutyrate (βOHB)	184.7	379.2	25.5	0.015
dihydroorotate	0.9	-5.1	15.3	0.015
isobutyrylglycine	57.5	44.2	-26.7	0.022
2-methylcitrate/homocitrate	6.2	28.3	-5.5	0.023
succinylcarnitine (C4-DC)	-15.0	-37.4	-11.2	0.024
sphingomyelin (d18:2/14:0, d18:1/14:1)	-14.9	-20.2	-2.3	0.024
indolelactate	22.6	30.1	4.0	0.024
androstenediol (3beta,17beta) disulfate (1)	4.5	6.5	-15.8	0.026
3-hydroxysebacate	44.6	89.5	-17.9	0.028
3-hydroxybutyrylcarnitine (1)	145.1	187.6	16.5	0.029
5alpha-androstan-3beta,17beta-diol disulfate	2.9	3.3	-13.4	0.029
6-bromotryptophan	1.9	-22.1	-0.3	0.029
propionylcarnitine (C3)	-23.7	-29.2	-6.7	0.030
pantothenate	6.7	12.2	-5.9	0.032
hexanoylglycine	119.4	138.6	113.9	0.033
citrate	34.1	52.0	10.9	0.041
mannonate	1.2	-4.2	14.0	0.046
tyrosine	-4.1	-9.7	2.1	0.046

myristoyl dihydrosphingomyelin (d18:0/14:0)	-21.1	-17.8	-3.7	0.046
N-acetyl glycine	53.5	37.6	12.5	0.046
aconitate [cis or trans]	28.4	57.2	18.9	0.046
ceramide (d16:1/24:1, d18:1/22:1)	-12.9	-20.0	3.0	0.046
creatine	-17.9	-26.7	-3.2	0.046
4-methylcatechol sulfate	-3.6	81.9	7.7	0.046
1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)	-29.9	-37.5	-12.6	0.046
5alpha-androstan-3beta,17alpha-diol disulfate	8.5	32.3	-2.1	0.048

ESM Table 9. Metabolites differently changed in evening samples with evening exercise compared to no exercise, using linear mixed model.

	Change (%) after morning exercise (EXam)	Change (%) after evening exercise (EXpm)	Change (%) after no exercise (CON)	<i>q</i> value between-group difference between EXpm and CON
androsterone sulfate	13.10	41.980	-7.239	<0.0001
epiandrosterone sulfate	15.16	48.003	-3.343	0.0004
5alpha-androstan-3alpha,17beta-diol monosulfate (1)	15.35	39.303	-9.318	0.0017
1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)	-10.85	-14.717	-1.195	0.0080
5alpha-androstan-3beta,17beta-diol monosulfate (2)	20.74	50.269	-11.331	0.0117
betaine	-2.82	4.880	-11.805	0.0129
alpha-hydroxyisovalerate	31.02	55.338	-14.765	0.0232