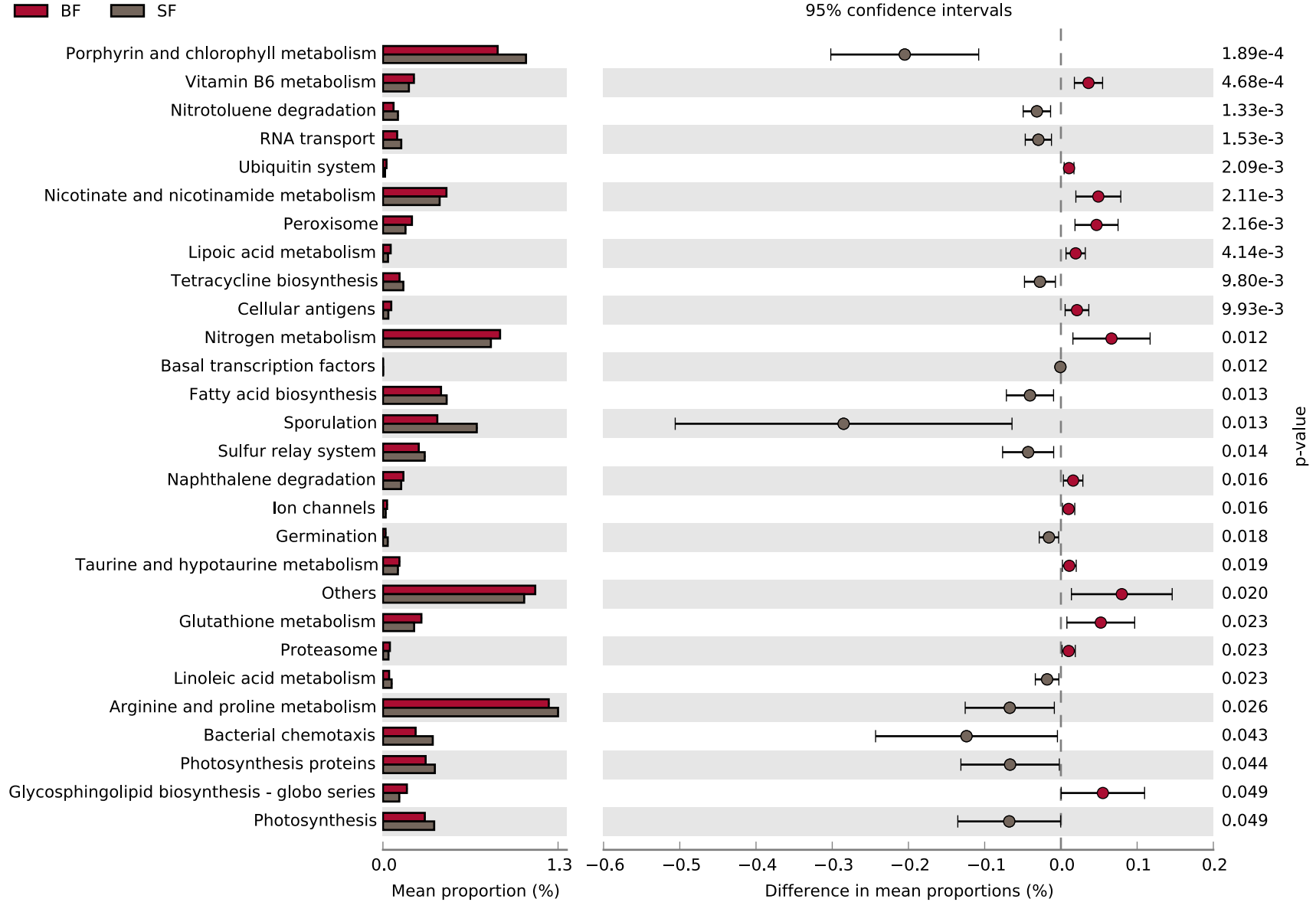
On-line Supplementary Material

Lauren Brink et al. Neonatal diet alters fecal microbiota and metabolome profiles over the first year of life in infants fed breast milk or formula.



Supplemental Figure 1: The figures shows the significant metabolic pathways of the corresponding OTUs generated by QIIME for microbial communities between BF and SF at 3 months of age.

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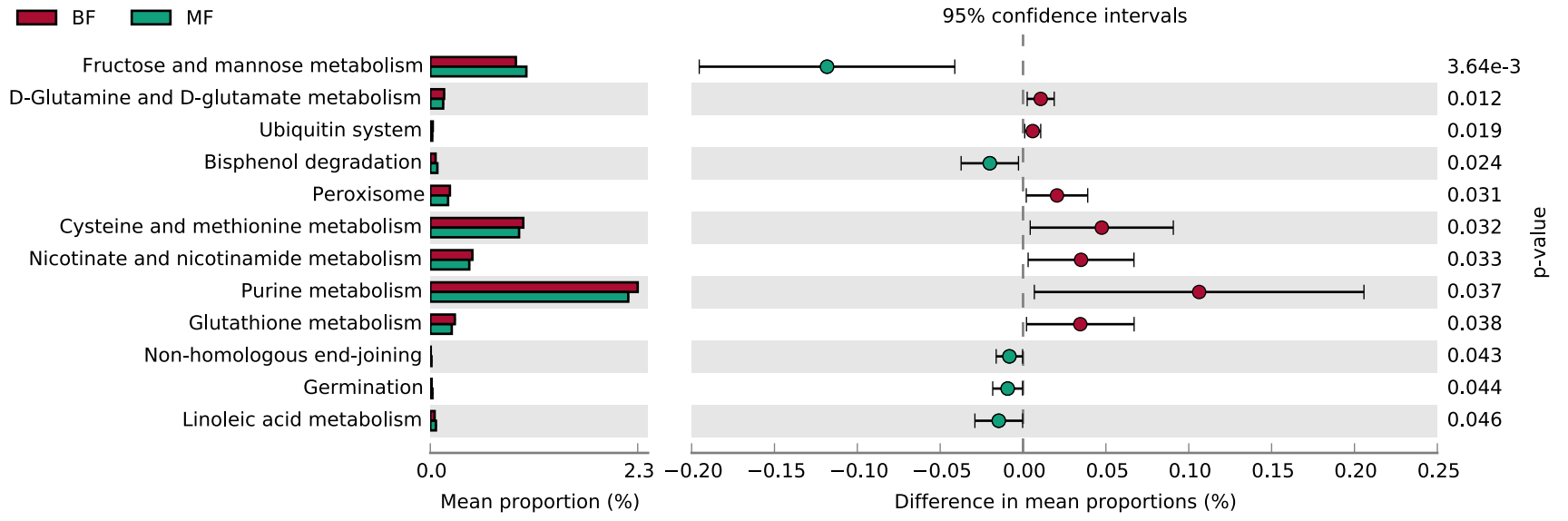

Supplemental Figure 2: The figures shows the significant metabolic pathways of the corresponding OTUs generated by QIIME for microbial communities between BF and MF at 6 months of age.

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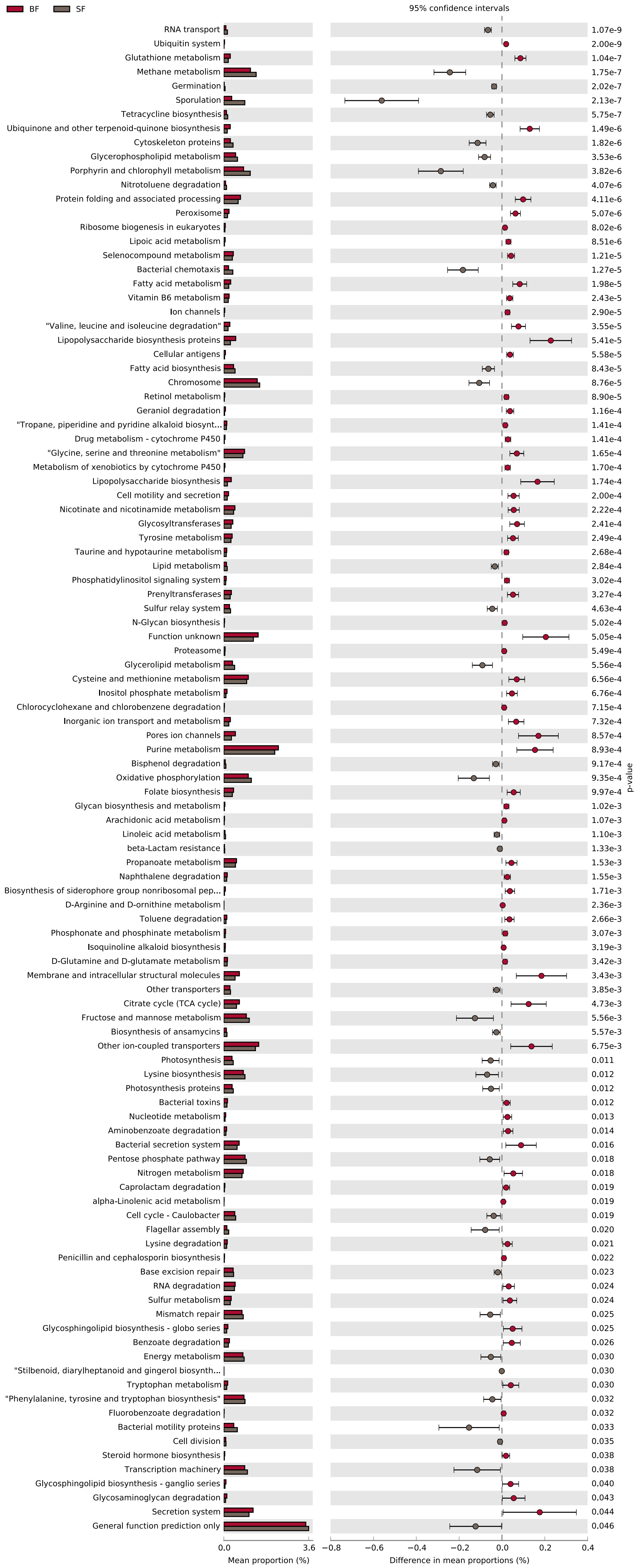

Supplemental Figure 3: The figures shows the significant metabolic pathways of the corresponding OTUs generated by QIIME for microbial communities between BF and SF at 6 months of age.

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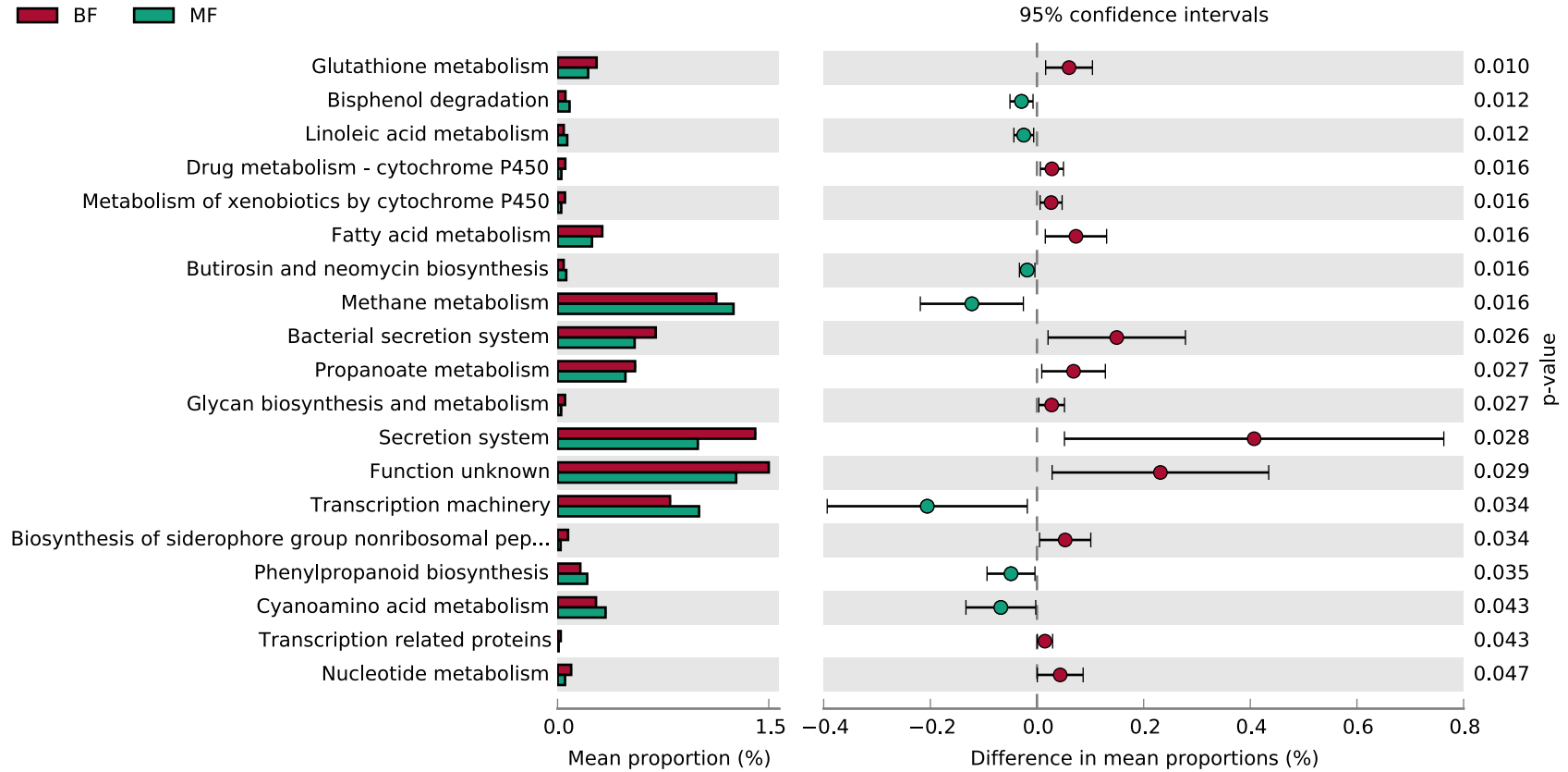

Supplemental Figure 4: The figures shows the significant metabolic pathways of the corresponding OTUs generated by QIIME for microbial communities between BF and MF at 9 months of age.

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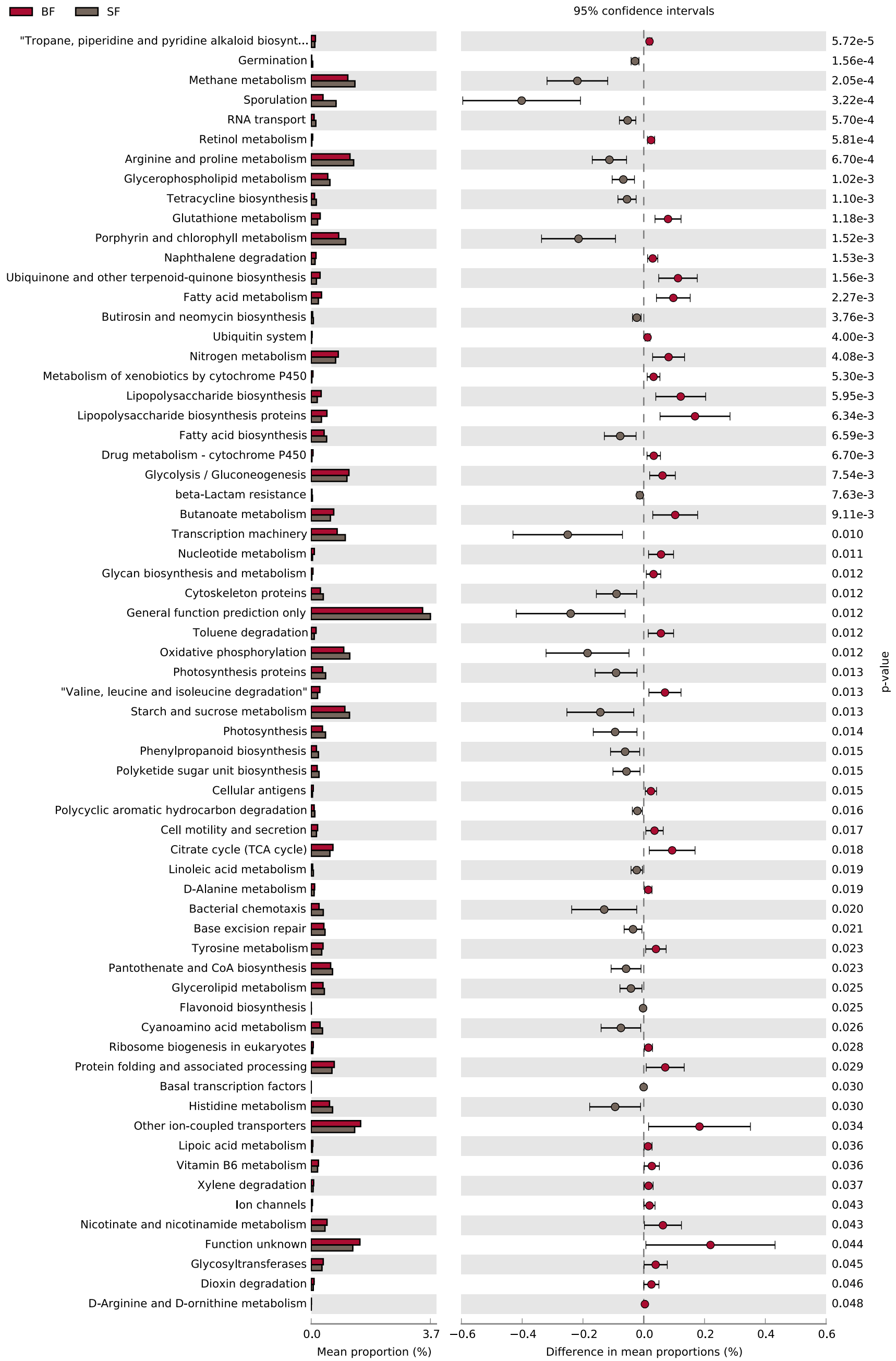

Supplemental Figure 5: The figures shows the significant metabolic pathways of the corresponding OTUs generated by QIIME for microbial communities between BF and SF at 9 months of age.

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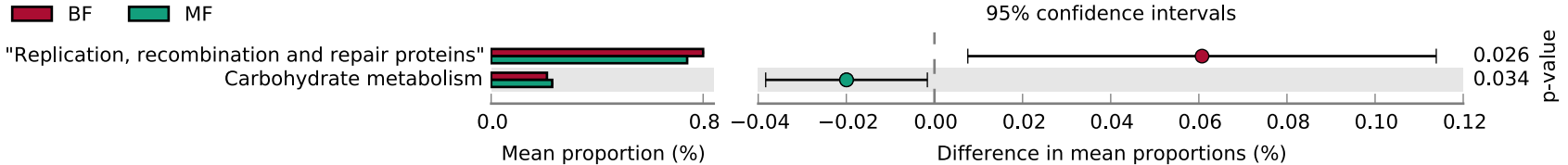

Supplemental Figure 6: The figures shows the significant metabolic pathways of the corresponding OTUs generated by QIIME for microbial communities between BF and MF at 12 months of age.

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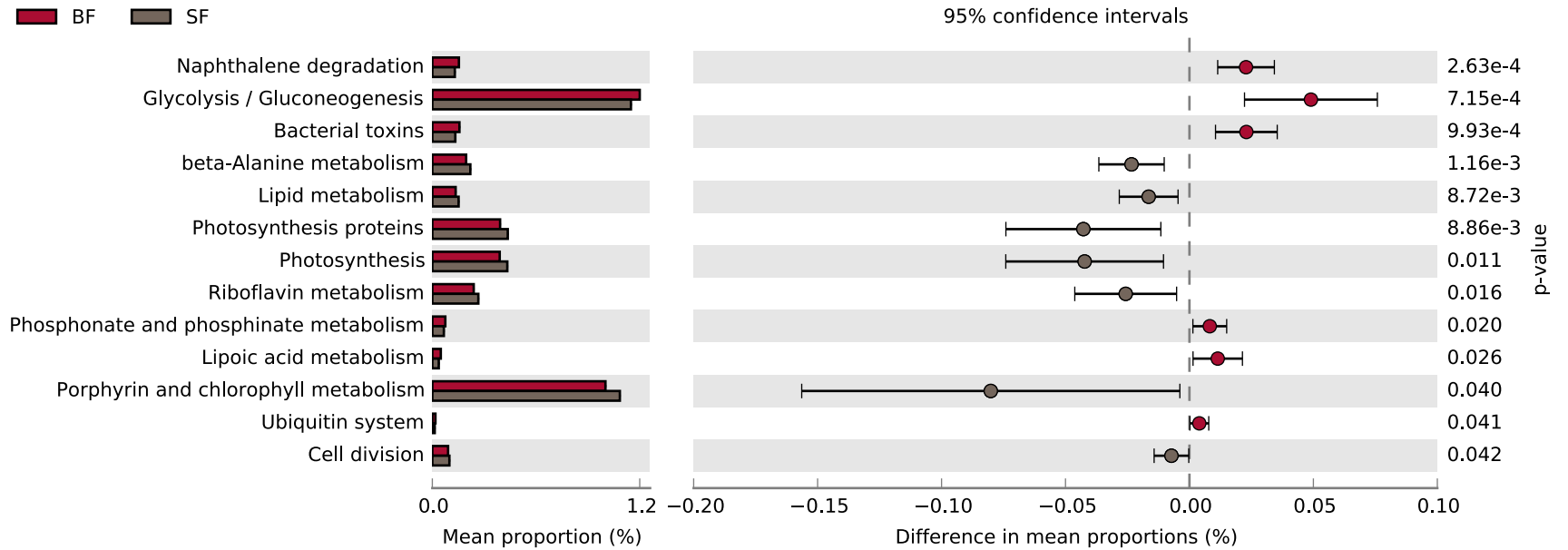

Supplemental Figure 7: The figures shows the significant metabolic pathways of the corresponding OTUs generated by QIIME for microbial communities between BF and SF at 12 months of age.

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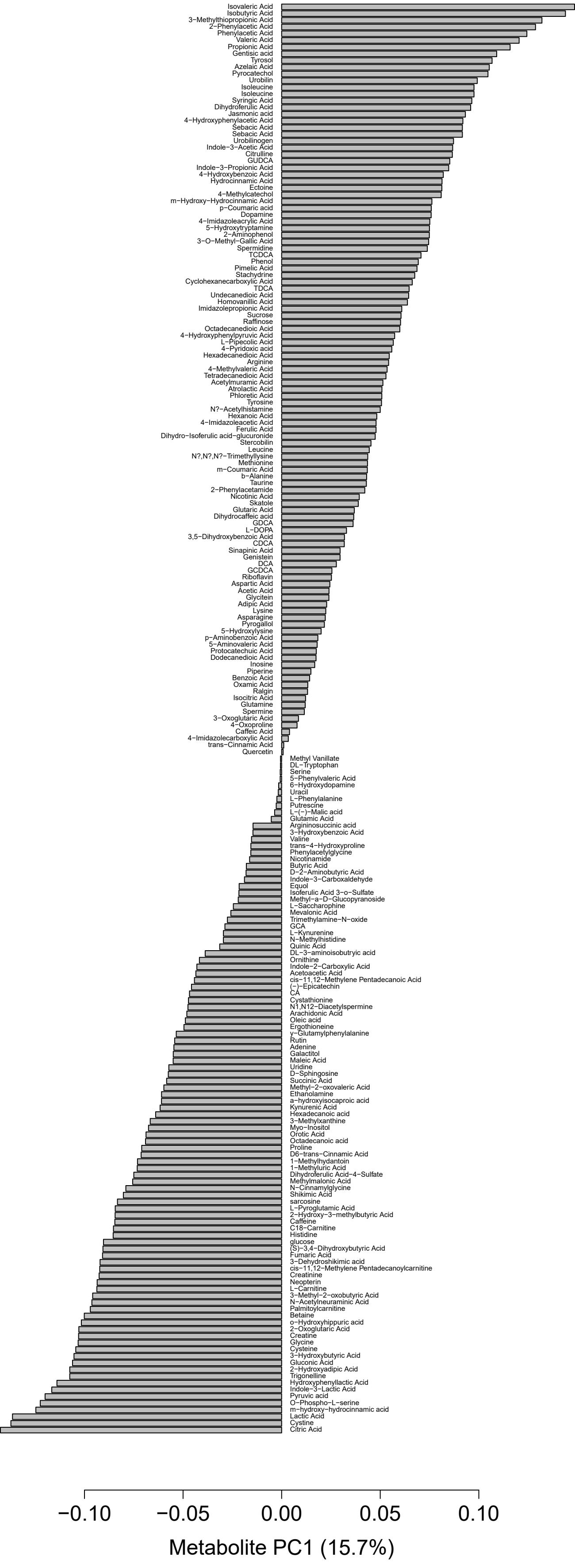

Supplemental Figure 8: PCA loading values associated with each metabolite along principal component 1. All metabolite were scaled to unit variance prior to PCA analysis. Largest absolute loading values (i.e., positive and negative values) contribute the greatest variance to principal component 1

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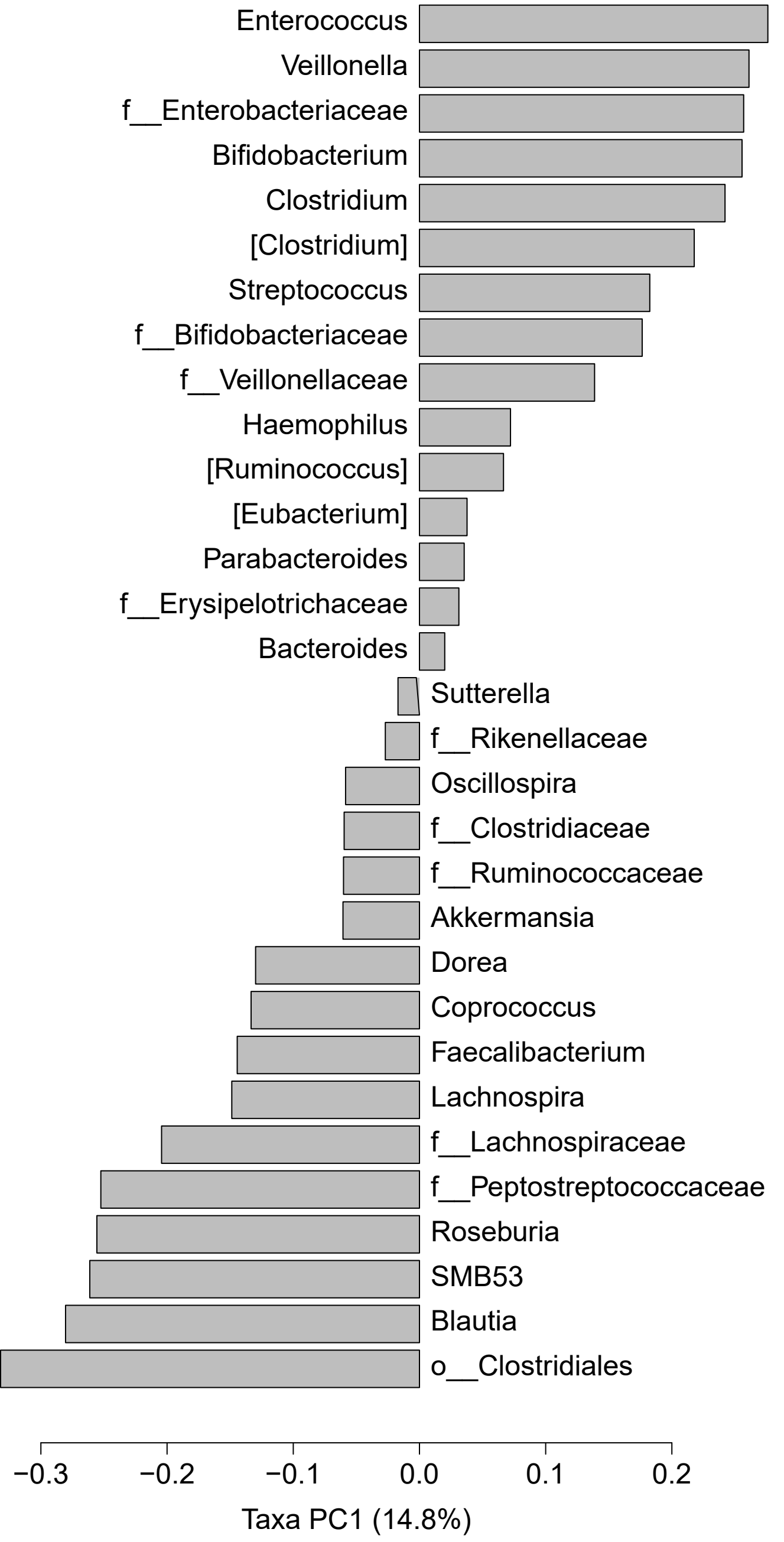

Supplemental Figure 9: PCA loading values associated with each genera along principal component 1. All genera were included in PCA. Data were centered-log transformed prior to PCA analysis. Zero counts were imputed using geometric Bayesian multiplicative imputation prior to transformation. Largest absolute loading values (i.e., positive and negative values) contribute the greatest variance to principal component 1.

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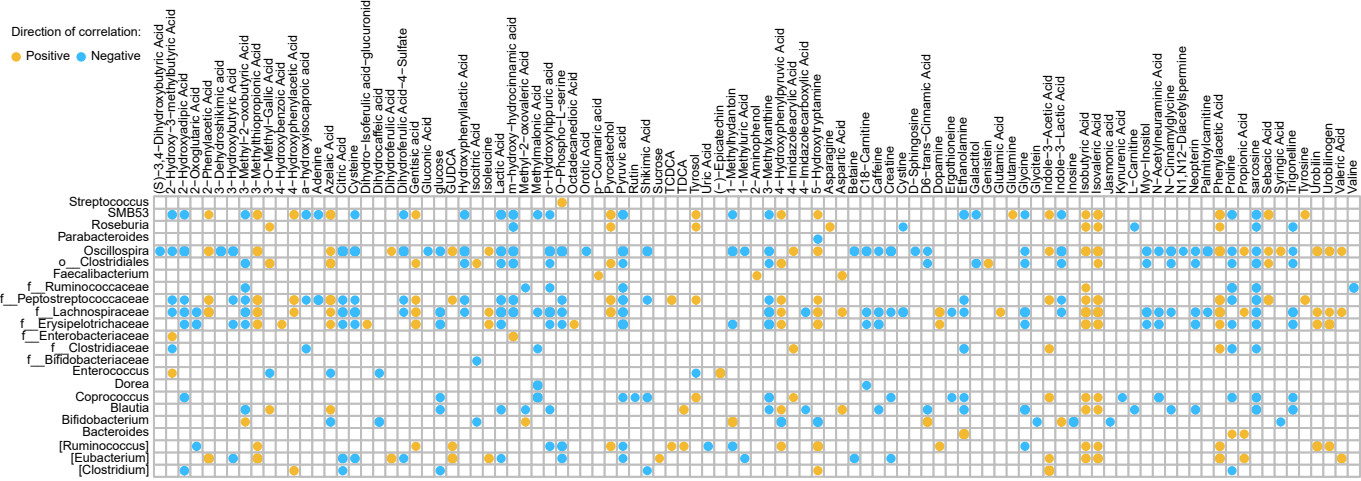

Supplemental Figure 10: Pearson Correlations of metabolites significantly affected by infant diet to center log transformed microbiome data at six months of age. Sample numbers were n=188. Data were presented at a significance level of FDR P<0.05.

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Supplementary Table 1. List of metabolite standards used for identification with mass spectrometry[1].

Metabolite	Alternate name	Formula	MW	M-H	M+H	RT
(-)-Epicatechin	(-)-Catechuic acid	C15H14O6	290.080	289.072	291.086	6.563
(+/-)-Catechin	(+)-Catechol	C15H14O6	290.078	289.072	291.086	6.002
(±)-Jasmonic acid		C12H18O3	210.125	209.118	211.133	9.368
(S)-(+)-2-Methylbutyric Acid	(S)-2-Methylbutanoic Acid	C5H10O2	102.068	101.061	103.075	7.216
(S)-3,4-Dihydroxybutyric Acid	2-Deoxytetronic Acid	C4H8O4	120.042	119.035	121.050	0.758
11-Bromoundecanoic Acid		C11H21BrO2	264.073	263.065	265.080	11.310
1-Methylhydantoin	1-Methylimidazolidine-2,4-dione	C4H6N2O2	114.043	113.036	115.050	1.240
1-Methyluric Acid	1-Mehtyl-2,6,8-trihydroxypurine	C6H6N4O3	182.043	181.037	183.051	2.896
2,3-Dihydroxybenzoic Acid		C7H6O4	154.026	153.019	155.034	7.152
2,5-Furandicarboxylic Acid	Dehydromucic Acid	C6H4O5	156.005	154.999	157.013	6.025
2-Aminophenol		C6H7NO	109.053	108.045	110.060	0.569
2-Butyl-3-(4-hydroxybenzoyl)benzofuran	(2-Butylbenzofuran-3-yl)(4-hydroxyphenyl)ketone	C19H18O3	294.126	293.118	295.133	11.318
2-Ethylhexanoic Acid		C8H16O2	144.116	143.108	145.122	10.060
2-Heptyl-3-Hydroxyl-4-Quinolone		C16H21NO2	259.157	258.150	260.165	10.321
2-Hydroxy-3-methylbutyric Acid	a-Hydroxyisovaleric Acid	C5H10O3	118.062	117.056	119.070	4.606
2-Hydroxyadipic Acid	2-Hydroxyhexanedioic Acid	C6H10O5	162.052	161.046	163.060	2.131
2-Hydroxybenzoic Acid	o-Salicylic Acid	C7H6O3	138.031	137.024	139.039	9.148
2-Oxoglutaric Acid	a-Ketoglutaric Acid	C5H6O5	146.021	145.014	147.029	2.951
2-Phenylacetamide	Acetanilide	C8H9NO	135.069	134.061	136.076	6.006
2-Phenylacetic Acid	a-Toluate	C8H8O2	136.052	135.045	137.060	8.158
3,4-Dihydroxybenzoic Acid	Protocatechuic Acid	C7H6O4	154.026	153.019	155.034	4.309
3,5-Dihydroxybenzoic Acid	a-Resorcylic Acid	C7H6O4	154.026	153.019	155.034	4.153
3-Dehydroquinic acid		C7H10O6	190.048	189.040	191.055	0.991
3-Dehydroshikimic acid		C7H8O5	172.038	171.030	173.044	1.589

3-Hydroxybenzoic Acid	m-Salicylic Acid	C7H6O3	138.032	137.024	139.039	6.310
3-Hydroxybutyric Acid	DL-b-Hydroxybutryic Acid	C4H8O3	104.048	103.040	105.055	1.517
3-Hydroxy-DL-Kynurenine	Hydroxykynurenine	C10H12N2O4	224.080	223.072	225.087	1.110
3-Methyl-2-oxobutyric Acid	α-Ketoisovaleric acid	C5H8O3	116.047	115.040	117.055	6.216
3-Methylthiopropionic Acid	4-Thiapentanoic Acid	C4H8O2S	120.024	119.017	121.032	5.092
3-Methylxanthine		C6H6N4O2	166.050	165.042	167.056	3.336
3-O-Methyl-Gallic Acid	3,4-dihydroxy-5-methoxybenzoic Acid	C8H8O5	184.038	183.030	185.044	5.290
3-Oxoglutaric Acid	b-Ketoglutaric Acid	C5H6O5	146.021	145.014	147.029	1.543
4-Ethylphenol		C8H10O	122.073	121.066	123.080	9.165
4-Ethylphenyl Sulfate	4-EPS	C8H10O4S	202.029	201.023	203.037	10.843
4-Hydroxybenzoic Acid	p-Salicylic Acid	C7H6O3	138.031	137.024	139.039	5.576
4-Hydroxyphenylacetic Acid	p-hydroxyphenylacetic Acid	C8H8O3	152.048	151.040	153.055	5.891
4-Hydroxyphenylpyruvic Acid	4-Hydroxyphenylpyruvate	C9H8O4	180.042	179.035	181.050	*8.220 pos; 8.514 neg*
4-Imidazoleacetic Acid		C5H6N2O2	126.042	125.036	127.050	0.457
4-Imidazoleacrylic Acid	Urocanic Acid	C6H6N2O2	138.042	137.036	139.050	0.538
4-Imidazolecarboxylic Acid		C4H4N2O2	112.027	111.020	113.035	0.566
4-Methylcatechol	3,4-dihydroxytoluene	C7H8O2	124.053	123.045	125.060	6.833
4-Methylvaleric Acid	Isocaproic Acid	C6H12O2	116.083	115.076	117.091	8.880
4-Oxoproline		C5H7NO3	129.043	128.035	130.050	0.561
4-Pyridoxic acid		C8H9NO4	183.054	182.046	184.060	2.618
5-Aminolevulinic acid		C5H9NO3	131.059	130.051	132.066	0.407
5-Aminovaleric Acid	5-Aminovalerate	C5H11NO2	117.078	116.072	118.086	0.433
5-Hydroxyindole		C8H7NO	133.052	132.045	134.060	5.250
5-Hydroxyindoleacetic Acid	5HIAA	C10H9NO3	191.059	190.051	192.066	5.732
5-Hydroxylysine		C6H14N2O3	162.100	161.093	163.108	0.375
5-Hydroxytryptamine	5HT	C10H12N2O	176.094	175.088	177.102	0.920
5-Hydroxytryptophan	5HTP	C11H12N2O3	220.084	219.078	221.092	1.815

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6-Hydroxydopamine	Oxidopamine	C8H11NO3	169.073	168.067	170.081	0.450
6-Sulfatoxymelatonin	6-Hydroxymelatonin Sulfate	C13H16N2O6S	328.072	327.066	329.080	8.467
7α-Hydroxy-4-cholesten-3-one	C4	C27H44O2	400.334	399.327	401.341	13.443
Acetic Acid	Ethanoic Acid	C2H4O2	60.021	59.014	61.028	0.977
Acetoacetic Acid	Diacetic Acid	C4H6O3	102.031	101.024	103.039	1.476
Acetylcholine		C7H16NO2	146.119	145.111	147.125	0.424
Acetylmuramic Acid		C11H19NO8	293.112	292.104	294.118	2.650
Adenine		C5H5N5	135.055	134.047	136.062	0.550
Adenosine		C10H13N5O4	267.097	266.089	268.104	1.761
Adipic Acid	Hexanedioic Acid	C6H10O4	146.057	145.051	147.065	4.939
a-Hydroxyhippuric Acid	Benzoylaminohydroxyacetic Acid	C9H9NO4	195.053	194.046	196.060	8.884
a-Hydroxyisobutyric Acid	2-Hydroxybutanoic Acid	C4H8O3	104.048	103.040	105.055	1.851
a-Hydroxyisocaproic Acid	2-Hydroxy-4-methylvaleric acid	C6H12O3	132.078	131.071	133.086	6.660
Amantadine	1-Adamantylamine	C10H17N	151.136	150.129	152.143	4.612
aMCA	alpha-Muricholic Acid	C24H40O5	408.288	407.280	409.295	9.787
Aminomalonic Acid	2-aminopropanedioic acid	C3H5NO4	119.021	118.015	120.029	0.880
Anserine	β-alanyl-N-methylhistidine	C10H16N4O3	240.123	239.115	241.130	0.364
Arachidic Acid	Eicosanoic Acid	C20H40O2	312.302	311.296	313.310	14.538
Arachidonic Acid	Vitamin F	C20H32O2	304.241	303.233	305.248	12.674
Arginine	ARG	C6H14N4O2	174.112	173.104	175.119	0.388
Argininosuccinic acid		C10H18N4O6	290.123	289.115	291.130	0.529
Asparagine	ASN	C4H8N2O3	132.054	131.046	133.061	0.527
Aspartic Acid	ASP	C4H7NO4	133.038	132.030	134.045	0.608
Atrolactic Acid	2-Phenyllactic Acid	C9H10O3	166.062	165.056	167.070	7.466
Azelaic Acid	Nonanedioic Acid	C9H16O4	188.104	187.098	189.112	8.470
b-Alanine		C3H7NO2	89.047	88.040	90.055	0.417
Benalfocin	SKF 86466	C11H14ClN	195.081	194.074	196.089	5.037
Benzoic Acid	Benzenecarboxylic Acid	C7H6O2	122.036	121.030	123.044	8.190
Betaine	Trimethylglycine	C5H11NO2	117.078	116.072	118.086	0.567

bMCA	beta-Muricholic Acid	C24H40O5	408.288	407.280	409.295	9.903
b-Pseudouridine		C9H12N2O6	244.070	243.062	245.077	0.912
Butylamine	1-Aminobutane	C4H11N	73.089	72.082	74.096	0.531
Butyric Acid	Butanoic Acid	C4H8O2	88.053	87.045	89.060	4.976
CA	Cholic Acid	C24H40O5	408.288	407.280	409.295	10.179
Caffeic Acid	3,4-dihyroxycinnamate	C9H8O4	180.042	179.035	181.050	6.443
Caffeine		C8H10N4O2	194.080	193.073	195.088	6.051
CDCA	Chenodeoxycholic acid	C24H40O4	392.293	391.285	393.300	10.944
CDCA-S	Chenodeoxycholic Acid-3-Sulfate	C24H40O7S	472.250	471.242	473.257	13.059
Chlorogenic acid	3-(3,4-Dihydroxycinnamoyl)quinic acid	C16H18O9	354.096	353.088	355.102	6.653
cis-11,12-Methylene Pentadecanoic Acid		C16H30O2	254.224		255.232	12.655
cis-11,12-Methylene Pentadecanoylcarnitine		C23H43NO4	397.319		398.326	10.061
cis-13,14-Methylene Heptadecanoic Acid		C18H34O2	282.255		283.263	13.239
cis-13,14-Methylene Heptadecanoylcarnitine		C25H47NO4	425.350		426.358	9.434
cis-3,4-Methylene Heptanoic acid		C8H14O2	142.099	141.092	143.107	9.643
cis-3,4-Methylene heptanoylcarnitine		C15H27N04	285.194		286.201	7.291
Citric Acid		C6H8O7	192.026	191.020	193.034	1.761
Citrulline		C6H13N3O3	175.096	174.088	176.103	0.542
Clomipramine		C19H23ClN2	314.156	313.148	315.162	8.939
CMPF	3-Carboxy-4-methyl-5-propyl-2-furanpropionic Acid	C12H16O5	240.099	239.092	241.107	9.701
Cortisone	17α,21-dihydroxypregn-4-ene-3,11,20-trione	C21H28O5	360.194	359.186	361.201	9.046
Creatine		C4H9N3O2	131.070	130.062	132.077	0.523
Creatinine		C4H7N3O	113.059	112.052	114.066	0.404

Crotonobetaine	Croton Betaine	C7H13NO2	143.094	142.087	144.102	0.439
Cyclohexanecarboxylic Acid		C7H12O2	128.084	127.076	129.091	8.945
Cyclopropylacetic acid		C5H8O2	100.052		101.060	5.573
Cyclopropylacetylcarnitine		C12H21NO4	243.147		244.154	1.611
Cystathionine		C7H14N2O4S	222.068	221.060	223.075	0.500
Cysteine	CYS	C3H7NO2S	121.020	120.012	122.027	0.575
Cystine	oxidized cysteine	C6H12N2O4S2	240.023	239.017	241.031	0.518
D-(+)-Glucose		C6H12O6	180.063	179.056	181.071	0.585
D-2-Aminobutyric Acid		C4H9NO2	103.064	102.056	104.071	0.554
DCA	Deoxycholic acid	C24H40O4	392.293	391.285	393.300	11.036
Decanoic Acid	Capric Acid	C10H20O2	172.147	171.139	173.154	11.074
Difenpiramide		C19H16N2O	288.127	287.119	289.134	10.225
Dihydro Isoferulic Acid 3-o-b-D-Glucuronide	5-(2-Carboxyethyl)-2-methoxyphenyl beta-D-glucopyranosiduronic acid	C16H20O10	372.105	371.098	373.113	7.224
Dihydrocaffeic acid	3,4-Dihydroxyhydrocinnamic acid	C9H10O4	182.058	181.051	183.065	5.903
Dihydroferulic Acid	3-(4-hydroxy-3-methoxyphenyl) propionic Acid	C10H12O4	196.074	195.066	197.081	7.453
Dihydroferulic Acid-4-Sulfate	3-(3-methoxy-4-sulfooxyphenyl) propionic Acid	C10H12O7S	276.031	275.023	277.038	8.553
Dihydrozeatin Riboside		C15H23N5O5	353.170	352.163	354.177	5.836
Dikegulac	Diprogulic Acid	C12H18O7	274.106	273.098	275.113	8.663
Dimethylalanine	N,N-Dimethyl-L-alanine	C5H11NO2	117.080	116.072	118.086	0.606
DL-3-Aminoisobutyric Acid	3-aminoisobutanoic Acid	C4H9NO2	103.064	102.056	104.071	0.441
Dodecanedioic Acid		C12H22O4	230.151	229.145	231.159	9.802
Dodecanoic Acid	Lauric Acid	C12H24O2	200.178	199.170	201.185	11.819
Dopamine		C8H11NO2	153.078	152.072	154.086	0.486
D-Sedoheptulose-7-Phosphate		C7H15O10P	290.041	289.033	291.048	1.461
D-Sphingosine		C18H37O2N	299.283	298.275	300.290	9.838
Ectoine		C6H10N2O2	142.075	141.067	143.082	0.568
Enanthic Acid	Heptanoic Acid	C7H14O2	130.099	129.092	131.107	9.703

Equol		C15H14O3	242.094	241.087	243.102	9.407
Equol-4'-Sulfate		C15H14O6S	322.051	321.044	323.058	10.650
Ergothioneine		C9H15N3O2S	229.089	228.081	230.096	*0.648*
Estriol	Oestriol	C18H24O3	288.172	287.165	289.180	8.768
Ethanolamine	2-aminoethanol	C2H7NO	61.053	60.045	62.060	0.404
Ethyl-b-D-Glucuronide		C8H14O7	222.073	221.067	223.081	2.106
Ferulic Acid	4-Hydroxy-3-methoxycinnamic Acid	C10H10O4	194.057	193.051	195.065	7.888
Folic Acid	Folate	C19H19N7O6	441.139	440.132	442.147	6.134
Fructose		C6H12O6	180.063	179.056	181.071	0.600
Fumaric Acid	trans-Butenedioic Acid	C4H4O4	116.010	115.004	117.018	2.134
Galactitol	Dulcitol	C6H14O6	182.078	181.072	183.086	0.580
Gallic Acid	3,4,5-Trihydroxybenzoic Acid	C7H6O5	170.022	169.014	171.029	2.057
GCA	Glycocholic acid	C26H43NO6	465.310	464.302	466.316	9.688
GCDCA	Glycochenodeoxycholic Acid	C26H43NO5	449.315	448.307	450.321	10.271
GDCA	Glycodeoxycholic Acid	C26H43NO5	449.315	448.307	450.321	10.377
Genistein	4',5,7-Trihydroxyisoflavone	C15H10O5	270.053	269.046	271.060	9.451
Genistin	Genistein-7-Glucoside	C21H20O10	432.106	431.098	433.113	8.140
Gentisic acid	2,5-Dihydroxybenzoate	C7H6O4	154.027	153.019	155.034	6.472
GHCA	Glycohyocholic Acid	C26H43NO6	465.310	464.302	466.316	9.501
GHDCA	Glycohyodeoxycholic Acid	C26H43NO5	449.315	448.307	450.321	9.722
GLCA	Glycolithocholic Acid	C26H43NO4	433.320	432.312	434.326	11.136
Gluconic Acid		C6H12O7	196.058	195.051	197.066	0.770
Glutamic Acid	GLU	C5H9NO4	147.054	146.046	148.060	0.565
Glutamine	GLN	C5H10N2O3	146.070	145.062	147.076	0.534
Glutaric Acid	Pentanedioic Acid	C5H8O4	132.042	131.035	133.050	2.546
Glycerol-3-phosphate		C3H9O6P	172.013	173.021	171.006	1.668
Glycine	GLY	C2H5NO2	75.033	74.025	76.039	0.510
Glycitein	4',7-Dihydroxy-6-methoxyisoflavone	C16H12O5	284.069	283.061	285.076	9.010
Glycylvaline		C7H14N2O3	174.101	173.093	175.108	0.682

GUDCA	Glycoursodeoxycholic Acid	C26H43NO5	449.315	448.307	450.321	9.735
HCA	Hyocholic acid	C24H40O5	408.288	407.280	409.295	10.030
HDCA	Hyodeoxycholic acid	C24H40O4	392.293	391.285	393.300	10.340
Heneicosanoic Acid	Heneicosylic Acid	C21H42O2	326.318	325.311	327.326	15.153
Heptadecanoic Acid	Margaric Acid	C17H34O2	270.256	269.249		13.372
Hexadecanedioic Acid		C16H30O4	286.214	285.207	287.222	11.159
Hexadecanoic acid	Palmitic acid	C16H32O2	256.240	255.233	257.248	13.050
Hexanoic Acid	Caproic acid	C6H12O2	116.084	115.076	117.091	8.959
Histidine	HIS	C6H9N3O2	155.069	154.062	156.077	0.386
Hydrocinnamic Acid	Phenylpropionic Acid	C9H10O2	150.068	149.061	151.075	9.017
Hydroumbellic Acid	3-(2,4-dihydroxyphenyl)propanoic Acid	C9H10O4	182.058	181.051	183.065	5.971
Hydroxyphenyllactic Acid	DL-p-Hydroxyphenyllactic Acid	C9H10O4	182.058	181.051	183.065	5.385
Hypotaurine		C2H7NO2S	109.020	108.012	110.027	0.567
Imidazolepropionic Acid	Dihydrourocanic acid	C6H8N2O2	140.058	139.051	141.066	0.458
Indole		C8H7N	117.057	116.051	118.065	9.276
Indole-2-Carboxylic Acid		C9H7NO2	161.048	160.040	162.055	9.019
Indole-3-Acetic Acid	β-indole-3-acetic acid	C10H9NO2	175.064	174.056	176.071	8.349
Indole-3-Acrylic Acid	3-(1H-Indol-3-yl)-2-propenoic acid	C11H9NO2	187.064	186.056	188.071	8.857
Indole-3-Carboxaldehyde	b-Indolylaldehyde	C9H7NO	145.053	144.045	146.060	7.971
Indole-3-Lactic Acid		C11H11NO3	205.073	204.067	206.081	7.843
Indole-3-Pyruvic Acid		C11H9NO3	203.059	202.051	204.066	*9.126*
Indoxyl-b-D-Glucuronide		C14H15NO7	309.085	308.078	310.092	6.570
Inosine		C10H12N4O5	268.080	267.073	269.088	2.555
Isobutyric Acid	2-Methylpropanoic Acid	C4H8O2	88.053	87.045	89.060	5.058
Isocitric Acid		C6H8O7	192.028	191.020	193.034	1.203
Isoferulic Acid 3-o-Sulfate	3-[4-Methoxy-3-(sulfooxy)phenyl]-2-propenoic Acid	C10H10O7S	274.015	273.007	275.022	9.221
Isoferulic Acid-3-o-b-D-Glucuruonide		C16H18O10	370.091	369.083	371.097	7.177
Isoguanine	2-Hydroxyadenine	C5H5N5O	151.050	150.042	152.057	0.446

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Isoleucine	ILE	C6H13NO2	131.095	130.087	132.102	1.072
Isovaleric Acid	3-Methylbutanoic acid	C5H10O2	102.068	101.061	103.075	7.131
Kasugamycin		C14H25N3O9	379.160	378.152	380.166	0.390
Kynurenic Acid		C10H7NO3	189.043	188.035	190.050	7.517
Lactic Acid	2-Hydroxypropanoic acid	C3H6O3	90.032	89.024	91.039	1.015
L-a-Hydroxyglutaric Acid	2-Hydroxyglutaric Acid	C5H8O5	148.038	147.030	149.044	1.285
L-Alanine	ALA	C3H7NO2	89.048	88.040	90.055	0.522
LCA	Lithocholic Acid	C24H40O3	376.298	375.290	377.305	12.009
L-Carnitine		C7H15NO3	161.106	160.098	162.112	0.418
L-DOPA	3,4-Dihydroxy-L-Phenylalanine	C9H11NO4	197.069	196.062	198.076	0.809
Leucine	LEU	C6H13NO2	131.095	130.087	132.102	1.152
L-Glutathione Oxidized	GSSG	C20H32N6O12S2	612.151	611.145	613.159	2.109
L-Glutathione Reduced	GSH	C10H17N3O6S	307.083	306.077	308.091	1.130
L-Homocysteine		C4H9NO2S	135.035	134.028	136.043	0.590
L-Homoserine		C4H9NO3	119.059	118.051	120.066	0.524
L-Kynurenine		C10H12N2O3	208.085	207.078	209.092	2.025
L-Phenylalanine	PHE	C9H11NO2	165.080	164.072	166.086	2.482
L-Pipecolic Acid	L-Homoproline	C6H11NO2	129.078	128.072	130.086	0.737
L-Pyroglutamic Acid		C5H7NO3	129.042	128.035	130.050	1.577
L-Saccharophine		C11H20N2O6	276.133	275.125	277.139	0.556
Lysine	LYS	C6H14N2O2	146.106	145.098	147.113	0.381
Maleic Acid	cis-Butenedioic Acid	C4H4O4	116.010	115.004	117.018	4.726
Malic Acid	2-Hydroxybutanedioic Acid	C4H6O5	134.021	133.014	135.029	1.200
m-Coumaric Acid	trans-3-Hydroxycinnamic Acid	C9H8O3	164.047	163.040	165.055	8.010
Metconazole		C17H22ClN3O	319.146	318.138	320.152	10.872
Methionine	MET	C5H11NO2S	149.052	148.044	150.058	0.823
Methyl Vanillate		C9H10O4	182.058	181.051	183.065	8.615
Methyl-2-oxovaleric Acid	Ketoisoleucine	C6H10O3	130.062	129.056	131.070	8.222
Methyl-a-D-Glucopyranoside		C7H14O6	194.080	193.072	195.086	*0.827*

Methylguanidine		C2H7N3	73.065	72.057	74.071	0.398
Methylmalonic Acid	2-Methylpropanedioic Acid	C4H6O4	118.026	117.019	119.034	2.503
Methylsuccinic Acid		C5H8O4	132.042	131.035	133.050	3.661
Mevalonic Acid	MVA	C6H12O4	148.074	147.066	149.081	1.812
Mycophenolic Acid		C17H20O6	320.127	319.119	321.133	9.866
Mycophenolic Acid Glucuronide		C23H28O12	496.159	495.151	497.165	8.814
myo-Inositol		C6H12O6	180.063	179.056	181.071	0.553
Myristoyl-L-carnitine (C14)	C14-Carnitine	C21H41NO4	371.304	370.296	372.311	9.995
N-(3-Phenylpropionyl)glycine		C11H13NO3	207.090	206.082	208.097	8.026
N,N-dimethylglycine	N,N-Dimethylglycine	C4H9NO2	103.063	102.056	104.071	0.558
N1,N12-Diacetylspermine		C14H30N4O2	286.236	285.230	287.244	0.366
N-Acetyl-b-D-Glucosaminylamine	2-Acetamido-2-Deoxy-B-D-Glucopyranosylamine	C8H16N2O5	220.106	219.099	221.113	0.663
N-Acetyl-L-Methionine		C7H13NO3S	191.062	190.054	192.069	5.632
N-Acetylneuraminic Acid	NANA	C11H19NO9	309.105	308.099	310.113	1.204
Naltrindole		C26H26N2O3	414.195	413.187	415.202	7.909
N-Carbamoylsarcosine	3-Methylhydantoin	C4H8N2O3	132.054	131.046	133.061	1.151
N-Cinnamylglycine	Cinnamoylglycine	C11H11NO3	205.074	204.067	206.081	8.321
Neopterin		C9H11N5O4	253.082	252.074	254.088	0.885
Nicotinamide	Vitamin B3	C6H6N2O	122.047	121.041	123.055	0.948
Nicotinic Acid	3-Pyridinecarboxylic Acid	C6H5NO2	123.033	122.025	124.039	1.090
N-Methylhistidine		C7H11N3O2	169.085	168.078	170.092	0.389
Nonadecanoic Acid	Nonadecyclic Acid	C19H38O2	298.288	297.280		14.119
Nonanoic acid	Pelargonic Acid	C9H18O2	158.130	157.123		10.656
N-Palmitoyl serinol		C19H39NO3	329.292	328.286	330.300	11.928
Nε,Nε,Nε-Trimethyllysine	N6,N6,N6-trimethyllysine	C9H20N2O2	188.153	187.145	189.160	0.380
Nω-Acetylhistamine		C7H11N3O	153.090	152.083	154.097	0.444
o-Acetylserine	OASS	C5H9NO4	147.053	146.046	148.060	0.607
Octadecanedioic Acid		C18H34O4	314.245	313.238	315.253	11.788
Octadecanoic acid	Stearic Acid	C18H36O2	284.272	283.264	285.279	13.725

Octanoic Acid	Caprylic Acid	C8H16O2	144.114	143.108	145.122	10.262
o-Desmethylangolensin	o-DMA	C15H14O4	258.090	257.082	259.096	9.658
o-Hydroxyhippuric acid	Salicyluric Acid	C9H9NO4	195.054	194.046	196.060	7.368
Oleic Acid	(9Z)-Octadec-9-enoic acid	C18H34O2	282.256	281.249	283.263	13.119
O-Phospho-L-serine		C3H8NO6P	185.009	184.002	186.016	*1.244*
Ornithine	5-amino norvaline	C5H12N2O2	132.089	131.083	133.097	0.377
Orotic Acid		C5H4N2O4	156.018	155.010	157.024	2.881
Oxamic Acid	Aminooxoacetic Acid	C2H3NO3	89.011	88.004	90.019	1.539
Palmitoyl-L-carnitine (C16)	C16-Carnitine	C23H45NO4	399.335	398.328	400.342	10.434
p-Aminobenzoic Acid	4-aminobenzoic acid	C7H7NO2	137.048	136.040	138.055	3.725
p-Coumaric acid	4-Hydroxycinnamic acid	C9H8O3	164.048	163.040	165.055	7.405
p-Cresol Glucuronide		C13H16O7	284.089	283.082	285.097	7.668
p-Cresol Sulfate		C7H8O4S	188.015	187.007	189.022	9.538
Pentadecanoic Acid	Pentadecyclic Acid	C15H30O2	242.225	241.217		12.751
Penthiopyrad		C16H20F3N3OS	359.128	358.121	360.135	11.121
Phenethylamine		C8H11N	121.089	120.082	122.096	1.126
Phenol		C6H6O	94.042	93.035	95.049	*6.305*
Phenylacetaldehyde		C8H8O	120.058	119.050	121.065	8.741
Phenylacetic Acid		C8H8O2	136.053	135.045	137.060	8.137
Phenylacetylglutamine	N2-(2-Phenylacetyl)-L-glutamine	C13H16N2O4	264.110	263.104	265.118	6.538
Phenylacetylglycine	Phenaceturic Acid	C10H11NO3	193.074	192.067	194.081	6.816
Phenylethanolamine	2-Amino-1-Phenylethanol	C8H11NO	137.084	136.077	138.091	0.690
Phloretic Acid	Desaminotyrosine	C9H10O3	166.062	165.056	167.070	8.021
Phloroglucinol	1,3,5-Trihydroxybenzene	C6H6O3	126.032	125.024	127.039	1.426
Phosphorcreatine	Creatine Phosphate	C4H10N3O5P	211.036	210.029	212.043	*1.165*
Phytanic Acid		C20H40O2	312.303	311.296	313.310	*13.941*
Pimelic Acid	Heptanedioic Acid	C7H12O4	160.073	159.066	161.081	6.202
Piperine		C17H19NO3	285.137	284.129	286.144	10.373
Proline	PRO	C5H9NO2	115.064	114.056	116.071	0.610

Propachlor		C11H14ClNO	211.077	210.069	212.084	9.959
Propionic Acid	Propanoic Acid	C3H6O2	74.037	73.030	75.044	2.073
Protocatechuic Acid	3,4-Dihydroxybenzoic Acid	C7H6O4	154.026	153.019	155.034	4.289
Pyrocatechol	1,2-dihydroxybenzene	C6H6O2	110.037	109.030	111.044	4.205
Pyrogallol	1,2,3-Trihydroxybenzene	C6H6O3	126.032	125.024	127.039	1.869
Quercetin		C15H10O7	302.042	301.035	303.050	9.103
Quinic Acid		C7H12O6	192.064	191.056	193.071	0.847
rac-Methyl Ephedrine	DL-Methylephedrine	C11H17NO	179.132	178.124	180.138	2.043
Raffinose		C18H32O16	504.168	503.162	505.176	0.693
Ralgin		C12H16N2O2	220.122	219.114	221.128	7.987
Riboflavin	Vitamin B2	C17H20N4O6	376.138	375.131	377.146	6.705
Rutin	sophorin	C27H30O16	610.153	609.146	611.161	7.969
Sarcosine	N-Methylglycine	C3H7NO2	89.047	88.040	90.055	0.527
Sebacic Acid	Decanedioic Acid	C10H18O4	202.120	201.113	203.128	9.030
Seleno-L-cystine		C6H12N2O4[80]Se2	335.912	334.905	336.920	0.530
Serine	SER	C3H7NO3	105.043	104.035	106.050	0.522
Shikimic Acid		C7H10O5	174.052	173.046	175.060	0.853
Sinapinic Acid	3,5-Dimethoxy-4-hydroxycinnamic Acid	C11H12O5	224.068	223.061	225.076	8.025
Skatole	3-Methylindole	C9H9N	131.073	130.066	132.081	10.001
SN-38 carboxylate form		C22H20N2O6	408.132	407.125	409.139	*8.738*
Spermidine		C7H19N3	145.157	144.151	146.165	0.341
Spermine		C10H26N4	202.215	201.208	203.223	0.348
Sphingosine-1-phosphate	S1P	C18H38NO5P	379.248	378.241	380.256	10.746
SR95531	Gabazine	C15H17N3O3	287.128	286.120	288.134	6.522
Stachydrine		C7H13NO2	143.095	142.087	144.102	0.634
Stercobilin		C33H46N4O6	594.341	593.334	595.349	8.516
Suberic Acid	Octanedioic Acid	C8H14O4	174.090	173.082	175.096	7.584
Succinic Acid	Butanedioic Acid	C4H6O4	118.026	117.019	119.034	1.401
Sucrose		C12H22O11	342.116	341.109	343.123	0.670

Syringic Acid	3,5-Dimethoxy-4-hydroxybenzoic acid	C9H10O5	198.053	197.046	199.060	6.694
TaMCA	Tauro-alpha-Muricholic Acid	C26H45NO7S	515.292	514.284	516.299	10.084
Tartronic Acid	2-Hydroxymalonic Acid	C3H4O5	120.005	118.999	121.013	*1.597*
Taurine	2-aminoethanesulfonic acid	C2H7NO3S	125.014	124.007	126.022	0.565
TbMCA	Tauro-beta-Muricholic Acid	C26H45NO7S	515.292	514.284	516.299	10.180
TCA	Taurocholic acid	C26H45NO7S	515.292	514.284	516.299	10.800
TCDCA	Taurochenodeoxycholic Acid	C26H45NO6S	499.297	498.289	500.304	12.194
TDCA	Taurodeoxycholic acid	C26H45NO6S	499.297	498.289	500.304	14.930
Tetradecanedioic Acid		C14H26O4	258.183	257.176	259.190	10.490
Tetradecanoic Acid	Myristic Acid	C14H28O2	228.209	227.202	229.216	12.467
THCA	Taurohyocholic Acid	C26H45NO7S	515.292	514.284	516.299	10.401
THDCA	Taurohyodeoxycholic Acid	C26H45NO6S	499.297	498.289	500.304	10.754
Threonine	THR	C4H9NO3	119.059	118.051	120.066	0.535
Tiglic Acid	2,3-Dimethylacrylic Acid	C5H8O2	100.052	99.045	101.060	6.969
Tilivalline		C20H19N3O2	333.147	332.140	334.155	9.222
trans-3,4-Methylene heptanoic acid		C8H14O2	142.099	141.092	143.107	9.717
trans-3,4-Methylene heptanoylcarnitine		C15H27N04	285.194		286.201	7.464
trans-4-Hydroxyproline		C5H9NO3	131.059	130.051	132.066	0.551
trans-Cinnamic Acid	3-Phenylacrylic acid	C9H8O2	148.053	147.045	149.060	9.139
Tridecanoic Acid	Tridecyclic Acid	C13H26O2	214.194	213.186	215.201	12.158
Trigonelline	N-methylnicotinate	C7H7NO2	137.048	136.040	138.055	0.588
Trimethylamine	TMA	C3H9N	59.074	58.066	60.081	0.391
Trimethylamine-N-oxide	TMAO	C3H9NO	75.069	74.061	76.076	0.398
Tryptamine	1H-indole-3-ethanamine	C10H12N2	160.100	159.093	161.107	2.382
Tryptamine	1H-indole-3-ethanamine	C10H12N2	160.100	159.093	161.107	2.112
Tryptophan	TRP	C11H12N2O2	204.090	203.083	205.097	4.427
Tubermycin B	Phenazine-1-carboxylic Acid	C13H8N2O2	224.058	223.051	225.066	9.460
TUDCA	Tauroursodeoxycholic Acid	C26H45NO6S	499.297	498.289	500.304	10.878

Tyrosine	TYR	C9H11NO3	181.074	180.067	182.081	1.087
UDCA	Ursodeoxycholic acid	C24H40O4	392.293	391.285	393.300	10.324
UDCA-S	Ursodeoxycholic Acid-3-Sulfate	C24H40O7S	472.250	471.242	473.257	11.563
Undecanedioic Acid	1,9-Nonanedicarboxylic acid	C11H20O4	216.136	215.129	217.143	9.421
Undecanoic Acid	Undecyclic Acid	C11H22O2	186.163	185.155	187.169	11.458
Uracil		C4H4N2O2	112.027	111.020	113.035	0.905
Urea		CH4N2O	60.033	59.025	61.040	0.594
Uric Acid		C5H4N4O3	168.028	167.021	169.036	1.047
Uridine		C9H12N2O6	244.069	243.062	245.077	1.484
Urobilin	Urochrome	C33H42N4O6	590.311	589.303	591.318	8.423
Urobilinogen		C33H44N4O6	592.327	591.319	593.333	10.122
Urolithin A		C13H8O4	228.043	227.035	229.050	8.873
Valeric Acid	Pentanoic Acid	C5H10O2	102.069	101.061	103.075	7.444
Valine	VAL	C5H11NO2	117.078	116.072	118.086	0.666
Xanthurenic acid		C10H7NO4	205.038	204.030	206.045	7.233
y-Aminobutyric Acid	4-aminobutanoic Acid	C4H9NO2	103.064	102.056	104.071	0.406
y-Glutamylphenylalanine		C14H18N2O5	294.121	293.114	295.129	5.751
α-D(+)Mannose 1-phosphate	Mannose-1P	C6H13O9P	260.029	259.022	261.037	1.599
α-D-Glucose 1-phosphate		C6H13O9P	260.029	259.022	261.037	1.648

[1]M = formula mass, H = hydrogen, M+H = formula mass + hydrogen, M-H = formula mass – hydrogen, RT = retention time.

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Supplementary Table 2: Non-parametric assessment of diet in fecal genera from infants at age three, six, nine, and 12 months of age.[1]

Age	Genus	P-value	BF	NLB	MF	SF
3	SMB53	<0.001	0.015 (0, 0) a		0.057 (0, 0) a	0.373 (0, 1) b
3	f__Ruminococcaceae	<0.001	0.087 (0, 1) a		0.448 (0, 1) b	2.081 (1, 4) c
3	Veillonella	<0.001	0.175 (0, 1) a		1.72 (1, 2) b	4.455 (2, 14) b
3	f__Peptostreptococcaceae	<0.001	0.053 (0, 0) a		0.219 (0, 1) a	2.225 (1, 4) b
3	f__Clostridiaceae	0.002	0.026 (0, 0) a		0.279 (0, 1) b	0.672 (0, 3) b
3	Streptococcus	0.003	0.085 (0, 1) a		0.472 (0, 1) b	1.17 (0, 3) b
3	Bifidobacterium	0.021	13.791 (10, 34) a		24.195 (14, 36) a	7.919 (2, 12) b
3	[Clostridium]	0.033	0.024 (0, 0) a		0.575 (0, 3) b	0.327 (0, 3) b
3	Coprococcus	0.056	0.029 (0, 0) a		0.349 (0, 1) b	0.041 (0, 0) ab
3	Parabacteroides	0.061	0.051 (0, 0) a		1.807 (0, 4) b	0.138 (0, 1) ab
3	Sutterella	0.195	0.006 (0, 0) a		0.01 (0, 0) a	0 (0, 0) a
3	Bacteroides	0.218	29.645 (9, 59) a		13.239 (9, 36) a	17.172 (1, 27) a
3	f__Lachnospiraceae	0.242	0.571 (0, 1) a		0.905 (0, 2) a	1.665 (1, 3) a
3	Enterococcus	0.254	0.091 (0, 0) a		0.039 (0, 0) a	0.151 (0, 1) a
3	f__Veillonellaceae	0.263	0.035 (0, 0) a		0.307 (0, 1) a	0.008 (0, 0) a
3	Haemophilus	0.288	0.036 (0, 0) a		0.028 (0, 0) a	0.212 (0, 1) a
3	Blautia	0.305	0.222 (0, 1) a		0.215 (0, 0) a	0.725 (0, 13) a
3	f__Bifidobacteriaceae	0.363	0.028 (0, 0) a		0.075 (0, 0) a	0.019 (0, 0) a
3	[Eubacterium]	0.375	0.004 (0, 0) a		0.022 (0, 0) a	0.019 (0, 0) a
3	Roseburia	0.38	0 (0, 0) a		0.019 (0, 0) a	0 (0, 0) a
3	o__Clostridiales	0.387	0 (0, 0) a		0 (0, 0) a	0.004 (0, 0) a

3	f__Erysipelotrichaceae	0.405	0.114 (0, 1) a		0.142 (0, 0) a	0.276 (0, 3) a
3	Dorea	0.412	0.016 (0, 0) a		0.137 (0, 0) a	0.069 (0, 1) a
3	Akkermansia	0.444	0.003 (0, 0) a		0.028 (0, 0) a	0.022 (0, 0) a
3	f__Enterobacteriaceae	0.486	14.906 (3, 20) a		11.14 (5, 23) a	7.194 (3, 17) a
3	Faecalibacterium	0.59	0.057 (0, 0) a		0.086 (0, 2) a	0.042 (0, 0) a
3	f__Rikenellaceae	0.66	0.004 (0, 0) a		0 (0, 0) a	0 (0, 0) a
3	Oscillospira	0.691	0.103 (0, 0) a		0.076 (0, 0) a	0.135 (0, 0) a
3	Lachnospira	0.702	0.003 (0, 0) a		0 (0, 0) a	0 (0, 0) a
3	[Ruminococcus]	0.725	2.198 (0, 5) a		3.631 (1, 8) a	3.428 (1, 10) a
3	Clostridium	0.769	0.048 (0, 2) a		0.26 (0, 2) a	0.09 (0, 5) a
6	f__Peptostreptococcaceae	<0.001	0.033 (0, 1) a		0.285 (0, 1) a	2.383 (2, 3) b
6	SMB53	<0.001	0.007 (0, 0) a		0.071 (0, 0) a	0.616 (0, 1) b
6	Bifidobacterium	<0.001	23.625 (15, 40) a		27.52 (12, 35) a	3.361 (0, 7) b
6	f__Lachnospiraceae	<0.001	0.115 (0, 1) a		0.901 (0, 2) b	4.17 (2, 7) c
6	o__Clostridiales	<0.001	0 (0, 0) a		0 (0, 0) a	0.226 (0, 0) b
6	Oscillospira	<0.001	0.066 (0, 0) a		0.118 (0, 0) b	0.391 (0, 1) c
6	Coprococcus	<0.001	0.021 (0, 0) a		0.293 (0, 1) b	0.481 (0, 2) b
6	Blautia	<0.001	0.065 (0, 1) a		0.477 (0, 2) a	4.893 (2, 10) b
6	f__Erysipelotrichaceae	0.004	0.137 (0, 1) a		0.214 (0, 1) a	1.469 (1, 2) b
6	[Ruminococcus]	0.005	0.987 (0, 3) a		2.959 (1, 6) a	7.584 (3, 24) b
6	f__Clostridiaceae	0.007	0.024 (0, 0) a		0.158 (0, 1) ab	0.571 (0, 5) b
6	Roseburia	0.013	0 (0, 0) a		0 (0, 0) a	0.088 (0, 2) b
6	Enterococcus	0.017	0.044 (0, 0) a		0.04 (0, 0) a	0 (0, 0) b

6	f__Ruminococcaceae	0.019	0.436 (0, 1) a		0.657 (0, 1) b	0.9 (0, 2) b
6	[Clostridium]	0.049	0.051 (0, 0) a		0.41 (0, 1) ab	0.299 (0, 1) b
6	[Eubacterium]	0.105	0.006 (0, 0) a		0.078 (0, 1) a	0.118 (0, 0) a
6	f__Bifidobacteriaceae	0.106	0.014 (0, 0) a		0.041 (0, 0) a	0.009 (0, 0) a
6	Dorea	0.136	0.041 (0, 0) a		0.064 (0, 0) a	0.363 (0, 2) a
6	f__Enterobacteriaceae	0.211	7.038 (5, 13) a		5.521 (3, 8) a	3.376 (1, 11) a
6	Veillonella	0.39	1.984 (0, 7) a		1.518 (0, 5) a	0.886 (0, 1) a
6	f__Rikenellaceae	0.417	0 (0, 0) a		0 (0, 0) a	0 (0, 0) a
6	Akkermansia	0.477	0.007 (0, 0) a		0.022 (0, 0) a	0 (0, 0) a
6	Clostridium	0.529	0.085 (0, 1) a		0.172 (0, 1) a	0.016 (0, 1) a
6	Faecalibacterium	0.533	0.067 (0, 0) a		0.392 (0, 3) a	0.132 (0, 6) a
6	Bacteroides	0.554	29.429 (11, 52) a		29.711 (13, 44) a	20.299 (1, 44) a
6	Sutterella	0.652	0 (0, 0) a		0 (0, 0) a	0 (0, 0) a
6	Lachnospira	0.715	0 (0, 0) a		0 (0, 0) a	0 (0, 0) a
6	Streptococcus	0.726	0.141 (0, 1) a		0.293 (0, 1) a	0.29 (0, 1) a
6	f__Veillonellaceae	0.726	0.065 (0, 7) a		0.232 (0, 5) a	0.055 (0, 1) a
6	Haemophilus	0.924	0.024 (0, 0) a		0.092 (0, 0) a	0.032 (0, 1) a
6	Parabacteroides	0.949	0.03 (0, 3) a		0.358 (0, 3) a	0.026 (0, 1) a
9	o__Clostridiales	<0.001	0 (0, 0) a		0 (0, 0) a	0.228 (0, 0) b
9	SMB53	<0.001	0 (0, 0) a		0.076 (0, 0) a	1.227 (1, 2) b
9	Blautia	<0.001	0.061 (0, 1) a		0.146 (0, 1) a	5.076 (3, 10) b
9	f__Peptostreptococcaceae	0.005	0.064 (0, 1) a		0.282 (0, 1) a	2.447 (1, 7) b
9	f__Lachnospiraceae	0.007	0.512 (0, 1) a		3.021 (2, 6) b	3.488 (2, 8) b

9	f__Veillonellaceae	0.01	0.027 (0, 2) a		7.207 (1, 18) b	0 (0, 0) a
9	Dorea	0.019	0.019 (0, 0) a		0.014 (0, 0) a	0.73 (0, 1) b
9	Clostridium	0.026	1.096 (0, 4) a		0.047 (0, 0) b	0.032 (0, 0) b
9	Akkermansia	0.038	0 (0, 0) a		0.017 (0, 0) b	0.107 (0, 2) b
9	Bifidobacterium	0.038	17.951 (11, 38) a		11.847 (10, 31) a	6.065 (3, 17) b
9	Lachnospira	0.054	0 (0, 0) a		0 (0, 1) a	0.368 (0, 5) b
9	Enterococcus	0.099	0.028 (0, 0) a		0.014 (0, 0) ab	0 (0, 0) b
9	Parabacteroides	0.127	0.004 (0, 0) a		0.082 (0, 4) a	0.535 (0, 2) a
9	Roseburia	0.132	0.006 (0, 0) a		0 (0, 0) a	0.016 (0, 1) a
9	Oscillospira	0.14	0.075 (0, 0) a		0.153 (0, 0) a	0.495 (0, 1) a
9	Veillonella	0.188	2.556 (1, 8) a		0.52 (0, 2) a	0.207 (0, 2) a
9	Coprococcus	0.222	0.283 (0, 1) a		0.226 (0, 1) a	0.412 (0, 2) a
9	f__Clostridiaceae	0.237	0.1 (0, 0) a		0.119 (0, 2) a	0.259 (0, 1) a
9	[Clostridium]	0.243	0.432 (0, 2) a		0.087 (0, 0) a	0.09 (0, 0) a
9	f__Bifidobacteriaceae	0.287	0.039 (0, 0) a		0.136 (0, 0) a	0.025 (0, 0) a
9	[Ruminococcus]	0.303	1.468 (0, 4) a		1.303 (1, 4) a	2.693 (2, 4) a
9	f__Enterobacteriaceae	0.31	2.891 (1, 24) a		1.705 (1, 4) a	1.854 (1, 3) a
9	[Eubacterium]	0.342	0.034 (0, 0) a		0.007 (0, 0) a	0.064 (0, 0) a
9	Faecalibacterium	0.429	0.023 (0, 2) a		6.68 (0, 13) a	0.071 (0, 7) a
9	Bacteroides	0.501	19.803 (0, 44) a		18.571 (8, 44) a	35.402 (9, 49) a
9	Streptococcus	0.524	0.064 (0, 0) a		0.106 (0, 1) a	0.183 (0, 1) a
9	Sutterella	0.79	0 (0, 0) a		0 (0, 0) a	0.005 (0, 0) a
9	Haemophilus	0.846	0.213 (0, 2) a		0.489 (0, 1) a	0.168 (0, 1) a

9	f__Ruminococcaceae	0.877	0.875 (1, 3) a		1.164 (1, 1) a	1.056 (0, 3) a
9	f__Rikenellaceae	0.971	0.003 (0, 0) a		0.012 (0, 0) a	0.004 (0, 0) a
9	f__Erysipelotrichaceae	0.989	0.252 (0, 0) a		0.169 (0, 0) a	0.165 (0, 0) a
12	o__Clostridiales	<0.001	0.005 (0, 0) a	0.018 (0, 0) a	0.015 (0, 0) a	0.218 (0, 0) b
12	Blautia	0.004	0.481 (0, 3) a	1.906 (0, 4) ab	0.969 (0, 3) a	4.819 (2, 7) b
12	Bifidobacterium	0.008	14.202 (13, 19) a	8.631 (4, 12) ab	15.18 (6, 23) a	4.604 (2, 6) b
12	f__Lachnospiraceae	0.012	1.267 (1, 2) a	1.473 (1, 3) ab	2.894 (2, 5) bc	3.836 (2, 6) c
12	Veillonella	0.047	0.836 (0, 4) a	0.415 (0, 1) ab	0.36 (0, 1) ab	0.25 (0, 0) b
12	Dorea	0.056	0.233 (0, 1) ab	0.933 (0, 2) b	0.153 (0, 0) a	0.496 (0, 1) ab
12	f__Erysipelotrichaceae	0.143	0.22 (0, 1) a	0.358 (0, 3) a	0.187 (0, 1) a	0.174 (0, 0) a
12	Parabacteroides	0.153	0.022 (0, 1) a	0.091 (0, 11) a	0.857 (0, 5) a	4.118 (0, 8) a
12	[Clostridium]	0.174	0.223 (0, 1) a	0.188 (0, 1) a	0.019 (0, 0) a	0.026 (0, 0) a
12	Akkermansia	0.192	0 (0, 0) a	0.036 (0, 2) a	0.007 (0, 0) a	0.143 (0, 1) a
12	f__Peptostreptococcaceae	0.225	0.608 (0, 2) a	0.821 (0, 1) a	0.643 (0, 1) a	2.025 (0, 3) a
12	f__Clostridiaceae	0.259	0.056 (0, 1) a	0.115 (0, 1) a	0.066 (0, 0) a	0.845 (0, 2) a
12	Roseburia	0.275	0.057 (0, 0) a	0 (0, 0) a	0.009 (0, 0) a	0.092 (0, 1) a
12	Clostridium	0.295	0.281 (0, 1) a	0.05 (0, 0) a	0.018 (0, 0) a	0.009 (0, 0) a
12	Faecalibacterium	0.391	0.234 (0, 15) a	6.724 (3, 17) a	2.669 (0, 4) a	1.942 (0, 8) a
12	Enterococcus	0.395	0.017 (0, 0) a	0 (0, 0) a	0 (0, 0) a	0.018 (0, 0) a
12	[Eubacterium]	0.4	0.038 (0, 0) a	0.134 (0, 0) a	0.042 (0, 0) a	0.07 (0, 0) a
12	f__Enterobacteriaceae	0.51	2.863 (1, 6) a	1.358 (1, 2) a	0.971 (0, 4) a	2.076 (0, 7) a
12	[Ruminococcus]	0.574	2.749 (1, 4) a	2.842 (2, 10) a	1.285 (1, 4) a	2.322 (1, 3) a
12	Haemophilus	0.577	0.622 (0, 1) a	0.163 (0, 1) a	0.186 (0, 1) a	0.081 (0, 1) a
12	Lachnospira	0.599	0.033 (0, 0) a	0.003 (0, 0) a	0.009 (0, 0) a	0.032 (0, 1) a
12	SMB53	0.649	0.137 (0, 0) a	0.163 (0, 1) a	0.12 (0, 0) a	0.348 (0, 1) a

12	f__Bifidobacteriaceae	0.697	0 (0, 0) a	0.015 (0, 0) a	0.032 (0, 0) a	0.008 (0, 0) a
12	Bacteroides	0.709	39.689 (12, 55) a	44.608 (35, 56) a	48.214 (32, 59) a	45.92 (35, 56) a
12	f__Ruminococcaceae	0.74	0.945 (1, 2) a	1.217 (1, 3) a	0.51 (0, 3) a	1.434 (0, 6) a
12	f__Rikenellaceae	0.805	0 (0, 0) a	0.005 (0, 0) a	0.019 (0, 1) a	0.013 (0, 0) a
12	Oscillospira	0.892	0.144 (0, 1) a	0.179 (0, 1) a	0.14 (0, 0) a	0.211 (0, 0) a
12	Streptococcus	0.931	0.279 (0, 1) a	0.377 (0, 1) a	0.184 (0, 1) a	0.267 (0, 1) a
12	f__Veillonellaceae	0.984	0.091 (0, 10) a	0.339 (0, 3) a	0.176 (0, 3) a	0.149 (0, 0) a
12	Sutterella	0.988	0.008 (0, 1) a	0.011 (0, 1) a	0 (0, 1) a	0.009 (0, 1) a
12	Coprococcus	1	0.47 (0, 1) a	0.398 (0, 1) a	0.249 (0, 2) a	0.418 (0, 2) a

[1] Data are presented as median (25^{th} quartile, 75^{th} quartile). Differences in diet were assessed by Kruskal-Wallis test on percent abundances. Post-hoc analysis of pairwise differences in diet were assessed by Dunn's test. Medians without a common letter are statistically significant. Sample size range from 10 to 20 per diet group at three, six, nine and 12 months of age. BF = Breast-fed, MF = milk formula fed, NLB = no longer breastfeeding, SF = soy formula fed.

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Supplementary Table 3: Dietary pairwise comparison of genera in infants at three, six, nine, and 12 months of age.[1]

Genus	Base Mean	Log2 Fold Change	Log2 Fold Change SE	Stat	*P-value*	FDR	Comparison	Age
[Clostridium]	173.400	-1.400	1.200	-1.200	0.234	0.234	BF vs MF	3
[Clostridium]	173.400	-0.700	1.100	-0.700	0.507	0.507	BF vs SF	3
[Clostridium]	173.400	0.700	1.200	0.600	0.548	0.548	MF vs SF	3
[Eubacterium]	3.900	-2.700	1.200	-2.300	0.024	0.024	BF vs MF	3
[Eubacterium]	3.900	-0.400	1.100	-0.300	0.744	0.744	BF vs SF	3
[Eubacterium]	3.900	2.400	1.200	2.000	0.041	0.041	MF vs SF	3
[Ruminococcus]	782.200	0.000	0.900	0.000	0.965	0.965	BF vs MF	3
[Ruminococcus]	782.200	0.900	0.800	1.200	0.242	0.242	BF vs SF	3
[Ruminococcus]	782.200	0.900	0.900	1.000	0.313	0.313	MF vs SF	3
Akkermansia	17.900	-0.200	1.400	-0.100	1	1	BF vs MF	3
Akkermansia	17.900	0.800	1.200	0.600	1	1	BF vs SF	3
Akkermansia	17.900	0.900	1.400	0.700	1	1	MF vs SF	3
Bacteroides	4668.900	1.800	0.900	2.000	0.045	0.045	BF vs MF	3
Bacteroides	4668.900	2.600	0.800	3.300	<0.01	<0.01	BF vs SF	3
Bacteroides	4668.900	0.900	0.900	1.000	0.332	0.332	MF vs SF	3
Bifidobacterium	2220.500	0.600	0.600	1.000	0.317	0.317	BF vs MF	3
Bifidobacterium	2220.500	2.800	0.500	5.200	<0.01	<0.01	BF vs SF	3
Bifidobacterium	2220.500	2.200	0.600	3.600	<0.01	<0.01	MF vs SF	3
Blautia	170.100	0.600	1.100	0.500	0.608	0.608	BF vs MF	3
Blautia	170.100	-1.800	1.000	-1.700	0.084	0.084	BF vs SF	3
Blautia	170.100	-2.400	1.100	-2.100	0.038	0.038	MF vs SF	3
Clostridium	498.800	2.300	1.600	1.500	1	1	BF vs MF	3
Clostridium	498.800	3.300	1.400	2.400	1	1	BF vs SF	3
Clostridium	498.800	1.000	1.500	0.600	1	1	MF vs SF	3
Coprococcus	57.700	-2.200	1.100	-2.100	0.04	0.04	BF vs MF	3
Coprococcus	57.700	-0.100	0.900	-0.100	0.957	0.957	BF vs SF	3
Coprococcus	57.700	2.100	1.000	2.000	0.043	0.043	MF vs SF	3

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Dorea	24.000	-1.400	1.200	-1.100	0.263	0.263	BF vs MF	3
Dorea	24.000	-1.700	1.100	-1.600	0.119	0.119	BF vs SF	3
Dorea	24.000	-0.300	1.200	-0.300	0.781	0.781	MF vs SF	3
Enterococcus	69.800	5.000	1.100	4.500	<0.01	<0.01	BF vs MF	3
Enterococcus	69.800	2.200	1.000	2.300	0.023	0.023	BF vs SF	3
Enterococcus	69.800	-2.800	1.100	-2.500	0.012	0.012	MF vs SF	3
f__Bifidobacteriaceae	11.500	-1.100	1.100	-1.000	0.334	0.334	BF vs MF	3
f__Bifidobacteriaceae	11.500	1.300	1.000	1.300	0.196	0.196	BF vs SF	3
f__Bifidobacteriaceae	11.500	2.300	1.100	2.100	0.032	0.032	MF vs SF	3
f__Clostridiaceae	59.200	-2.100	1.000	-2.100	0.036	0.036	BF vs MF	3
f__Clostridiaceae	59.200	-3.100	0.900	-3.600	<0.01	<0.01	BF vs SF	3
f__Clostridiaceae	59.200	-1.100	1.000	-1.100	0.266	0.266	MF vs SF	3
f__Enterobacteriaceae	2411.700	2.100	0.700	3.200	<0.01	<0.01	BF vs MF	3
f__Enterobacteriaceae	2411.700	3.000	0.600	5.000	<0.01	<0.01	BF vs SF	3
f__Enterobacteriaceae	2411.700	0.900	0.700	1.300	0.195	0.195	MF vs SF	3
f__Erysipelotrichaceae	182.400	2.900	1.200	2.400	0.016	0.016	BF vs MF	3
f__Erysipelotrichaceae	182.400	0.700	1.100	0.700	0.493	0.493	BF vs SF	3
f__Erysipelotrichaceae	182.400	-2.100	1.200	-1.800	0.072	0.072	MF vs SF	3
f__Lachnospiraceae	122.600	-0.400	0.700	-0.600	0.539	0.539	BF vs MF	3
f__Lachnospiraceae	122.600	0.100	0.600	0.100	0.891	0.891	BF vs SF	3
f__Lachnospiraceae	122.600	0.500	0.700	0.700	0.457	0.457	MF vs SF	3
f__Peptostreptococcaceae	143.000	-3.500	1.000	-3.500	<0.01	<0.01	BF vs MF	3
f__Peptostreptococcaceae	143.000	-4.500	0.900	-5.200	<0.01	<0.01	BF vs SF	3
f__Peptostreptococcaceae	143.000	-1.100	1.000	-1.100	0.26	0.26	MF vs SF	3
f__Rikenellaceae	32.500	1.000	1.900	0.500	0.612	0.612	BF vs MF	3
f__Rikenellaceae	32.500	-1.600	1.700	-0.900	0.347	0.347	BF vs SF	3
f__Rikenellaceae	32.500	-2.500	1.900	-1.400	0.175	0.175	MF vs SF	3
f__Ruminococcaceae	120.100	-0.700	0.700	-0.900	0.352	0.352	BF vs MF	3

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f__Ruminococcaceae	120.100	-1.700	0.600	-2.700	<0.01	<0.01	BF vs SF	3
f__Ruminococcaceae	120.100	-1.100	0.700	-1.500	0.139	0.139	MF vs SF	3
f__Veillonellaceae	166.700	-0.600	1.400	-0.400	1	1	BF vs MF	3
f__Veillonellaceae	166.700	2.800	1.200	2.300	1	1	BF vs SF	3
f__Veillonellaceae	166.700	3.500	1.400	2.500	1	1	MF vs SF	3
Faecalibacterium	142.500	-1.600	1.300	-1.200	0.228	0.228	BF vs MF	3
Faecalibacterium	142.500	0.500	1.200	0.400	0.664	0.664	BF vs SF	3
Faecalibacterium	142.500	2.100	1.300	1.600	0.109	0.109	MF vs SF	3
Haemophilus	93.400	3.400	1.400	2.500	0.012	0.012	BF vs MF	3
Haemophilus	93.400	-0.200	1.200	-0.200	0.838	0.838	BF vs SF	3
Haemophilus	93.400	-3.700	1.300	-2.700	<0.01	<0.01	MF vs SF	3
Lachnospira	24.600	-1.900	1.700	-1.100	0.266	0.266	BF vs MF	3
Lachnospira	24.600	-3.400	1.500	-2.200	0.026	0.026	BF vs SF	3
Lachnospira	24.600	-1.500	1.700	-0.900	0.379	0.379	MF vs SF	3
o__Clostridiales	5.100	0.300	1.500	0.200	0.847	0.847	BF vs MF	3
o__Clostridiales	5.100	-2.100	1.300	-1.600	0.113	0.113	BF vs SF	3
o__Clostridiales	5.100	-2.400	1.500	-1.600	0.102	0.102	MF vs SF	3
Oscillospira	23.900	-0.100	0.900	-0.200	0.875	0.875	BF vs MF	3
Oscillospira	23.900	0.800	0.800	1.000	0.317	0.317	BF vs SF	3
Oscillospira	23.900	1.000	0.900	1.100	0.288	0.288	MF vs SF	3
Parabacteroides	365.300	-4.900	1.200	-4.200	<0.01	<0.01	BF vs MF	3
Parabacteroides	365.300	-0.400	1.100	-0.400	0.679	0.679	BF vs SF	3
Parabacteroides	365.300	4.500	1.200	3.800	<0.01	<0.01	MF vs SF	3
Roseburia	4.400	1.100	1.400	0.800	0.426	0.426	BF vs MF	3
Roseburia	4.400	2.200	1.200	1.800	0.066	0.066	BF vs SF	3
Roseburia	4.400	1.200	1.400	0.900	0.393	0.393	MF vs SF	3
SMB53	21.000	-2.200	0.800	-2.600	0.01	0.01	BF vs MF	3
SMB53	21.000	-3.700	0.700	-4.900	<0.01	<0.01	BF vs SF	3
SMB53	21.000	-1.500	0.800	-1.900	0.064	0.064	MF vs SF	3

Streptococcus	143.700	0.800	0.800	1.000	0.333	0.333	BF vs MF	3
Streptococcus	143.700	-1.100	0.700	-1.500	0.124	0.124	BF vs SF	3
Streptococcus	143.700	-1.900	0.800	-2.400	0.018	0.018	MF vs SF	3
Sutterella	14.500	0.900	1.600	0.600	0.578	0.578	BF vs MF	3
Sutterella	14.500	0.500	1.400	0.300	0.741	0.741	BF vs SF	3
Sutterella	14.500	-0.400	1.600	-0.300	0.79	0.79	MF vs SF	3
Veillonella	409.600	0.300	0.900	0.400	0.719	0.719	BF vs MF	3
Veillonella	409.600	-1.100	0.800	-1.400	0.164	0.164	BF vs SF	3
Veillonella	409.600	-1.400	0.900	-1.600	0.106	0.106	MF vs SF	3
[Clostridium]	67.200	-1.900	0.800	-2.400	0.017	0.017	BF vs MF	6
[Clostridium]	67.200	-1.100	0.800	-1.300	0.201	0.201	BF vs SF	6
[Clostridium]	67.200	0.800	0.800	0.900	0.345	0.345	MF vs SF	6
[Eubacterium]	57.200	-3.300	1.000	-3.200	<0.01	<0.01	BF vs MF	6
[Eubacterium]	57.200	-1.200	1.100	-1.100	0.288	0.288	BF vs SF	6
[Eubacterium]	57.200	2.100	1.100	1.900	0.056	0.056	MF vs SF	6
[Ruminococcus]	754.200	0.000	0.700	0.000	0.998	0.998	BF vs MF	6
[Ruminococcus]	754.200	0.300	0.700	0.400	0.708	0.708	BF vs SF	6
[Ruminococcus]	754.200	0.300	0.700	0.400	0.709	0.709	MF vs SF	6
Akkermansia	30.400	-4.000	1.200	-3.400	<0.01	<0.01	BF vs MF	6
Akkermansia	30.400	0.400	1.300	0.300	0.745	0.745	BF vs SF	6
Akkermansia	30.400	4.400	1.300	3.500	<0.01	<0.01	MF vs SF	6
Bacteroides	6063.500	0.200	0.700	0.200	0.817	0.817	BF vs MF	6
Bacteroides	6063.500	1.400	0.800	1.800	0.069	0.069	BF vs SF	6
Bacteroides	6063.500	1.200	0.800	1.600	0.108	0.108	MF vs SF	6
Bifidobacterium	3587.600	1.300	0.500	2.400	0.016	0.016	BF vs MF	6
Bifidobacterium	3587.600	4.400	0.600	8.000	<0.01	<0.01	BF vs SF	6
Bifidobacterium	3587.600	3.200	0.600	5.700	<0.01	<0.01	MF vs SF	6
Blautia	195.800	0.500	0.900	0.600	0.564	0.564	BF vs MF	6
Blautia	195.800	-1.400	0.900	-1.600	0.12	0.12	BF vs SF	6
Blautia	195.800	-1.900	0.900	-2.100	0.036	0.036	MF vs SF	6

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Clostridium	105.600	1.900	0.900	2.000	0.051	0.051	BF vs MF	6
Clostridium	105.600	1.200	1.000	1.200	0.25	0.25	BF vs SF	6
Clostridium	105.600	-0.700	1.000	-0.700	0.509	0.509	MF vs SF	6
Coprococcus	72.900	-3.900	0.800	-5.200	<0.01	<0.01	BF vs MF	6
Coprococcus	72.900	-3.600	0.800	-4.500	<0.01	<0.01	BF vs SF	6
Coprococcus	72.900	0.300	0.800	0.300	0.741	0.741	MF vs SF	6
Dorea	34.200	0.900	0.800	1.100	0.272	0.272	BF vs MF	6
Dorea	34.200	-0.400	0.900	-0.500	0.601	0.601	BF vs SF	6
Dorea	34.200	-1.300	0.800	-1.500	0.122	0.122	MF vs SF	6
Enterococcus	37.500	1.400	1.000	1.400	0.15	0.15	BF vs MF	6
Enterococcus	37.500	5.700	1.100	5.300	<0.01	<0.01	BF vs SF	6
Enterococcus	37.500	4.300	1.100	4.000	<0.01	<0.01	MF vs SF	6
f__Bifidobacteriaceae	13.100	-0.500	0.900	-0.600	0.53	0.53	BF vs MF	6
f__Bifidobacteriaceae	13.100	3.000	1.000	3.100	<0.01	<0.01	BF vs SF	6
f__Bifidobacteriaceae	13.100	3.500	1.000	3.700	<0.01	<0.01	MF vs SF	6
f__Clostridiaceae	93.700	-1.000	0.900	-1.200	0.236	0.236	BF vs MF	6
f__Clostridiaceae	93.700	-2.700	0.900	-2.900	<0.01	<0.01	BF vs SF	6
f__Clostridiaceae	93.700	-1.700	0.900	-1.800	0.075	0.075	MF vs SF	6
f__Enterobacteriaceae	2226.100	0.600	0.600	1.000	0.335	0.335	BF vs MF	6
f__Enterobacteriaceae	2226.100	3.000	0.700	4.300	<0.01	<0.01	BF vs SF	6
f__Enterobacteriaceae	2226.100	2.400	0.700	3.400	<0.01	<0.01	MF vs SF	6
f__Erysipelotrichaceae	90.900	0.100	0.700	0.200	0.844	0.844	BF vs MF	6
f__Erysipelotrichaceae	90.900	-0.000	0.700	-0.000	0.975	0.975	BF vs SF	6
f__Erysipelotrichaceae	90.900	-0.200	0.700	-0.200	0.83	0.83	MF vs SF	6
f__Lachnospiraceae	213.400	-0.300	0.600	-0.500	0.628	0.628	BF vs MF	6
f__Lachnospiraceae	213.400	-1.600	0.700	-2.400	0.019	0.019	BF vs SF	6
f__Lachnospiraceae	213.400	-1.300	0.700	-1.900	0.056	0.056	MF vs SF	6
f__Peptostreptococcaceae	84.800	0.500	0.700	0.700	0.456	0.456	BF vs MF	6

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f__Peptostreptococcaceae	84.800	-1.100	0.700	-1.600	0.116	0.116	BF vs SF	6
f__Peptostreptococcaceae	84.800	-1.600	0.700	-2.300	0.023	0.023	MF vs SF	6
f__Rikenellaceae	4.300	-1.100	2.200	-0.500	0.627	0.627	BF vs MF	6
f__Rikenellaceae	4.300	4.900	2.500	2.000	0.049	0.049	BF vs SF	6
f__Rikenellaceae	4.300	6.000	2.500	2.400	0.016	0.016	MF vs SF	6
f__Ruminococcaceae	130.700	-0.500	0.600	-0.800	0.406	0.406	BF vs MF	6
f__Ruminococcaceae	130.700	-0.600	0.700	-0.900	0.367	0.367	BF vs SF	6
f__Ruminococcaceae	130.700	-0.100	0.700	-0.100	0.895	0.895	MF vs SF	6
f__Veillonellaceae	966.600	1.400	1.100	1.200	0.218	0.218	BF vs MF	6
f__Veillonellaceae	966.600	4.500	1.200	3.700	<0.01	<0.01	BF vs SF	6
f__Veillonellaceae	966.600	3.100	1.200	2.500	0.012	0.012	MF vs SF	6
Faecalibacterium	245.100	-1.200	1.100	-1.100	0.265	0.265	BF vs MF	6
Faecalibacterium	245.100	-1.100	1.200	-0.900	0.359	0.359	BF vs SF	6
Faecalibacterium	245.100	0.100	1.200	0.100	0.908	0.908	MF vs SF	6
Haemophilus	67.600	2.300	1.000	2.200	0.026	0.026	BF vs MF	6
Haemophilus	67.600	1.200	1.100	1.100	0.273	0.273	BF vs SF	6
Haemophilus	67.600	-1.100	1.100	-1.000	0.334	0.334	MF vs SF	6
Lachnospira	9.400	2.600	1.700	1.600	0.111	0.111	BF vs MF	6
Lachnospira	9.400	-2.600	1.700	-1.500	0.129	0.129	BF vs SF	6
Lachnospira	9.400	-5.300	1.800	-3.000	<0.01	<0.01	MF vs SF	6
o__Clostridiales	7.800	0.600	1.000	0.600	0.578	0.578	BF vs MF	6
o__Clostridiales	7.800	-2.400	1.100	-2.300	0.023	0.023	BF vs SF	6
o__Clostridiales	7.800	-3.000	1.100	-2.800	<0.01	<0.01	MF vs SF	6
Oscillospira	27.700	-1.200	0.600	-2.000	0.047	0.047	BF vs MF	6
Oscillospira	27.700	-1.400	0.700	-2.100	0.035	0.035	BF vs SF	6
Oscillospira	27.700	-0.200	0.600	-0.300	0.793	0.793	MF vs SF	6
Parabacteroides	478.600	-0.300	1.300	-0.200	0.832	0.832	BF vs MF	6
Parabacteroides	478.600	0.200	1.400	0.200	0.871	0.871	BF vs SF	6

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Parabacteroides	478.600	0.500	1.400	0.400	0.719	0.719	MF vs SF	6
Roseburia	35.200	-2.800	1.600	-1.700	0.091	0.091	BF vs MF	6
Roseburia	35.200	-4.300	1.800	-2.400	0.016	0.016	BF vs SF	6
Roseburia	35.200	-1.500	1.800	-0.800	0.398	0.398	MF vs SF	6
SMB53	18.600	-0.300	0.700	-0.400	0.724	0.724	BF vs MF	6
SMB53	18.600	-2.000	0.800	-2.600	<0.01	<0.01	BF vs SF	6
SMB53	18.600	-1.800	0.800	-2.300	0.023	0.023	MF vs SF	6
Streptococcus	123.000	0.700	0.700	1.000	0.34	0.34	BF vs MF	6
Streptococcus	123.000	2.000	0.800	2.600	<0.01	<0.01	BF vs SF	6
Streptococcus	123.000	1.300	0.800	1.800	0.078	0.078	MF vs SF	6
Sutterella	80.700	-4.600	1.600	-2.900	<0.01	<0.01	BF vs MF	6
Sutterella	80.700	-4.700	1.700	-2.800	<0.01	<0.01	BF vs SF	6
Sutterella	80.700	-0.100	1.700	-0.000	0.967	0.967	MF vs SF	6
Veillonella	597.600	1.400	0.700	2.000	0.048	0.048	BF vs MF	6
Veillonella	597.600	3.800	0.800	4.800	<0.01	<0.01	BF vs SF	6
Veillonella	597.600	2.300	0.800	3.000	<0.01	<0.01	MF vs SF	6
[Clostridium]	59.000	1.900	0.900	2.000	0.041	0.041	BF vs MF	9
[Clostridium]	59.000	3.900	1.000	4.100	<0.01	<0.01	BF vs SF	9
[Clostridium]	59.000	1.900	0.900	2.100	0.039	0.039	MF vs SF	9
[Eubacterium]	10.100	0.400	1.100	0.400	0.705	0.705	BF vs MF	9
[Eubacterium]	10.100	0.500	1.100	0.400	0.671	0.671	BF vs SF	9
[Eubacterium]	10.100	0.100	1.100	0.000	0.963	0.963	MF vs SF	9
[Ruminococcus]	257.300	-0.400	0.800	-0.500	0.621	0.621	BF vs MF	9
[Ruminococcus]	257.300	-0.000	0.800	-0.000	0.966	0.966	BF vs SF	9
[Ruminococcus]	257.300	0.300	0.700	0.500	0.648	0.648	MF vs SF	9
Akkermansia	101.300	-4.400	1.900	-2.300	0.022	0.022	BF vs MF	9
Akkermansia	101.300	-8.000	1.900	-4.100	<0.01	<0.01	BF vs SF	9
Akkermansia	101.300	-3.600	1.900	-1.900	0.055	0.055	MF vs SF	9
Bacteroides	2768.500	-0.600	0.800	-0.700	0.478	0.478	BF vs MF	9
Bacteroides	2768.500	-0.100	0.800	-0.100	0.896	0.896	BF vs SF	9

Bacteroides	2768.500	0.500	0.800	0.600	0.559	0.559	MF vs SF	9
Bifidobacterium	3091.200	0.200	0.800	0.200	0.821	0.821	BF vs MF	9
Bifidobacterium	3091.200	2.200	0.900	2.600	<0.01	<0.01	BF vs SF	9
Bifidobacterium	3091.200	2.000	0.800	2.400	0.016	0.016	MF vs SF	9
Blautia	312.900	0.700	1.200	0.600	0.56	0.56	BF vs MF	9
Blautia	312.900	-2.200	1.200	-1.900	0.062	0.062	BF vs SF	9
Blautia	312.900	-2.900	1.200	-2.500	0.013	0.013	MF vs SF	9
Clostridium	153.300	3.400	1.200	2.800	<0.01	<0.01	BF vs MF	9
Clostridium	153.300	3.300	1.200	2.700	<0.01	<0.01	BF vs SF	9
Clostridium	153.300	-0.100	1.200	-0.100	0.94	0.94	MF vs SF	9
Coprococcus	67.300	-0.300	1.000	-0.300	0.743	0.743	BF vs MF	9
Coprococcus	67.300	-1.000	1.000	-1.000	0.317	0.317	BF vs SF	9
Coprococcus	67.300	-0.600	1.000	-0.700	0.496	0.496	MF vs SF	9
Dorea	38.900	-0.300	1.100	-0.300	0.764	0.764	BF vs MF	9
Dorea	38.900	-0.700	1.100	-0.600	0.537	0.537	BF vs SF	9
Dorea	38.900	-0.400	1.100	-0.300	0.748	0.748	MF vs SF	9
Enterococcus	11.700	2.000	1.300	1.600	0.12	0.12	BF vs MF	9
Enterococcus	11.700	4.000	1.300	3.100	<0.01	<0.01	BF vs SF	9
Enterococcus	11.700	2.100	1.300	1.600	0.116	0.116	MF vs SF	9
f__Bifidobacteriaceae	18.400	0.500	1.100	0.500	0.635	0.635	BF vs MF	9
f__Bifidobacteriaceae	18.400	1.400	1.100	1.300	0.208	0.208	BF vs SF	9
f__Bifidobacteriaceae	18.400	0.900	1.100	0.800	0.428	0.428	MF vs SF	9
f__Clostridiaceae	66.900	-1.400	1.000	-1.300	0.182	0.182	BF vs MF	9
f__Clostridiaceae	66.900	-0.600	1.000	-0.600	0.552	0.552	BF vs SF	9
f__Clostridiaceae	66.900	0.800	1.000	0.700	0.454	0.454	MF vs SF	9
f__Enterobacteriaceae	1007.200	3.600	0.800	4.500	<0.01	<0.01	BF vs MF	9
f__Enterobacteriaceae	1007.200	3.900	0.800	4.900	<0.01	<0.01	BF vs SF	9
f__Enterobacteriaceae	1007.200	0.400	0.800	0.500	0.65	0.65	MF vs SF	9
f__Erysipelotrichaceae	32.600	1.300	0.800	1.600	0.108	0.108	BF vs MF	9

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f__Erysipelotrichaceae	32.600	1.100	0.800	1.400	0.16	0.16	BF vs SF	9
f__Erysipelotrichaceae	32.600	-0.200	0.800	-0.200	0.835	0.835	MF vs SF	9
f__Lachnospiraceae	335.100	-0.700	0.900	-0.700	0.456	0.456	BF vs MF	9
f__Lachnospiraceae	335.100	-1.000	0.900	-1.100	0.275	0.275	BF vs SF	9
f__Lachnospiraceae	335.100	-0.300	0.900	-0.400	0.726	0.726	MF vs SF	9
f__Peptostreptococcaceae	140.700	-1.400	1.100	-1.200	0.222	0.222	BF vs MF	9
f__Peptostreptococcaceae	140.700	-3.400	1.100	-3.000	<0.01	<0.01	BF vs SF	9
f__Peptostreptococcaceae	140.700	-2.000	1.100	-1.800	0.072	0.072	MF vs SF	9
f__Rikenellaceae	23.500	-0.300	1.600	-0.200	1	1	BF vs MF	9
f__Rikenellaceae	23.500	-0.700	1.600	-0.400	1	1	BF vs SF	9
f__Rikenellaceae	23.500	-0.400	1.600	-0.200	1	1	MF vs SF	9
f__Ruminococcaceae	256.900	-0.600	0.900	-0.700	1	1	BF vs MF	9
f__Ruminococcaceae	256.900	-0.500	0.900	-0.500	1	1	BF vs SF	9
f__Ruminococcaceae	256.900	0.100	0.900	0.100	1	1	MF vs SF	9
f__Veillonellaceae	1022.100	-0.300	1.700	-0.200	0.856	0.856	BF vs MF	9
f__Veillonellaceae	1022.100	4.600	1.700	2.700	<0.01	<0.01	BF vs SF	9
f__Veillonellaceae	1022.100	4.900	1.700	2.900	<0.01	<0.01	MF vs SF	9
Faecalibacterium	479.800	-1.200	1.500	-0.800	0.43	0.43	BF vs MF	9
Faecalibacterium	479.800	0.900	1.500	0.600	0.533	0.533	BF vs SF	9
Faecalibacterium	479.800	2.100	1.400	1.400	0.153	0.153	MF vs SF	9
Haemophilus	179.500	1.500	1.200	1.200	0.224	0.224	BF vs MF	9
Haemophilus	179.500	3.800	1.200	3.000	<0.01	<0.01	BF vs SF	9
Haemophilus	179.500	2.300	1.200	1.800	0.065	0.065	MF vs SF	9
Lachnospira	142.400	-3.500	1.600	-2.100	0.035	0.035	BF vs MF	9
Lachnospira	142.400	-4.400	1.600	-2.700	<0.01	<0.01	BF vs SF	9
Lachnospira	142.400	-0.900	1.600	-0.600	0.571	0.571	MF vs SF	9
o__Clostridiales	7.400	0.500	1.200	0.400	0.678	0.678	BF vs MF	9
o__Clostridiales	7.400	-3.000	1.100	-2.700	<0.01	<0.01	BF vs SF	9

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o__Clostridiales	7.400	-3.500	1.100	-3.100	<0.01	<0.01	MF vs SF	9
Oscillospira	36.200	0.100	0.900	0.100	0.89	0.89	BF vs MF	9
Oscillospira	36.200	-0.300	0.900	-0.400	0.715	0.715	BF vs SF	9
Oscillospira	36.200	-0.500	0.900	-0.500	0.61	0.61	MF vs SF	9
Parabacteroides	523.900	-8.000	1.500	-5.200	1	1	BF vs MF	9
Parabacteroides	523.900	-4.700	1.500	-3.100	1	1	BF vs SF	9
Parabacteroides	523.900	3.300	1.500	2.200	1	1	MF vs SF	9
Roseburia	45.700	-2.800	1.600	-1.700	0.083	0.083	BF vs MF	9
Roseburia	45.700	-4.000	1.600	-2.500	0.013	0.013	BF vs SF	9
Roseburia	45.700	-1.200	1.600	-0.800	0.44	0.44	MF vs SF	9
SMB53	43.300	-1.900	1.000	-1.900	0.057	0.057	BF vs MF	9
SMB53	43.300	-4.300	1.000	-4.200	<0.01	<0.01	BF vs SF	9
SMB53	43.300	-2.300	1.000	-2.400	0.017	0.017	MF vs SF	9
Streptococcus	70.400	0.200	1.200	0.200	0.875	0.875	BF vs MF	9
Streptococcus	70.400	1.700	1.200	1.500	0.146	0.146	BF vs SF	9
Streptococcus	70.400	1.500	1.100	1.300	0.189	0.189	MF vs SF	9
Sutterella	69.900	-0.500	2.000	-0.200	0.809	0.809	BF vs MF	9
Sutterella	69.900	-1.800	2.000	-0.900	0.376	0.376	BF vs SF	9
Sutterella	69.900	-1.300	2.000	-0.700	0.514	0.514	MF vs SF	9
Veillonella	335.600	1.600	1.000	1.600	0.114	0.114	BF vs MF	9
Veillonella	335.600	3.400	1.000	3.300	<0.01	<0.01	BF vs SF	9
Veillonella	335.600	1.700	1.000	1.700	0.089	0.089	MF vs SF	9
[Clostridium]	87.700	-0.700	1.100	-0.600	0.553	0.553	BF vs MF	12
[Clostridium]	87.700	2.600	1.200	2.100	0.033	0.033	BF vs NLB	12
[Clostridium]	87.700	1.000	1.100	0.900	0.377	0.377	BF vs SF	12
[Clostridium]	87.700	3.200	1.200	2.600	<0.01	<0.01	MF vs NLB	12
[Clostridium]	87.700	1.700	1.100	1.500	0.129	0.129	MF vs SF	12
[Clostridium]	87.700	-1.600	1.200	-1.300	0.205	0.205	NLB vs SF	12
[Eubacterium]	15.000	-0.100	0.800	-0.200	0.868	0.868	BF vs MF	12

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[Eubacterium]	15.000	-0.300	0.800	-0.300	0.743	0.743	BF vs NLB	12
[Eubacterium]	15.000	1.100	0.800	1.400	0.161	0.161	BF vs SF	12
[Eubacterium]	15.000	-0.100	0.800	-0.200	0.865	0.865	MF vs NLB	12
[Eubacterium]	15.000	1.200	0.800	1.600	0.107	0.107	MF vs SF	12
[Eubacterium]	15.000	1.400	0.900	1.600	0.112	0.112	NLB vs SF	12
[Ruminococcus]	484.900	-1.000	0.600	-1.800	0.078	0.078	BF vs MF	12
[Ruminococcus]	484.900	-0.200	0.600	-0.300	0.764	0.764	BF vs NLB	12
[Ruminococcus]	484.900	0.100	0.600	0.200	0.854	0.854	BF vs SF	12
[Ruminococcus]	484.900	0.800	0.600	1.300	0.191	0.191	MF vs NLB	12
[Ruminococcus]	484.900	1.200	0.600	2.000	0.046	0.046	MF vs SF	12
[Ruminococcus]	484.900	0.300	0.700	0.500	0.647	0.647	NLB vs SF	12
Akkermansia	94.100	3.000	1.400	2.200	0.03	0.03	BF vs MF	12
Akkermansia	94.100	-1.200	1.500	-0.800	0.442	0.442	BF vs NLB	12
Akkermansia	94.100	0.400	1.400	0.300	0.754	0.754	BF vs SF	12
Akkermansia	94.100	-4.200	1.500	-2.700	<0.01	<0.01	MF vs NLB	12
Akkermansia	94.100	-2.600	1.400	-1.900	0.058	0.058	MF vs SF	12
Akkermansia	94.100	1.600	1.600	1.000	0.303	0.303	NLB vs SF	12
Bacteroides	6744.100	-1.100	0.600	-1.900	0.059	0.059	BF vs MF	12
Bacteroides	6744.100	-0.100	0.600	-0.200	0.826	0.826	BF vs NLB	12
Bacteroides	6744.100	0.400	0.600	0.700	0.501	0.501	BF vs SF	12
Bacteroides	6744.100	1.000	0.700	1.500	0.134	0.134	MF vs NLB	12
Bacteroides	6744.100	1.500	0.600	2.600	<0.01	<0.01	MF vs SF	12
Bacteroides	6744.100	0.500	0.700	0.800	0.41	0.41	NLB vs SF	12
Bifidobacterium	1396.600	0.000	0.600	0.000	0.965	0.965	BF vs MF	12
Bifidobacterium	1396.600	1.300	0.600	2.000	0.044	0.044	BF vs NLB	12
Bifidobacterium	1396.600	2.300	0.600	3.900	<0.01	<0.01	BF vs SF	12
Bifidobacterium	1396.600	1.300	0.600	1.900	0.052	0.052	MF vs NLB	12
Bifidobacterium	1396.600	2.300	0.600	4.000	<0.01	<0.01	MF vs SF	12
Bifidobacterium	1396.600	1.000	0.700	1.600	0.12	0.12	NLB vs SF	12
Blautia	359.800	-0.600	0.800	-0.800	0.439	0.439	BF vs MF	12

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Blautia	359.800	-1.500	0.800	-1.800	0.064	0.064	BF vs NLB	12
Blautia	359.800	-1.600	0.800	-2.000	0.041	0.041	BF vs SF	12
Blautia	359.800	-0.900	0.800	-1.100	0.265	0.265	MF vs NLB	12
Blautia	359.800	-1.000	0.700	-1.300	0.186	0.186	MF vs SF	12
Blautia	359.800	-0.100	0.900	-0.100	0.952	0.952	NLB vs SF	12
Clostridium	119.500	1.100	1.400	0.800	0.423	0.423	BF vs MF	12
Clostridium	119.500	2.300	1.500	1.500	0.13	0.13	BF vs NLB	12
Clostridium	119.500	5.600	1.400	4.000	<0.01	<0.01	BF vs SF	12
Clostridium	119.500	1.200	1.500	0.800	0.448	0.448	MF vs NLB	12
Clostridium	119.500	4.500	1.400	3.300	<0.01	<0.01	MF vs SF	12
Clostridium	119.500	3.400	1.600	2.200	0.03	0.03	NLB vs SF	12
Coprococcus	106.800	-0.400	0.700	-0.500	0.605	0.605	BF vs MF	12
Coprococcus	106.800	0.600	0.800	0.800	0.437	0.437	BF vs NLB	12
Coprococcus	106.800	-0.100	0.700	-0.200	0.872	0.872	BF vs SF	12
Coprococcus	106.800	1.000	0.800	1.200	0.217	0.217	MF vs NLB	12
Coprococcus	106.800	0.300	0.700	0.400	0.717	0.717	MF vs SF	12
Coprococcus	106.800	-0.700	0.800	-0.900	0.369	0.369	NLB vs SF	12
Dorea	59.000	-0.400	0.700	-0.500	0.611	0.611	BF vs MF	12
Dorea	59.000	-1.600	0.700	-2.100	0.034	0.034	BF vs NLB	12
Dorea	59.000	-0.600	0.700	-0.900	0.381	0.381	BF vs SF	12
Dorea	59.000	-1.200	0.800	-1.600	0.105	0.105	MF vs NLB	12
Dorea	59.000	-0.300	0.700	-0.400	0.7	0.7	MF vs SF	12
Dorea	59.000	1.000	0.800	1.300	0.207	0.207	NLB vs SF	12
Enterococcus	9.300	3.500	1.400	2.500	0.011	0.011	BF vs MF	12
Enterococcus	9.300	1.700	1.400	1.200	0.225	0.225	BF vs NLB	12
Enterococcus	9.300	-1.400	1.300	-1.100	0.292	0.292	BF vs SF	12
Enterococcus	9.300	-1.800	1.500	-1.200	0.245	0.245	MF vs NLB	12
Enterococcus	9.300	-4.900	1.300	-3.600	<0.01	<0.01	MF vs SF	12
Enterococcus	9.300	-3.100	1.500	-2.100	0.034	0.034	NLB vs SF	12
f__Bifidobacteriaceae	7.300	-0.200	1.100	-0.200	0.862	0.862	BF vs MF	12

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f__Bifidobacteriaceae	7.300	0.300	1.200	0.200	0.805	0.805	BF vs NLB	12
f__Bifidobacteriaceae	7.300	1.100	1.200	1.000	0.325	0.325	BF vs SF	12
f__Bifidobacteriaceae	7.300	0.500	1.200	0.400	0.689	0.689	MF vs NLB	12
f__Bifidobacteriaceae	7.300	1.300	1.100	1.200	0.232	0.232	MF vs SF	12
f__Bifidobacteriaceae	7.300	0.800	1.300	0.700	0.513	0.513	NLB vs SF	12
f__Clostridiaceae	174.200	-0.100	1.100	-0.100	0.923	0.923	BF vs MF	12
f__Clostridiaceae	174.200	-0.100	1.200	-0.100	0.959	0.959	BF vs NLB	12
f__Clostridiaceae	174.200	-2.700	1.100	-2.400	0.016	0.016	BF vs SF	12
f__Clostridiaceae	174.200	0.000	1.200	0.000	0.97	0.97	MF vs NLB	12
f__Clostridiaceae	174.200	-2.600	1.100	-2.400	0.017	0.017	MF vs SF	12
f__Clostridiaceae	174.200	-2.600	1.200	-2.100	0.033	0.033	NLB vs SF	12
f__Enterobacteriaceae	444.900	0.000	0.700	0.100	0.946	0.946	BF vs MF	12
f__Enterobacteriaceae	444.900	1.300	0.800	1.800	0.077	0.077	BF vs NLB	12
f__Enterobacteriaceae	444.900	0.200	0.700	0.200	0.829	0.829	BF vs SF	12
f__Enterobacteriaceae	444.900	1.300	0.800	1.700	0.093	0.093	MF vs NLB	12
f__Enterobacteriaceae	444.900	0.100	0.700	0.200	0.878	0.878	MF vs SF	12
f__Enterobacteriaceae	444.900	-1.200	0.800	-1.500	0.128	0.128	NLB vs SF	12
f__Erysipelotrichaceae	59.000	0.600	0.600	1.000	0.32	0.32	BF vs MF	12
f__Erysipelotrichaceae	59.000	-0.700	0.700	-1.000	0.301	0.301	BF vs NLB	12
f__Erysipelotrichaceae	59.000	1.800	0.700	2.800	<0.01	<0.01	BF vs SF	12
f__Erysipelotrichaceae	59.000	-1.300	0.700	-1.900	0.055	0.055	MF vs NLB	12
f__Erysipelotrichaceae	59.000	1.200	0.600	1.900	0.061	0.061	MF vs SF	12
f__Erysipelotrichaceae	59.000	2.500	0.700	3.500	<0.01	<0.01	NLB vs SF	12
f__Lachnospiraceae	402.100	-1.500	0.500	-3.100	<0.01	<0.01	BF vs MF	12
f__Lachnospiraceae	402.100	-0.000	0.500	-0.100	0.948	0.948	BF vs NLB	12
f__Lachnospiraceae	402.100	-0.700	0.500	-1.400	0.168	0.168	BF vs SF	12
f__Lachnospiraceae	402.100	1.400	0.500	2.700	<0.01	<0.01	MF vs NLB	12

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f__Lachnospiraceae	402.100	0.800	0.500	1.700	0.087	0.087	MF vs SF	12
f__Lachnospiraceae	402.100	-0.600	0.500	-1.200	0.236	0.236	NLB vs SF	12
f__Peptostreptococcaceae	116.600	-0.500	0.600	-0.900	0.369	0.369	BF vs MF	12
f__Peptostreptococcaceae	116.600	0.100	0.600	0.100	0.93	0.93	BF vs NLB	12
f__Peptostreptococcaceae	116.600	-0.700	0.600	-1.300	0.183	0.183	BF vs SF	12
f__Peptostreptococcaceae	116.600	0.500	0.600	0.900	0.366	0.366	MF vs NLB	12
f__Peptostreptococcaceae	116.600	-0.200	0.500	-0.500	0.648	0.648	MF vs SF	12
f__Peptostreptococcaceae	116.600	-0.800	0.600	-1.300	0.196	0.196	NLB vs SF	12
f__Rikenellaceae	59.600	-3.600	1.700	-2.100	0.032	0.032	BF vs MF	12
f__Rikenellaceae	59.600	-4.400	1.800	-2.400	0.016	0.016	BF vs NLB	12
f__Rikenellaceae	59.600	-2.300	1.700	-1.400	0.177	0.177	BF vs SF	12
f__Rikenellaceae	59.600	-0.800	1.900	-0.400	0.676	0.676	MF vs NLB	12
f__Rikenellaceae	59.600	1.300	1.600	0.800	0.425	0.425	MF vs SF	12
f__Rikenellaceae	59.600	2.100	1.900	1.100	0.266	0.266	NLB vs SF	12
f__Ruminococcaceae	231.800	0.000	0.600	0.100	0.951	0.951	BF vs MF	12
f__Ruminococcaceae	231.800	0.300	0.700	0.400	0.665	0.665	BF vs NLB	12
f__Ruminococcaceae	231.800	0.100	0.600	0.100	0.903	0.903	BF vs SF	12
f__Ruminococcaceae	231.800	0.300	0.700	0.400	0.712	0.712	MF vs NLB	12
f__Ruminococcaceae	231.800	0.000	0.600	0.100	0.95	0.95	MF vs SF	12
f__Ruminococcaceae	231.800	-0.200	0.700	-0.300	0.758	0.758	NLB vs SF	12
f__Veillonellaceae	440.000	0.600	1.300	0.500	0.64	0.64	BF vs MF	12
f__Veillonellaceae	440.000	1.400	1.500	1.000	0.325	0.325	BF vs NLB	12
f__Veillonellaceae	440.000	2.000	1.400	1.400	0.152	0.152	BF vs SF	12
f__Veillonellaceae	440.000	0.800	1.500	0.500	0.588	0.588	MF vs NLB	12
f__Veillonellaceae	440.000	1.300	1.300	1.000	0.315	0.315	MF vs SF	12
f__Veillonellaceae	440.000	0.500	1.500	0.300	0.73	0.73	NLB vs SF	12
Faecalibacterium	949.700	-0.100	1.000	-0.100	0.944	0.944	BF vs MF	12
Faecalibacterium	949.700	-0.500	1.100	-0.500	0.641	0.641	BF vs NLB	12

Faecalibacterium	949.700	0.900	1.000	0.900	0.373	0.373	BF vs SF	12
Faecalibacterium	949.700	-0.400	1.100	-0.400	0.693	0.693	MF vs NLB	12
Faecalibacterium	949.700	1.000	1.000	1.000	0.321	0.321	MF vs SF	12
Faecalibacterium	949.700	1.400	1.100	1.300	0.208	0.208	NLB vs SF	12
Haemophilus	122.600	-0.100	0.900	-0.100	0.884	0.884	BF vs MF	12
Haemophilus	122.600	2.000	1.000	2.000	0.051	0.051	BF vs NLB	12
Haemophilus	122.600	2.100	0.900	2.200	0.025	0.025	BF vs SF	12
Haemophilus	122.600	2.100	1.000	2.100	0.04	0.04	MF vs NLB	12
Haemophilus	122.600	2.200	0.900	2.500	0.013	0.013	MF vs SF	12
Haemophilus	122.600	0.100	1.000	0.100	0.886	0.886	NLB vs SF	12
Lachnospira	33.300	-0.300	1.300	-0.200	0.85	0.85	BF vs MF	12
Lachnospira	33.300	3.000	1.400	2.000	0.041	0.041	BF vs NLB	12
Lachnospira	33.300	-0.100	1.300	-0.100	0.931	0.931	BF vs SF	12
Lachnospira	33.300	3.200	1.500	2.200	0.029	0.029	MF vs NLB	12
Lachnospira	33.300	0.100	1.300	0.100	0.917	0.917	MF vs SF	12
Lachnospira	33.300	-3.100	1.500	-2.100	0.039	0.039	NLB vs SF	12
o__Clostridiales	12.400	-0.200	0.900	-0.200	0.804	0.804	BF vs MF	12
o__Clostridiales	12.400	-0.600	1.000	-0.600	0.538	0.538	BF vs NLB	12
o__Clostridiales	12.400	-1.800	0.900	-1.900	0.056	0.056	BF vs SF	12
o__Clostridiales	12.400	-0.400	1.000	-0.400	0.706	0.706	MF vs NLB	12
o__Clostridiales	12.400	-1.500	0.900	-1.700	0.087	0.087	MF vs SF	12
o__Clostridiales	12.400	-1.200	1.000	-1.100	0.257	0.257	NLB vs SF	12
Oscillospira	39.200	-0.900	0.700	-1.400	0.151	0.151	BF vs MF	12
Oscillospira	39.200	-0.000	0.700	-0.000	0.991	0.991	BF vs NLB	12
Oscillospira	39.200	0.300	0.700	0.500	0.63	0.63	BF vs SF	12
Oscillospira	39.200	0.900	0.700	1.300	0.195	0.195	MF vs NLB	12
Oscillospira	39.200	1.300	0.600	2.000	0.049	0.049	MF vs SF	12
Oscillospira	39.200	0.300	0.700	0.400	0.654	0.654	NLB vs SF	12

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Parabacteroides	397.800	-1.800	1.300	-1.400	0.154	0.154	BF vs MF	12
Parabacteroides	397.800	-1.800	1.400	-1.300	0.199	0.199	BF vs NLB	12
Parabacteroides	397.800	-2.700	1.300	-2.100	0.038	0.038	BF vs SF	12
Parabacteroides	397.800	0.000	1.400	0.000	0.974	0.974	MF vs NLB	12
Parabacteroides	397.800	-0.900	1.300	-0.700	0.488	0.488	MF vs SF	12
Parabacteroides	397.800	-0.900	1.400	-0.600	0.522	0.522	NLB vs SF	12
Roseburia	36.600	-0.800	1.300	-0.700	0.504	0.504	BF vs MF	12
Roseburia	36.600	2.300	1.400	1.600	0.1	0.1	BF vs NLB	12
Roseburia	36.600	-0.500	1.300	-0.400	0.673	0.673	BF vs SF	12
Roseburia	36.600	3.100	1.400	2.200	0.026	0.026	MF vs NLB	12
Roseburia	36.600	0.300	1.200	0.200	0.805	0.805	MF vs SF	12
Roseburia	36.600	-2.800	1.400	-2.000	0.048	0.048	NLB vs SF	12
SMB53	32.300	-0.200	0.600	-0.400	0.7	0.7	BF vs MF	12
SMB53	32.300	-0.400	0.700	-0.500	0.599	0.599	BF vs NLB	12
SMB53	32.300	-1.000	0.600	-1.500	0.128	0.128	BF vs SF	12
SMB53	32.300	-0.100	0.700	-0.200	0.87	0.87	MF vs NLB	12
SMB53	32.300	-0.700	0.600	-1.200	0.241	0.241	MF vs SF	12
SMB53	32.300	-0.600	0.700	-0.900	0.384	0.384	NLB vs SF	12
Streptococcus	78.300	-0.700	0.800	-0.900	0.349	0.349	BF vs MF	12
Streptococcus	78.300	1.200	0.800	1.400	0.161	0.161	BF vs NLB	12
Streptococcus	78.300	1.100	0.800	1.400	0.174	0.174	BF vs SF	12
Streptococcus	78.300	1.900	0.900	2.200	0.026	0.026	MF vs NLB	12
Streptococcus	78.300	1.800	0.800	2.400	0.018	0.018	MF vs SF	12
Streptococcus	78.300	-0.100	0.900	-0.100	0.899	0.899	NLB vs SF	12
Sutterella	190.600	-1.100	1.700	-0.600	0.537	0.537	BF vs MF	12
Sutterella	190.600	0.400	1.900	0.200	0.847	0.847	BF vs NLB	12
Sutterella	190.600	1.700	1.700	1.000	0.329	0.329	BF vs SF	12
Sutterella	190.600	1.400	1.900	0.800	0.453	0.453	MF vs NLB	12
Sutterella	190.600	2.800	1.700	1.600	0.101	0.101	MF vs SF	12
Sutterella	190.600	1.300	1.900	0.700	0.486	0.486	NLB vs SF	12
Veillonella	152.700	2.800	0.700	3.800	<0.01	<0.01	BF vs MF	12

Veillonella	152.700	2.600	0.800	3.300	<0.01	<0.01	BF vs NLB	12
Veillonella	152.700	3.900	0.700	5.200	<0.01	<0.01	BF vs SF	12
Veillonella	152.700	-0.200	0.800	-0.300	0.789	0.789	MF vs NLB	12
Veillonella	152.700	1.100	0.700	1.500	0.143	0.143	MF vs SF	12
Veillonella	152.700	1.300	0.800	1.500	0.121	0.121	NLB vs SF	12

[1]Output from DESeq2 package in R in which pairwise comparisons by diet were performed. BF = Breast-fed, f = family, FDR = false discovery rate, MF = milk formula fed, NLB = no longer breastfeeding, o = order, SE = standard error of mean, SF = soy formula fed. Data are presented at the genera taxonomic level. Sample size range from 10 to 20 per diet group at three, six, nine and 12 months of age.

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Supplementary Table 4: Dietary differences in fecal metabolites (Negative Mode) from infants at three, six, nine, and 12 months of age.[1]

Age	Metabolite	BF	MF	NLB	SF	P-value	FDR
3	(S)-3,4-Dihydroxybutyric Acid	20 (1.79)a	20.8 (1.03)a		19.3 (3.64)a	0.496	0.57
3	2-Hydroxy-3-methylbutyric Acid	21.8 (2.57)a	21.3 (0.969)a		18.4 (1)b	<0.01	<0.01
3	2-Hydroxyadipic Acid	17.8 (2.09)a	16.9 (1.38)a		15.8 (1.49)b	<0.01	0.02
3	2-Oxoglutaric Acid	18.7 (4.17)a	17 (1.58)a		14.7 (1.88)b	<0.01	0.021
3	2-Phenylacetic Acid	10.8 (3.77)a	13.8 (0.933)a		14.9 (1.59)b	<0.01	<0.01
3	3-Dehydroshikimic acid	13.2 (2.78)a	13.7 (3.64)a		10.9 (0.765)b	<0.01	<0.01
3	3-Hydroxybenzoic Acid	10.1 (0.947)a	9.91 (0.168)a		9.78 (0.397)a	0.14	0.215
3	3-Hydroxybutyric Acid	15.9 (2.64)a	15.3 (2.01)a		12.5 (2.72)b	<0.01	<0.01
3	3-Methyl-2-oxobutyric Acid	20 (2.49)a	18.4 (1)a		15.2 (1.83)b	<0.01	<0.01
3	3-Methylthiopropionic Acid	8.93 (3.88)a	12.7 (1.61)b		14.6 (0.923)c	<0.01	<0.01
3	3-O-Methyl-Gallic Acid	9.47 (1.69)a	9.31 (1.14)a		15.5 (4.46)b	<0.01	<0.01
3	3-Oxoglutaric Acid	9.45 (1.53)a	9.36 (1.67)a		8.82 (1.44)a	0.357	0.439
3	3,5-Dihydroxybenzoic Acid	12.8 (2.89)a	11.9 (1.76)a		15.7 (2.27)b	<0.01	<0.01
3	4-Hydroxybenzoic Acid	15.7 (1.13)a	15.2 (1.46)a		17 (1.08)b	<0.01	0.013
3	4-Hydroxyphenylacetic Acid	14.7 (1.11)a	17.1 (1.88)ab		19.2 (2.24)b	<0.01	<0.01
3	4-Methylcatechol	8.09 (0.778)a	8.35 (0.447)ab		9.54 (3.07)b	0.042	0.089
3	4-Methylvaleric Acid	8.5 (1.08)a	10.6 (3.85)a		8.57 (2.42)a	0.483	0.558
3	5-Phenylvaleric Acid	11.5 (0.995)a	11.6 (0.273)a		10.3 (1.23)b	<0.01	<0.01
3	a-hydroxyisocaproic acid	22.3 (3.76)a	22.4 (0.859)a		19 (2.32)b	<0.01	0.017
3	Acetoacetic Acid	13 (0.589)a	12.9 (0.361)a		11.6 (0.98)b	<0.01	0.011
3	Adenine	11.8 (1.62)ab	12.3 (0.779)a		11.3 (1.28)b	0.013	0.033

3	Adipic Acid	16.8 (0.565)a	15.9 (0.649)b		15.9 (0.789)b	<0.01	<0.01
3	Arachidonic Acid	13.8 (5.33)a	12.9 (2.32)a		13.6 (5.09)a	0.461	0.54
3	Argininosuccinic acid	13.2 (1.94)a	13.5 (0.537)a		13.8 (0.593)a	0.211	0.293
3	Atrolactic Acid	21.3 (2.69)a	20.6 (2.82)a		18.3 (4.26)a	0.371	0.451
3	Azelaic Acid	17.2 (0.631)a	17.8 (0.0924)a		20.7 (1.16)b	<0.01	<0.01
3	Benzoic Acid	13.1 (0.808)a	11.4 (1.34)b		11.8 (1.28)b	<0.01	0.014
3	Butyric Acid	13.1 (1.74)a	11.2 (0.987)b		11.2 (1)b	0.018	0.042
3	CA	22 (0.81)a	21.8 (0.979)a		21.9 (1.28)a	0.553	0.622
3	Caffeic Acid	9.26 (2.1)a	8.83 (2.02)a		12.2 (3.42)b	<0.01	<0.01
3	CDCA	18.7 (2.02)a	19 (0.761)a		20.8 (1.31)b	<0.01	<0.01
3	cis-11,12-Methylene Pentadecanoic Acid	7.22 (0.606)a	6.6 (0.287)b		6.97 (0.7)ab	0.036	0.078
3	Citric Acid	18.7 (2.38)a	15.7 (3.16)ab		16.8 (5.25)b	0.069	0.13
3	Cysteine	14.7 (1.08)a	14.8 (0.416)a		13.5 (0.479)b	<0.01	<0.01
3	DCA	18.1 (4)a	18.6 (4.87)ab		15.2 (3.4)b	0.078	0.144
3	Dihydro-Isoferulic acid-glucuronide	9.09 (1.63)a	9.15 (0.592)a		10.1 (4.84)a	0.081	0.145
3	Dihydrocaffeic acid	12.6 (1.79)a	13.4 (2.06)a		17.9 (3.57)b	<0.01	<0.01
3	Dihydroferulic Acid	9.65 (0.678)a	13.1 (1.06)b		15.4 (2.53)b	<0.01	<0.01
3	Dihydroferulic Acid-4-Sulfate	8.86 (2.93)a	8.65 (1.57)a		8.2 (2.37)a	0.999	0.999
3	Dodecanedioic Acid	14.4 (0.519)a	14.1 (0.841)ab		13.8 (1.49)b	0.064	0.124
3	Fumaric Acid	16.6 (2.09)a	16 (1.15)ab		15.4 (1.45)b	0.096	0.161
3	GCA	17.4 (3.14)a	17 (1.21)a		17.3 (2.39)a	0.808	0.85
3	GCDCA	14.3 (1.52)a	14.3 (1.63)a		15 (1.29)a	0.155	0.231
3	GDCA	7.27 (3.48)a	8.16 (3.14)a		7.69 (1.81)a	0.873	0.908

3	Gentisic acid	8.65 (1.25)a	8.41 (1.1)a		13.2 (0.734)b	<0.01	<0.01
3	Gluconic Acid	19 (1.34)a	17.8 (1.13)ab		16.7 (1.83)b	0.027	0.062
3	glucose	21.7 (1.31)a	19.8 (0.453)b		19 (0.923)b	<0.01	<0.01
3	GUDCA	9.41 (4.05)a	11.1 (3.32)a		12.4 (3.25)a	0.122	0.193
3	Hexadecanedioic Acid	12.3 (0.491)ab	13 (0.562)a		12.1 (0.557)b	0.049	0.099
3	Hexadecanoic acid	11.3 (0.426)a	11 (0.104)a		11.5 (1.76)a	0.277	0.363
3	Homovanillic Acid	10.4 (2.29)a	10.1 (1.15)a		9.27 (2.03)a	0.604	0.67
3	Hydrocinnamic Acid	7.02 (0.55)a	10.7 (3.56)b		10.2 (2.16)b	0.018	0.042
3	Hydroxyphenyllactic Acid	23.2 (3.95)a	22.1 (2.08)a		16.8 (1.17)b	<0.01	<0.01
3	Indole-2-Carboxylic Acid	8.73 (2.71)a	14.1 (4.53)b		10.5 (2.24)a	<0.01	<0.01
3	Indole-3-Carboxaldehyde	15.5 (1.86)a	15.6 (0.531)ab		14.7 (1.3)b	0.064	0.124
3	Isocitric Acid	13 (1.62)a	13.1 (1)a		14.9 (0.781)b	<0.01	<0.01
3	Isoferulic Acid 3-o-Sulfate	8.51 (1.53)a	10.2 (1.88)a		10.7 (3.23)a	0.225	0.31
3	Isoleucine	16.4 (2.23)a	17.3 (0.799)a		16.9 (1.62)a	0.141	0.215
3	L-(-)-Malic acid	20 (1.62)a	20.3 (0.979)a		19.9 (1.32)a	0.643	0.702
3	Lactic Acid	23.1 (5.2)a	22.3 (2.6)a		17.3 (1.52)b	<0.01	<0.01
3	Leucine	18.8 (2.04)a	18.5 (1.11)a		18.2 (2.26)a	0.921	0.938
3	m-Coumaric Acid	9.34 (0.889)a	9.26 (0.418)a		9.35 (1.39)a	0.761	0.805
3	m-hydroxy-hydrocinnamic acid	22.8 (2.56)a	22.2 (1.07)a		17.7 (2.25)b	<0.01	<0.01
3	Maleic Acid	12.4 (0.98)a	12.5 (0.239)a		11.6 (0.626)b	<0.01	0.019
3	Methyl-2-oxovaleric Acid	20.9 (2.8)a	19.9 (0.684)a		17 (2.8)b	<0.01	<0.01
3	Methyl-a-D-Glucopyranoside	16 (4.2)a	16.6 (0.743)a		15.5 (2.06)a	0.25	0.335
3	Methyl Vanillate	8.8 (1.2)a	8.9 (0.762)a		8.69 (0.736)a	0.325	0.408
3	Methylmalonic Acid	16 (1.98)a	14.7 (1.26)b		12.8 (2.54)c	<0.01	<0.01

3	Mevalonic Acid	14.2 (4.59)a	15.6 (2.71)a		13.7 (1.76)a	0.277	0.363
3	o-Hydroxyhippuric acid	12.1 (3.58)a	9.62 (3.37)ab		8.51 (2.81)b	<0.01	0.016
3	O-Phospho-L-serine	12.3 (2.42)a	9.74 (1.75)b		9.41 (3.61)b	<0.01	0.019
3	Octadecanedioic Acid	12 (1.5)a	13.6 (1.49)b		14.4 (1.47)b	<0.01	<0.01
3	Octadecanoic acid	10.9 (0.487)a	10.6 (0.333)a		10.6 (2.33)a	0.266	0.351
3	Orotic Acid	17.2 (2.83)a	20.6 (1.53)b		16.2 (2.76)a	<0.01	<0.01
3	Oxamic Acid	10.4 (1.06)a	13.4 (1.95)b		11.7 (0.754)c	<0.01	<0.01
3	p-Coumaric acid	11.2 (0.827)a	12.8 (0.924)b		15.9 (3.19)c	<0.01	<0.01
3	Phenol	7.15 (1.23)a	7.5 (1.64)ab		8.91 (1.35)b	0.015	0.036
3	Pimelic Acid	14.5 (1.13)ab	14.1 (0.744)a		14.6 (1.17)b	0.085	0.151
3	Pyrocatechol	10.9 (1.99)a	10.5 (1.26)a		15.3 (4.07)b	<0.01	<0.01
3	Pyrogallol	10.5 (3.47)a	10.6 (0.816)a		9.89 (3.35)a	0.689	0.737
3	Pyruvic acid	16.1 (4.83)a	13.8 (2.25)b		13.7 (1.32)b	<0.01	0.011
3	Quercetin	8.09 (0.793)a	8.34 (0.792)ab		8.49 (0.565)b	0.013	0.033
3	Quinic Acid	17.2 (2.08)a	17 (1.3)ab		15.4 (1.73)b	0.07	0.131
3	Raffinose	14.6 (1.97)a	18.7 (0.697)b		18.5 (1.54)b	<0.01	<0.01
3	Rutin	7.16 (1.45)a	6.54 (0.273)ab		5.99 (0.644)b	0.091	0.155
3	Shikimic Acid	14.6 (1.43)a	14.1 (1.2)a		12.2 (1.02)b	<0.01	<0.01
3	Stercobilin	6.63 (2.48)a	6.11 (0.315)b		6.86 (0.583)a	0.013	0.033
3	Succinic Acid	24.9 (2.34)a	23.1 (1.4)ab		20.6 (3.05)b	<0.01	<0.01
3	Sucrose	17.9 (1.01)a	19.7 (1.11)b		18.5 (0.964)c	<0.01	0.011
3	TCDCA	10 (1.56)a	11.2 (2.84)a		15.1 (3.86)b	<0.01	0.012
3	TDCA	8.98 (2.16)a	10.8 (2.61)ab		13 (2.75)b	<0.01	<0.01
3	Tetradecanedioic Acid	12.7 (0.566)a	13.1 (0.613)a		12.2 (0.662)b	0.033	0.073

3	Tyrosol	11.7 (0.722)ab	11.6 (1.42)a		14.6 (5.72)b	0.07	0.131
3	Undecanedioic Acid	15.2 (0.363)ab	14.6 (0.937)a		16.2 (1.96)b	0.015	0.036
3	Uric Acid	20.3 (3.32)a	14.5 (1.31)b		16 (2.98)b	<0.01	<0.01
3	Uridine	17.6 (2.9)a	17.2 (2.05)a		16.2 (1.37)a	0.206	0.289
6	(S)-3,4-Dihydroxybutyric Acid	20.8 (0.923)a	19.9 (2.15)a		18.3 (2.98)b	<0.01	0.024
6	2-Hydroxy-3-methylbutyric Acid	22.3 (1.83)a	20.7 (1.64)b		19.9 (1.3)c	<0.01	<0.01
6	2-Hydroxyadipic Acid	20.4 (4.12)a	16.7 (1.22)b		15.9 (2.15)b	<0.01	<0.01
6	2-Oxoglutaric Acid	17.5 (3.11)a	15.3 (1.63)b		14.6 (2.08)b	<0.01	<0.01
6	2-Phenylacetic Acid	11.3 (4.89)a	14.1 (0.871)a		15.3 (1.3)b	<0.01	<0.01
6	3-Dehydroshikimic acid	14.1 (2.69)a	12.3 (3.03)b		10.9 (2.63)c	<0.01	<0.01
6	3-Hydroxybenzoic Acid	10.3 (0.804)a	10.2 (0.646)a		10.3 (0.622)a	0.327	0.408
6	3-Hydroxybutyric Acid	17.7 (3.14)a	15 (3.09)b		12.5 (4.7)c	<0.01	<0.01
6	3-Methyl-2-oxobutyric Acid	20 (1.9)a	18.2 (2.06)b		16.5 (1.95)c	<0.01	<0.01
6	3-Methylthiopropionic Acid	8.61 (5.33)a	13.1 (1.95)b		13.8 (1.11)b	<0.01	0.015
6	3-O-Methyl-Gallic Acid	11.1 (1.93)a	10.2 (2.82)a		14.6 (4.8)b	<0.01	<0.01
6	3-Oxoglutaric Acid	9.59 (1.66)a	9.17 (1.99)a		9.54 (2.3)a	0.299	0.385
6	3,5-Dihydroxybenzoic Acid	15.1 (1.91)a	13.9 (2.93)b		15.1 (1.59)a	<0.01	0.019
6	4-Hydroxybenzoic Acid	15.9 (2.07)a	17.3 (2.56)a		17.7 (1.87)b	<0.01	0.014
6	4-Hydroxyphenylacetic Acid	14.4 (3.6)a	16.8 (2.34)a		18.8 (3.9)b	<0.01	<0.01
6	4-Methylcatechol	8.97 (1.75)a	9.26 (1.68)a		10.7 (2.69)a	0.105	0.174
6	4-Methylvaleric Acid	8.98 (2.35)a	9.75 (3.33)a		9.58 (2.53)a	0.404	0.484
6	5-Phenylvaleric Acid	11.3 (1.22)a	11.7 (1.15)a		10.9 (1.66)a	0.12	0.19
6	a-hydroxyisocaproic acid	22.3 (1.77)a	21.8 (1.47)a		20.3 (1.17)b	<0.01	<0.01
6	Acetoacetic Acid	13.1 (1.02)a	12.3 (0.885)b		11.7 (0.949)c	<0.01	<0.01

6	Adenine	12.3 (1.56)a	13.1 (1.18)a		11.6 (0.682)b	<0.01	0.015
6	Adipic Acid	16.9 (0.483)a	15.8 (0.89)b		16.4 (1.26)ab	<0.01	0.025
6	Arachidonic Acid	12.8 (2.73)a	11 (1.59)a		10.8 (2.49)a	0.47	0.546
6	Argininosuccinic acid	13.8 (1.67)a	12.5 (1.19)b		13.3 (1.3)a	<0.01	0.02
6	Atrolactic Acid	21.7 (2.61)a	22 (3.32)a		22.6 (1.05)a	0.177	0.253
6	Azelaic Acid	17.9 (0.93)a	18.2 (0.959)a		20.7 (0.814)b	<0.01	<0.01
6	Benzoic Acid	11.4 (1.97)a	11.7 (0.927)a		11.8 (1.56)a	0.908	0.934
6	Butyric Acid	13.3 (0.927)a	11.9 (1.35)b		11.3 (2.09)b	<0.01	<0.01
6	CA	22.2 (0.841)a	21.7 (1.23)a		21.7 (0.965)a	0.138	0.212
6	Caffeic Acid	12.4 (4.63)a	11.5 (3.27)a		12.5 (2.63)a	0.19	0.269
6	CDCA	18.6 (0.969)a	18.7 (2.43)a		19.9 (3.08)a	0.242	0.327
6	cis-11,12-Methylene Pentadecanoic Acid	6.63 (0.876)a	6.5 (0.444)a		6.22 (0.595)a	0.08	0.145
6	Citric Acid	18.5 (3.93)a	14.4 (4.68)b		12.4 (0.994)b	<0.01	<0.01
6	Cysteine	15 (0.789)a	13.9 (1.48)b		13.5 (0.885)c	<0.01	<0.01
6	DCA	16.1 (4.97)a	16.7 (5.9)a		14.6 (1.25)a	0.599	0.668
6	Dihydro-Isoferulic acid-glucuronide	10.2 (1.3)a	9.48 (1.29)a		11.6 (1.84)b	<0.01	<0.01
6	Dihydrocaffeic acid	15.2 (4.6)a	15 (4.38)a		19.2 (3.81)b	<0.01	<0.01
6	Dihydroferulic Acid	13 (5.21)a	15.7 (2.83)b		16.7 (1.18)c	<0.01	<0.01
6	Dihydroferulic Acid-4-Sulfate	9.81 (3.9)a	7.82 (1.6)b		7.72 (0.935)b	0.013	0.033
6	Dodecanedioic Acid	14.4 (0.574)a	13.9 (1.08)a		14 (0.981)a	0.286	0.373
6	Fumaric Acid	15.6 (1.35)a	14.3 (2.16)ab		14 (1.69)b	0.039	0.082
6	GCA	17.2 (2.14)a	16.9 (2.81)a		16.5 (2.23)a	0.418	0.496
6	GCDCA	14.3 (2.42)a	15 (3.02)a		15.5 (2.14)a	0.19	0.269

6	GDCA	7.14 (3.15)a	7.62 (3.27)a		7.06 (0.964)a	0.395	0.474
6	Gentisic acid	10.1 (2.07)a	11.5 (2.91)a		13.5 (1.53)b	<0.01	<0.01
6	Gluconic Acid	18.9 (1.47)a	17.6 (1.19)b		17.1 (3.05)b	<0.01	<0.01
6	glucose	21.4 (1.18)a	19.8 (1.24)b		19.5 (1.22)b	<0.01	<0.01
6	GUDCA	9.16 (5.04)a	12.1 (2.61)b		13.9 (2.62)b	0.025	0.058
6	Hexadecanedioic Acid	11.9 (1.3)a	12.6 (0.707)a		12.4 (1.38)a	0.156	0.231
6	Hexadecanoic acid	11.2 (0.538)a	10.8 (0.453)b		10.8 (0.688)b	0.047	0.097
6	Homovanillic Acid	11.2 (0.776)a	11.1 (2.03)a		12 (1.83)a	0.11	0.179
6	Hydrocinnamic Acid	7.84 (3.73)a	11.2 (4.02)b		11.5 (4.23)ab	0.062	0.12
6	Hydroxyphenyllactic Acid	23.2 (1.81)a	21.6 (3.4)b		17.8 (2.09)c	<0.01	<0.01
6	Indole-2-Carboxylic Acid	12.4 (2.25)ab	12.1 (5.02)a		9.59 (1.65)b	0.044	0.092
6	Indole-3-Carboxaldehyde	16 (2.01)a	16.8 (2.72)a		15.3 (1.66)a	0.166	0.24
6	Isocitric Acid	13.3 (1.45)a	13.1 (1.4)a		14.5 (0.798)b	<0.01	<0.01
6	Isoferulic Acid 3-o-Sulfate	11.9 (4.73)a	9.98 (4.41)a		11.2 (5.31)a	0.365	0.446
6	Isoleucine	16.2 (2.26)a	17.9 (1.6)b		18 (2.42)b	<0.01	0.025
6	L-(-)-Malic acid	19.8 (2.09)a	18.6 (2.23)a		19.9 (1.17)a	0.366	0.446
6	Lactic Acid	25.4 (3.58)a	19.9 (3.06)b		17.7 (1.47)c	<0.01	<0.01
6	Leucine	19.1 (1.22)a	18.9 (1.71)a		19.1 (1.88)a	0.824	0.864
6	m-Coumaric Acid	9.48 (1.34)a	9.35 (0.788)a		9.91 (1.88)a	0.164	0.238
6	m-hydroxy-hydrocinnamic acid	23.2 (2.22)a	20.8 (2.47)b		17.6 (3.34)c	<0.01	<0.01
6	Maleic Acid	12.4 (1.53)a	12.2 (0.938)ab		12.1 (0.68)b	0.052	0.104
6	Methyl-2-oxovaleric Acid	20.9 (1.21)a	20 (1.71)b		18.6 (2.29)c	<0.01	<0.01
6	Methyl-a-D-Glucopyranoside	20.3 (2.93)a	16.7 (3.98)b		16.2 (3.68)b	0.058	0.113
6	Methyl Vanillate	9.34 (1.16)a	9.14 (1.24)a		8.91 (1.54)a	0.92	0.938

6	Methylmalonic Acid	16.9 (1.12)a	14 (1.19)b		13.3 (1.68)b	<0.01	<0.01
6	Mevalonic Acid	13.7 (3.38)ab	14.5 (2.14)a		12.8 (1.55)b	0.038	0.082
6	o-Hydroxyhippuric acid	13 (2.67)a	10.5 (3.51)b		9.25 (1.3)c	<0.01	<0.01
6	O-Phospho-L-serine	12.6 (3.8)a	9.54 (4.31)b		7.95 (2.12)b	<0.01	<0.01
6	Octadecanedioic Acid	11.8 (0.931)a	12.9 (1.54)b		12.9 (2.13)b	0.013	0.033
6	Octadecanoic acid	10.6 (0.609)a	10.6 (0.524)a		10.3 (0.476)a	0.116	0.187
6	Orotic Acid	18.6 (2.3)a	18.8 (2.85)a		16.6 (1.11)b	0.018	0.044
6	Oxamic Acid	11 (1.56)a	13.4 (2.69)b		11.7 (1.62)c	<0.01	<0.01
6	p-Coumaric acid	13.8 (2.18)a	14.6 (1.86)b		15 (1.84)b	0.011	0.028
6	Phenol	7.93 (1.84)a	7.97 (2.68)a		8.98 (1.91)a	0.143	0.216
6	Pimelic Acid	15 (0.605)ab	14.5 (0.792)a		15.5 (1.48)b	0.019	0.044
6	Pyrocatechol	13.1 (2.44)a	12.5 (2.91)a		17 (1.13)b	<0.01	<0.01
6	Pyrogallol	11 (2.14)a	9.31 (2.78)b		11.2 (1.92)a	<0.01	0.012
6	Pyruvic acid	19.1 (5.4)a	14.4 (0.92)b		13.1 (2.02)c	<0.01	<0.01
6	Quercetin	8.1 (0.761)ab	7.9 (0.436)a		8.58 (0.447)b	<0.01	<0.01
6	Quinic Acid	19.4 (4.52)a	17.7 (1.44)b		17.8 (1.98)b	0.018	0.043
6	Raffinose	16.4 (2.21)a	18.7 (0.654)b		17.9 (1.27)c	<0.01	<0.01
6	Rutin	7.15 (1.47)a	6.23 (0.477)b		6.14 (0.694)b	<0.01	0.019
6	Shikimic Acid	15.6 (1.99)a	13.4 (1.5)b		12.5 (1.5)b	<0.01	<0.01
6	Stercobilin	6.47 (1.24)ab	6.22 (0.382)a		6.75 (0.627)b	<0.01	0.021
6	Succinic Acid	22.3 (2.74)a	21.1 (2.9)ab		20.8 (1.29)b	0.07	0.131
6	Sucrose	18.1 (1.3)a	19.6 (1.22)b		19.2 (1.45)b	<0.01	0.011
6	TCDCA	10.2 (3.97)a	11.8 (4.21)a		15.6 (3.41)b	<0.01	0.013
6	TDCA	8.91 (2.14)a	10.4 (3.37)a		13.4 (3.44)b	<0.01	<0.01

6	Tetradecanedioic Acid	13 (1.42)a	13.4 (0.983)a		13.2 (0.938)a	0.339	0.42
6	Tyrosol	11.9 (2.11)a	13.5 (3.42)a		16.9 (5.7)b	<0.01	0.016
6	Undecanedioic Acid	15 (0.522)ab	14.4 (1.35)a		15.5 (1.48)b	0.038	0.082
6	Uric Acid	20 (4.59)a	14.9 (2.29)b		16.4 (2.89)b	<0.01	<0.01
6	Uridine	17 (3.91)a	15.7 (1.68)a		16 (1.19)a	0.24	0.327
9	(S)-3,4-Dihydroxybutyric Acid	21.1 (2.99)a	22.1 (3.39)a		18.2 (1.48)b	<0.01	<0.01
9	2-Hydroxy-3-methylbutyric Acid	22.3 (3.08)a	21.2 (1.83)a		19.1 (1.86)b	<0.01	<0.01
9	2-Hydroxyadipic Acid	18.6 (2)a	17.2 (1.62)b		15.7 (3.22)c	<0.01	<0.01
9	2-Oxoglutaric Acid	15.3 (2.18)a	14.5 (2.97)b		13.1 (1.63)b	<0.01	0.018
9	2-Phenylacetic Acid	13.9 (1.92)a	14.1 (0.884)a		15.9 (1.97)b	<0.01	<0.01
9	3-Dehydroshikimic acid	14.7 (2.25)a	13.6 (2.39)a		11.3 (1.95)b	<0.01	<0.01
9	3-Hydroxybenzoic Acid	10.6 (1.03)a	10.9 (0.996)a		10.5 (0.729)a	0.12	0.191
9	3-Hydroxybutyric Acid	15.2 (3.9)a	15.1 (3.75)a		13.6 (4.23)a	0.211	0.293
9	3-Methyl-2-oxobutyric Acid	17.1 (2.18)a	15.9 (3.21)b		15.4 (3.77)b	<0.01	0.024
9	3-Methylthiopropionic Acid	13 (3.79)a	12 (3.23)a		14 (0.664)b	<0.01	0.025
9	3-O-Methyl-Gallic Acid	14.1 (1)a	11.1 (3.4)b		16.3 (2.45)c	<0.01	<0.01
9	3-Oxoglutaric Acid	11.1 (1.77)a	11.9 (1.37)a		11.1 (3)a	0.294	0.38
9	3,5-Dihydroxybenzoic Acid	17.4 (1.83)a	16.4 (2.48)b		15.8 (1.48)b	<0.01	0.018
9	4-Hydroxybenzoic Acid	18.7 (1.51)a	17.8 (0.936)a		18.4 (1.08)a	0.474	0.55
9	4-Hydroxyphenylacetic Acid	17.6 (2.5)a	17 (3.12)a		17.9 (2.63)a	0.679	0.731
9	4-Methylcatechol	10.8 (2.19)a	9.89 (1.67)a		11.2 (3.87)a	0.581	0.65
9	4-Methylvaleric Acid	9.4 (2.75)a	8.88 (1.45)a		9.9 (1.29)a	0.717	0.763
9	5-Phenylvaleric Acid	11.2 (1.17)ab	11.8 (0.75)a		10.6 (0.927)b	0.092	0.156
9	a-hydroxyisocaproic acid	22.7 (3.21)a	21.8 (0.686)a		19.2 (1.83)b	<0.01	<0.01

9	Acetoacetic Acid	12.8 (1.06)a	12.4 (0.605)ab		11.9 (0.669)b	<0.01	0.025
9	Adenine	13 (3.23)a	12.7 (3.89)a		11.1 (0.555)b	<0.01	<0.01
9	Adipic Acid	16.9 (0.598)a	16.2 (0.557)b		16.4 (1.41)ab	0.05	0.101
9	Arachidonic Acid	11.8 (0.626)a	10.9 (1.18)b		11.2 (0.87)b	<0.01	0.011
9	Argininosuccinic acid	13.1 (0.979)a	12.4 (1.24)a		13.1 (0.781)a	0.415	0.494
9	Atrolactic Acid	22.9 (1.24)a	22.3 (1.78)a		22.9 (1.06)a	0.683	0.733
9	Azelaic Acid	18.2 (1.28)a	18.3 (0.588)a		20.6 (1.25)b	<0.01	<0.01
9	Benzoic Acid	11.8 (0.913)a	12.4 (2.17)a		12.1 (1.1)a	0.655	0.71
9	Butyric Acid	12.8 (1.53)a	12.4 (1.11)ab		11.9 (2.48)b	0.077	0.143
9	CA	22.6 (0.993)a	21.6 (0.687)b		21.8 (0.403)b	<0.01	0.011
9	Caffeic Acid	14.5 (1.65)a	13.1 (1.54)a		13.7 (1.61)a	0.124	0.195
9	CDCA	19.7 (0.803)a	18.7 (1.39)a		19.8 (1.63)a	0.134	0.207
9	cis-11,12-Methylene Pentadecanoic Acid	6.72 (0.502)a	6.36 (0.198)b		6.17 (0.644)b	0.024	0.055
9	Citric Acid	14.8 (5.03)a	13.8 (5.07)a		12.3 (2.47)b	<0.01	0.024
9	Cysteine	14.4 (1.78)a	14.7 (2.06)a		13.6 (0.69)a	0.383	0.464
9	DCA	15.9 (3.43)a	16.6 (4.2)a		16 (3.17)a	0.947	0.952
9	Dihydro-Isoferulic acid-glucuronide	11.6 (1.68)a	10.4 (1.22)a		11.4 (1.4)a	0.106	0.174
9	Dihydrocaffeic acid	18.5 (5.03)a	16.5 (4.84)a		18.2 (6.05)a	0.856	0.895
9	Dihydroferulic Acid	17.3 (2.59)a	14.7 (3.59)a		15.8 (2.32)a	0.226	0.31
9	Dihydroferulic Acid-4-Sulfate	9.65 (3.77)a	8.68 (3.77)a		7.99 (2.04)a	0.112	0.182
9	Dodecanedioic Acid	15.1 (1.12)a	14.6 (1.01)a		14.6 (1.77)a	0.58	0.65
9	Fumaric Acid	16.2 (1.16)a	14.2 (0.884)b		14.3 (1.75)b	<0.01	<0.01
9	GCA	17.5 (2)a	15.1 (1.25)b		16.4 (1.38)b	<0.01	<0.01

9	GCDCA	15.7 (1.69)a	14.4 (2.07)a		15.1 (0.807)a	0.11	0.179
9	GDCA	7.42 (3.15)a	7.65 (2.31)a		7.02 (2.94)a	0.95	0.953
9	Gentisic acid	13 (2.35)a	14.1 (0.965)a		13.4 (2.12)a	0.16	0.236
9	Gluconic Acid	19.7 (1.4)a	19.2 (2.5)b		16.2 (1.64)c	<0.01	<0.01
9	glucose	20.4 (1.2)a	20.2 (0.816)a		19.5 (1.03)a	0.334	0.416
9	GUDCA	13.9 (2.9)a	12.1 (3.34)a		13.6 (1.82)a	0.521	0.592
9	Hexadecanedioic Acid	12.8 (1.43)a	12.7 (0.46)a		13 (1.33)a	0.625	0.688
9	Hexadecanoic acid	11.2 (0.749)a	10.9 (0.432)b		10.6 (0.393)b	<0.01	0.012
9	Homovanillic Acid	12 (2.98)a	12.3 (3.35)a		13.7 (1.85)a	0.528	0.598
9	Hydrocinnamic Acid	10.6 (5.35)a	12 (3.46)a		11.2 (4.52)a	0.867	0.905
9	Hydroxyphenyllactic Acid	23.6 (3.68)a	20.8 (3.1)a		18.7 (1.56)b	<0.01	<0.01
9	Indole-2-Carboxylic Acid	9.56 (3.45)a	12.5 (5.13)a		10.5 (2.32)a	0.163	0.238
9	Indole-3-Carboxaldehyde	16.5 (2.2)a	15.1 (1.79)b		15.2 (2.01)b	0.038	0.082
9	Isocitric Acid	13.7 (1.73)a	13 (1.09)b		13.9 (0.888)a	<0.01	0.025
9	Isoferulic Acid 3-o-Sulfate	14.9 (5.22)a	13.6 (7.47)a		12 (5.13)a	0.652	0.709
9	Isoleucine	17.1 (3.39)a	17.6 (2.49)ab		18.7 (1.89)b	0.049	0.1
9	L-(-)-Malic acid	20.5 (1.74)a	19.7 (2.22)a		19.6 (1.36)a	0.304	0.389
9	Lactic Acid	20.2 (4.48)a	18.9 (3.23)a		18 (2.21)b	<0.01	0.021
9	Leucine	18.3 (1.46)a	18.5 (1.85)a		19.7 (1.24)b	0.048	0.098
9	m-Coumaric Acid	9.92 (0.73)a	9.67 (2.16)a		9.54 (1.61)a	0.909	0.934
9	m-hydroxy-hydrocinnamic acid	21.8 (2.43)a	19.9 (1.97)a		16.7 (1.3)b	<0.01	<0.01
9	Maleic Acid	12.4 (0.693)a	12.4 (1.12)a		12.3 (1.72)a	0.635	0.695
9	Methyl-2-oxovaleric Acid	19.4 (1.95)a	17.7 (3.26)b		18.1 (3.01)b	0.011	0.03
9	Methyl-a-D-Glucopyranoside	19.4 (2.43)a	16.8 (4.6)a		17.5 (3.02)a	0.129	0.203

9	Methyl Vanillate	9.93 (1.24)a	9.59 (0.726)a		8.95 (1.4)a	0.241	0.327
9	Methylmalonic Acid	16 (1.66)a	12.8 (1.87)b		13.7 (1.64)b	<0.01	<0.01
9	Mevalonic Acid	15.1 (2.87)a	13.8 (1.55)a		12.9 (0.891)a	0.086	0.151
9	o-Hydroxyhippuric acid	11.6 (1.41)a	10 (4)ab		9.18 (0.705)b	<0.01	0.015
9	O-Phospho-L-serine	11 (4.56)a	10.1 (2.03)ab		8.9 (2.35)b	0.097	0.163
9	Octadecanedioic Acid	12.4 (1.86)a	12.9 (1.6)a		13.6 (0.945)a	0.214	0.297
9	Octadecanoic acid	10.9 (0.474)a	10.5 (0.429)b		10.2 (0.657)c	<0.01	<0.01
9	Orotic Acid	18.1 (2.76)a	17.4 (2.5)a		15.2 (1.39)b	0.014	0.034
9	Oxamic Acid	12.9 (2.88)a	13.7 (1.92)a		11.1 (1.94)b	0.042	0.089
9	p-Coumaric acid	16.1 (2.9)a	16.4 (1.9)a		15 (2.11)a	0.518	0.59
9	Phenol	8.46 (3.17)a	8.72 (5.87)a		8.76 (2.35)a	0.518	0.59
9	Pimelic Acid	15.5 (1.67)a	15.4 (0.521)a		15.6 (2.02)a	0.63	0.692
9	Pyrocatechol	15.8 (1.35)a	15.1 (3.22)a		17.2 (0.688)b	0.018	0.042
9	Pyrogallol	10.8 (1.7)a	10.9 (2.31)ab		12.4 (2.55)b	0.054	0.107
9	Pyruvic acid	16.7 (2.35)a	14.1 (1.6)b		13.9 (1.23)b	<0.01	0.015
9	Quercetin	8.42 (1.35)ab	8.05 (0.791)a		8.48 (0.408)b	0.081	0.145
9	Quinic Acid	19.8 (1.59)a	18.6 (1.93)ab		18.4 (0.93)b	0.024	0.057
9	Raffinose	18.4 (3.06)a	18.2 (0.908)a		17.9 (1.25)a	0.715	0.762
9	Rutin	7.59 (1.98)a	6.23 (0.45)a		6.37 (1.85)a	0.09	0.154
9	Shikimic Acid	15 (1.3)a	14 (1.86)a		13.1 (0.832)b	<0.01	0.012
9	Stercobilin	6.92 (0.906)a	6.65 (0.49)a		6.78 (1.12)a	0.942	0.95
9	Succinic Acid	21.2 (2.45)a	20.8 (1.96)a		21.3 (5.23)a	0.417	0.496
9	Sucrose	19.7 (1.85)a	19.4 (0.77)a		19.8 (1.27)a	0.88	0.911
9	TCDCA	14.2 (2.66)a	11.6 (1.38)b		13.7 (4.75)a	<0.01	0.026

9	TDCA	10.1 (2.01)a	10.6 (3.18)a		13.5 (3.63)a	0.18	0.256
9	Tetradecanedioic Acid	13.6 (0.39)a	13.2 (0.865)b		13.4 (1.06)ab	0.047	0.097
9	Tyrosol	14.5 (2.35)a	15.5 (2.1)ab		17.6 (4.64)b	0.031	0.07
9	Undecanedioic Acid	15.4 (1.47)a	15.2 (1.63)a		16.7 (0.914)b	<0.01	<0.01
9	Uric Acid	15.9 (2.85)a	14.5 (2.91)a		15.9 (3.29)a	0.17	0.243
9	Uridine	15.9 (3.14)a	16.4 (2.41)a		15.7 (1.37)a	0.253	0.338
12	(S)-3,4-Dihydroxybutyric Acid	20 (3.31)a	17.3 (2.58)a	18.7 (1.47)a	17.3 (2.57)a	0.089	0.153
12	2-Hydroxy-3-methylbutyric Acid	20.8 (1.86)a	19.2 (2.38)a	20.4 (0.538)a	19.2 (3.81)a	0.082	0.146
12	2-Hydroxyadipic Acid	18.2 (2.69)a	15.6 (1.09)b	16.6 (2.64)ab	16.5 (2.1)ab	0.011	0.03
12	2-Oxoglutaric Acid	14.1 (2.47)a	12.1 (1.45)a	12.8 (1.21)a	13.5 (1.42)a	0.13	0.203
12	2-Phenylacetic Acid	15.2 (2.07)a	13.9 (2.65)a	13.9 (2)a	14.9 (1.91)a	0.465	0.543
12	3-Dehydroshikimic acid	11.3 (3.01)a	11.8 (2.58)a	11.5 (2.12)a	11 (1.08)a	0.921	0.938
12	3-Hydroxybenzoic Acid	10.7 (0.882)a	10.4 (0.642)a	10.5 (0.542)a	10.6 (0.664)a	0.31	0.396
12	3-Hydroxybutyric Acid	15.3 (3.13)a	13.3 (4.18)a	15.4 (2.33)a	15.3 (3.74)a	0.439	0.517
12	3-Methyl-2-oxobutyric Acid	15.9 (4.64)a	15.4 (3.05)a	14.2 (5.52)a	15.6 (4.53)a	0.515	0.59
12	3-Methylthiopropionic Acid	13.3 (2.08)a	13.2 (3.36)a	13.5 (1.47)a	14 (2.08)a	0.672	0.725
12	3-O-Methyl-Gallic Acid	15.1 (1.2)a	10.5 (3.72)b	13.4 (4.93)a	16.3 (2.89)a	<0.01	<0.01
12	3-Oxoglutaric Acid	9.87 (1.82)a	9.57 (1.31)a	9.51 (2.09)a	9.94 (2.49)a	0.425	0.502
12	3,5-Dihydroxybenzoic Acid	17.4 (2.02)a	15.1 (1.15)b	17.6 (2.88)ac	15.8 (1.96)bc	<0.01	<0.01
12	4-Hydroxybenzoic Acid	19.1 (1.63)a	16.5 (2.03)b	18.6 (1.25)ac	17.7 (2.82)bc	0.023	0.055
12	4-Hydroxyphenylacetic Acid	18.1 (3.36)a	15.4 (2.23)b	18.1 (3.13)a	16.2 (1.7)ab	0.036	0.078
12	4-Methylcatechol	10.7 (2.54)ab	9.52 (1.51)a	11.9 (2.6)ab	12.4 (5.62)b	0.056	0.11
12	4-Methylvaleric Acid	9.68 (3.92)a	9.18 (1.69)a	9.91 (1.15)a	8.8 (1.41)a	0.388	0.469
12	5-Phenylvaleric Acid	10.6 (1.24)a	11.8 (0.708)b	11.1 (0.58)ab	11.3 (0.905)b	<0.01	<0.01
12	a-hydroxyisocaproic acid	21.3 (2.57)a	19.3 (2.63)a	21.1 (1.47)a	20 (3.57)a	0.17	0.243

12	Acetoacetic Acid	12.2 (1.43)a	11.5 (0.554)a	11.9 (1.23)a	12 (1.72)a	0.108	0.177
12	Adenine	12.2 (2.32)a	11.5 (2.25)a	12.8 (2.92)a	11.3 (0.84)a	0.149	0.223
12	Adipic Acid	16.5 (1.25)a	15.9 (1.69)a	16.5 (1.58)a	17.2 (1.42)a	0.106	0.174
12	Arachidonic Acid	11.7 (3.15)a	12 (1.64)a	11.3 (2.21)a	11.2 (1.87)a	0.623	0.688
12	Argininosuccinic acid	12.6 (1.82)a	12 (0.713)a	12.1 (1.56)a	12.7 (0.925)a	0.162	0.237
12	Atrolactic Acid	23.4 (1.44)ab	22.8 (0.871)c	24.2 (1.29)a	22.8 (1.15)bc	0.029	0.065
12	Azelaic Acid	18.6 (1.24)a	17.9 (1.82)a	18.8 (0.737)a	20.5 (0.66)b	<0.01	0.015
12	Benzoic Acid	12.6 (1.57)a	12.5 (1.07)a	12 (0.909)a	12.3 (0.862)a	0.318	0.403
12	Butyric Acid	12.7 (1.55)a	11.1 (1.4)b	12.4 (1.39)ab	12.3 (1.41)a	0.013	0.033
12	CA	22 (0.796)a	21.6 (0.709)b	22.4 (1.16)a	21.9 (1.38)ab	0.013	0.033
12	Caffeic Acid	14.8 (3.21)a	11.5 (3.69)b	13.7 (2.46)ab	13 (1.89)ab	0.052	0.104
12	CDCA	20.4 (1.73)a	19.6 (3.67)a	20.7 (1.98)a	19 (3.07)a	0.259	0.344
12	cis-11,12-Methylene Pentadecanoic Acid	6.91 (2.08)a	6.49 (0.946)a	6.61 (1.13)a	6.38 (0.5)a	0.327	0.408
12	Citric Acid	13.8 (3.94)a	12.3 (3.8)a	12.7 (1.43)a	12.5 (1.39)a	0.495	0.57
12	Cysteine	13.7 (1.16)a	12.4 (1.73)a	13.1 (1.16)a	13.6 (1.22)a	0.156	0.231
12	DCA	14.8 (3.58)a	20.6 (5.35)ab	15.4 (7.06)ab	20.6 (5.8)b	0.081	0.145
12	Dihydro-Isoferulic acid-glucuronide	11.1 (1.24)a	10.6 (0.66)a	11.3 (0.822)a	10.7 (1.31)a	0.265	0.351
12	Dihydrocaffeic acid	19.2 (4.97)a	15.5 (2.67)a	19.5 (3.28)a	16.7 (5.12)a	0.095	0.161
12	Dihydroferulic Acid	16.7 (2.25)a	14.2 (1.01)b	17.5 (1.59)a	16.2 (2.64)a	<0.01	<0.01
12	Dihydroferulic Acid-4-Sulfate	10 (3.3)a	9.07 (3.33)a	8.89 (2.6)a	7.94 (1.64)a	0.354	0.437
12	Dodecanedioic Acid	14.3 (1.13)a	14.2 (1.4)a	14.7 (1.7)a	14.7 (1.34)a	0.899	0.928
12	Fumaric Acid	14.1 (1.75)a	13.9 (2.05)a	13.7 (1.16)a	13.8 (1.05)a	0.929	0.941
12	GCA	17.7 (2.79)a	15.5 (1.81)b	19.6 (3.64)a	15.6 (1.84)b	<0.01	<0.01
12	GCDCA	17.1 (2.62)a	15 (2.09)b	18 (4.55)a	15.1 (2.17)b	<0.01	0.016
12	GDCA	9.62 (2.03)a	12.2 (4.66)a	11.9 (7.13)a	13.2 (6.12)a	0.088	0.153

12	Gentisic acid	13.8 (2.08)a	12.8 (2.47)a	14.7 (1.9)a	13.9 (1.8)a	0.255	0.341
12	Gluconic Acid	18.1 (3.89)a	16 (2.89)a	16.6 (1.08)a	16.4 (2.54)a	0.101	0.169
12	glucose	20.1 (0.917)ab	19.8 (1.37)a	20.6 (1.26)b	19.8 (0.944)ab	0.117	0.188
12	GUDCA	14.8 (1.69)ab	12.9 (2.15)c	16.4 (3.74)a	13.3 (1.89)bc	<0.01	0.012
12	Hexadecanedioic Acid	12.5 (1.5)a	13.3 (1.27)a	12.7 (0.899)a	12.3 (1.73)a	0.444	0.521
12	Hexadecanoic acid	11.1 (1.11)a	10.8 (0.605)a	11 (0.558)a	10.7 (0.25)a	0.081	0.145
12	Homovanillic Acid	13.2 (1.38)a	11.6 (2.39)a	13.6 (2.04)a	12.6 (1.82)a	0.289	0.375
12	Hydrocinnamic Acid	12.2 (4.75)a	11.9 (3.66)a	12.9 (2.19)a	11.6 (2.83)a	0.289	0.375
12	Hydroxyphenyllactic Acid	21.4 (3.65)a	16.9 (3.09)b	18.6 (0.768)b	18.9 (3.45)ab	0.035	0.078
12	Indole-2-Carboxylic Acid	10.8 (4.9)a	12.6 (4.79)a	11.5 (3.54)a	10.5 (1.42)a	0.324	0.407
12	Indole-3-Carboxaldehyde	15.5 (2.28)a	15.7 (1.95)a	14.4 (2.35)a	15.6 (1.65)a	0.73	0.774
12	Isocitric Acid	12.2 (0.824)a	13.1 (2.16)ab	12.9 (2.39)ab	14.3 (0.788)b	0.012	0.031
12	Isoferulic Acid 3-o-Sulfate	14.9 (6.13)a	12 (4.32)a	13.1 (6.11)a	10.6 (4.43)a	0.133	0.205
12	Isoleucine	17.3 (1.71)a	18.9 (3.78)a	18.8 (2.93)a	18.6 (2.24)a	0.665	0.72
12	L-(-)-Malic acid	18.6 (2.43)a	18.1 (2.05)a	19.8 (3.23)a	19.4 (1.21)a	0.132	0.205
12	Lactic Acid	18.8 (1.08)a	18.5 (5.26)a	18.9 (2.06)a	17.6 (1.57)a	0.361	0.443
12	Leucine	18.1 (1.42)a	18.8 (2.75)ab	20 (1.76)b	18.6 (1.33)ab	0.119	0.19
12	m-Coumaric Acid	9.88 (0.8)ab	9.58 (1.08)ab	9.4 (0.692)a	10.8 (1.91)b	0.066	0.127
12	m-hydroxy-hydrocinnamic acid	19.2 (3.67)a	15.9 (3.88)b	18.2 (3.02)ab	16.6 (4.32)ab	0.066	0.126
12	Maleic Acid	11.8 (0.688)a	11.4 (0.995)a	11.8 (0.913)a	12.5 (1.8)a	0.141	0.215
12	Methyl-2-oxovaleric Acid	18.8 (3.86)a	17.3 (3.27)a	16.4 (4.4)a	17.9 (4.06)a	0.923	0.938
12	Methyl-a-D-Glucopyranoside	18.8 (2.62)a	15.5 (2.25)b	17.6 (3.49)ab	16 (2.09)ab	0.027	0.062
12	Methyl Vanillate	11 (1.68)a	9.08 (0.957)b	10.1 (1.54)ab	9.39 (1.67)ab	<0.01	0.024
12	Methylmalonic Acid	14 (2.23)ab	12.8 (1.89)a	13 (3.29)ab	15.2 (1.14)b	0.088	0.153
12	Mevalonic Acid	13.6 (1.78)a	12.8 (1.87)a	12.9 (1.26)a	12.6 (1.76)a	0.534	0.603
12	o-Hydroxyhippuric acid	9.68 (2.15)a	9.9 (3.2)a	10.1 (1.21)a	9.31 (1.47)a	0.23	0.314

12	O-Phospho-L-serine	8.33 (1.42)a	8.54 (1.47)a	8.44 (1.97)a	10.1 (1.67)a	0.155	0.231
12	Octadecanedioic Acid	13.2 (2.09)a	13.6 (2.01)a	14 (2.08)a	12.5 (1.94)a	0.618	0.684
12	Octadecanoic acid	10.4 (0.694)a	10.4 (0.7)a	10.6 (0.349)a	10.4 (0.437)a	0.392	0.472
12	Orotic Acid	16.5 (1.83)a	16.3 (4.57)a	16.6 (3.34)a	16.5 (2.64)a	0.933	0.943
12	Oxamic Acid	12.8 (3.1)ab	12.3 (1.61)ab	13.7 (1.32)a	11.8 (1.28)b	0.038	0.082
12	p-Coumaric acid	15.8 (2.93)a	15.1 (2.44)a	16.4 (2.18)a	14.6 (1.55)a	0.144	0.218
12	Phenol	8.75 (3.39)a	10.4 (3.73)a	8.3 (3.33)a	11.1 (3.95)a	0.315	0.401
12	Pimelic Acid	16 (0.964)a	15.2 (1.52)a	15.5 (1.05)a	16.1 (1.89)a	0.169	0.243
12	Pyrocatechol	16.2 (1.86)a	14.3 (1.42)b	15.6 (2.86)a	17 (2.32)a	<0.01	<0.01
12	Pyrogallol	10.5 (2.69)a	10.1 (1.99)a	10.6 (2.49)a	11.9 (4.18)a	0.6	0.668
12	Pyruvic acid	14.6 (2.65)a	13 (2.31)ab	12.7 (2.43)b	13.9 (1.44)ab	0.071	0.131
12	Quercetin	9.22 (3.58)a	8.53 (1.66)a	8.24 (1.21)a	8.29 (0.835)a	0.3	0.386
12	Quinic Acid	19 (1.45)a	16.9 (1.75)b	18.3 (0.836)ab	18.5 (1.9)ab	<0.01	0.018
12	Raffinose	18 (1.04)ab	17.7 (1.56)a	18.4 (1.07)b	17.6 (1.94)a	0.035	0.077
12	Rutin	6.45 (2.97)a	6.03 (0.866)a	6.41 (1.62)a	6.15 (1.33)a	0.206	0.289
12	Shikimic Acid	13.6 (1.39)a	12.9 (1.68)a	14 (0.714)a	13.3 (2.95)a	0.32	0.404
12	Stercobilin	7.07 (0.895)a	6.66 (2.45)a	6.84 (0.82)a	6.91 (0.539)a	0.801	0.845
12	Succinic Acid	19.7 (2.75)ab	20.1 (4.17)a	19.9 (4.52)ab	24.2 (4.13)b	0.08	0.145
12	Sucrose	20.1 (1.02)ab	19.4 (2.09)a	20.9 (0.798)b	19.9 (1.6)ab	0.04	0.084
12	TCDCA	14.5 (3.01)ab	10.3 (2.61)c	15.8 (2.91)a	13.1 (3.56)b	<0.01	<0.01
12	TDCA	10.9 (1.93)ab	10.4 (2.66)a	12.8 (0.831)b	11.3 (3.64)ab	0.088	0.153
12	Tetradecanedioic Acid	13.4 (1.06)ab	13.4 (0.944)ab	13.8 (0.93)a	13 (0.588)b	0.068	0.13
12	Tyrosol	16.8 (2.91)a	15.7 (3.22)a	17.3 (2.84)a	17.2 (5.4)a	0.245	0.33
12	Undecanedioic Acid	15.6 (1.19)a	15.9 (1.79)a	15.7 (1.21)a	15.6 (2.02)a	0.877	0.911
12	Uric Acid	14.7 (1.86)a	17.3 (4.81)a	16.6 (2.28)a	16 (2.93)a	0.222	0.307
12	Uridine	15.4 (2.07)a	15.3 (1.57)a	15 (3.04)a	16.9 (2.32)a	0.09	0.154

On-line Supplementary Material

Lauren Brink et al. Neonatal diet alters fecal microbiota and metabolome profiles over the first year of life in infants fed breast milk or formula.

[1] Data are log transformed peak areas and presented as median (25^{th} quartile, 75^{th} quartile). Differences in diet were assessed by Kruskal-Wallis test on percent abundances. Post-hoc analysis of pairwise differences in diet were assessed by Dunn's test. Medians without a common letter differ. FDR calculated by Benjamini and Hochberg false discovery rate procedure. BF = Breast-fed, MF = milk formula fed, NLB = no longer breastfeeding, SF = soy formula fed.

On-line Supplementary Material

Lauren Brink et al. Neonatal diet alters fecal microbiota and metabolome profiles over the first year of life in infants fed breast milk or formula.

Supplementary Table 5: Dietary differences in fecal metabolites (Positive Mode) from infants at three, six, nine, and 12 months of age.[1]

Age	Metabolite	BF	MF	NLB	SF	*P*-value	FDR
3	(-)-Epicatechin	9.3 (1.45)ab	9.75 (1.96)a		8.88 (0.637)b	0.07	0.14
3	1-Methylhydantoin	17.4 (2.28)a	18.1 (2.81)a		16.2 (4.01)a	0.092	0.171
3	1-Methyluric Acid	19.9 (1.15)a	16.2 (1.49)b		15.9 (1.19)b	<0.01	<0.01
3	2-Aminophenol	14.3 (0.973)a	17.5 (0.914)b		14.8 (0.908)c	<0.01	<0.01
3	2-Phenylacetamide	12.3 (0.834)a	12.4 (1.01)a		12.6 (1.99)a	0.938	0.956
3	3-Methylxanthine	15.9 (2.31)a	11.2 (0.115)b		10.8 (0.668)b	<0.01	<0.01
3	4-Hydroxyphenylpyruvic Acid	11.6 (2.74)a	10.9 (0.906)a		15.9 (3.72)b	<0.01	<0.01
3	4-Imidazoleacetic Acid	14.8 (2.07)a	16 (2.4)a		15.9 (3.11)a	0.178	0.28
3	4-Imidazoleacrylic Acid	20.1 (1.4)a	21.5 (1.31)ab		22.3 (1.14)b	0.02	0.055
3	4-Imidazolecarboxylic Acid	15.3 (0.677)a	14.6 (1.1)b		14.5 (1.09)b	0.013	0.038
3	4-Oxoproline	22.8 (2.99)a	23.9 (0.82)a		23.3 (1.14)a	0.305	0.416
3	4-Pyridoxic acid	17.8 (1.46)a	20 (0.601)b		17.6 (0.961)a	<0.01	<0.01
3	5-Aminovaleric Acid	23.4 (6.86)a	23.4 (1.46)a		24.2 (1.93)a	0.207	0.309
3	5-Hydroxylysine	14.7 (1.69)a	15.4 (1.85)a		14.4 (1.28)a	0.112	0.194
3	5-Hydroxytryptamine	12.8 (2.79)a	12.1 (1.49)a		15.4 (3.64)a	0.104	0.188
3	6-Hydroxydopamine	17.5 (1.19)a	16.9 (0.691)a		16.6 (1.01)a	0.109	0.191
3	Acetic Acid	22.2 (1.48)a	22.9 (1.67)a		22.5 (2.14)a	0.542	0.648
3	Acetylmuramic Acid	19.4 (1.83)a	19.2 (1.02)a		20.4 (1.17)b	0.034	0.08
3	Arginine	16.9 (2.11)a	16.2 (0.851)a		19 (1.62)b	<0.01	0.017
3	Asparagine	16.4 (0.73)a	16.1 (0.327)a		17 (1.28)a	0.167	0.267
3	Aspartic Acid	20.6 (2.11)a	21.1 (1.28)a		21.4 (1.46)a	0.109	0.191

3	b-Alanine	16.6 (1.33)a	17.6 (0.92)a		17.5 (2.35)a	0.286	0.396
3	Betaine	23.5 (1.08)a	21.7 (2.35)b		20.7 (2.6)b	<0.01	0.018
3	C18-Carnitine	17.7 (3.38)a	12.7 (3.72)b		13.5 (2.95)b	<0.01	0.023
3	Caffeine	16.5 (1.15)a	10.1 (1.27)b		10.4 (1.18)b	<0.01	<0.01
3	cis-11,12-Methylene Pentadecanoylcarnitine	18 (3.34)a	13.9 (2.6)b		14.9 (2.15)b	0.023	0.06
3	Citrulline	21.4 (2.84)a	22.2 (1.57)ab		22.5 (1.39)b	0.095	0.173
3	Creatine	23.5 (2.73)a	18.6 (3.73)a		20.2 (6.87)a	0.092	0.171
3	Creatinine	19.5 (4.08)a	18.3 (1.55)a		16.3 (3.11)b	<0.01	0.02
3	Cyclohexanecarboxylic Acid	12.9 (1.27)a	13 (0.76)a		12.5 (1.02)a	0.645	0.733
3	Cystathionine	13.9 (1.84)a	13.8 (1.2)a		13.4 (0.873)a	0.704	0.773
3	Cystine	17.5 (0.829)a	15.6 (1.54)b		14.8 (0.589)c	<0.01	<0.01
3	D-2-Aminobutyric Acid	20.9 (1.47)a	21.2 (1.3)a		20.6 (0.795)a	0.617	0.713
3	D-Sphingosine	19.2 (2.34)a	16.1 (1.56)b		16.8 (2.04)b	<0.01	<0.01
3	D6-trans-Cinnamic Acid	16.3 (0.407)a	16.3 (0.258)a		15.3 (0.297)b	<0.01	<0.01
3	DL-3-aminoisobutryic acid	20.9 (2.77)a	20.5 (2.28)a		20.1 (2.82)a	0.765	0.826
3	DL-Tryptophan	23 (1.88)a	22.9 (1.11)a		22.9 (1.65)a	0.879	0.912
3	Dopamine	14.8 (1.22)a	17.4 (0.901)b		16.6 (0.617)b	<0.01	<0.01
3	Ectoine	14.1 (1.4)a	13.9 (0.56)a		14.1 (1.15)a	0.798	0.852
3	Equol	9.03 (0.728)a	8.89 (0.315)a		9.14 (0.582)a	0.666	0.748
3	Ergothioneine	16.2 (1.89)a	14.5 (0.882)b		14.3 (0.94)b	<0.01	0.02
3	Ethanolamine	18 (1.39)a	16.8 (1.5)b		14.9 (1.52)c	<0.01	<0.01
3	Ferulic Acid	11.1 (0.805)a	13.1 (1.42)b		13.7 (3.45)b	<0.01	<0.01
3	Galactitol	19.1 (2.12)a	22.3 (1.78)b		16.6 (1.09)c	<0.01	<0.01

3	Genistein	9.74 (2.14)a	9.68 (2.45)a		15.1 (3.56)b	<0.01	<0.01
3	Glutamic Acid	24.8 (2.77)a	25.6 (0.825)a		24.9 (1.07)a	0.321	0.431
3	Glutamine	20.7 (1.46)a	20.5 (2.4)a		20.6 (1.21)a	0.725	0.793
3	Glutaric Acid	14.8 (1.65)ab	14.5 (0.597)a		15.2 (1.38)b	0.045	0.099
3	Glycine	21.4 (1.01)a	20.3 (2.29)a		19.8 (1.23)b	<0.01	0.017
3	Glycitein	9.86 (1.91)a	8.56 (0.222)b		14.2 (4.38)c	<0.01	<0.01
3	Hexanoic Acid	10.1 (3.56)a	12.2 (3.77)a		11.7 (1.8)a	0.577	0.682
3	Histidine	20.3 (1.74)a	20.1 (3.33)a		18.4 (1.07)b	<0.01	0.028
3	Imidazolepropionic Acid	19.7 (3.6)a	22.2 (1.22)b		21.9 (1.93)ab	0.063	0.13
3	Indole-3-Acetic Acid	15 (2.79)a	16.7 (1.67)a		19 (3.05)b	<0.01	<0.01
3	Indole-3-Lactic Acid	21.9 (2.57)a	22.7 (2.03)a		17.6 (1.93)b	<0.01	<0.01
3	Indole-3-Propionic Acid	12 (1.68)a	13.3 (4.79)ab		16.7 (1.99)b	<0.01	0.03
3	Inosine	16 (3.19)a	17.1 (2.73)a		17.5 (1.4)a	0.559	0.664
3	Isobutyric Acid	16.5 (2.43)a	18.9 (1.18)b		19.5 (0.939)b	<0.01	<0.01
3	Isovaleric Acid	11.9 (2.17)a	16 (1.59)b		17.3 (1.04)c	<0.01	<0.01
3	Jasmonic acid	14 (1.14)a	14.4 (0.432)a		17.4 (1.92)b	<0.01	<0.01
3	Kynurenic Acid	21.9 (1.98)a	19.5 (1.12)b		20 (1.01)b	<0.01	<0.01
3	L-Carnitine	20.7 (1.35)a	20.2 (1.53)a		19.4 (1.4)b	0.014	0.041
3	L-DOPA	11.8 (1.15)a	14 (0.97)b		12.6 (1.2)a	<0.01	<0.01
3	L-Kynurenine	15.8 (1.12)a	16 (0.477)a		15.9 (0.969)a	0.929	0.949
3	L-Phenylalanine	25.6 (2.01)a	25.6 (1.12)a		25.2 (1.4)a	0.652	0.739
3	L-Pipecolic Acid	21.1 (2.65)a	24.8 (2.2)b		23 (0.865)c	<0.01	<0.01
3	L-Pyroglutamic Acid	23.6 (1.85)a	24.5 (1.95)a		22.4 (3.63)a	0.166	0.267
3	L-Saccharophine	14.5 (1.91)a	15.5 (1.03)a		14.9 (1.23)a	0.168	0.267

3	Lysine	20.2 (2.21)a	22.1 (0.978)b		20.9 (1.1)a	0.011	0.033
3	m-Hydroxy-Hydrocinnamic Acid	10.8 (1.42)a	10.8 (1.08)a		14.3 (3.54)b	<0.01	<0.01
3	Methionine	24.1 (2.22)a	23.9 (0.525)a		23.7 (1.27)a	0.667	0.748
3	Myo-Inositol	21.3 (1.36)a	19.1 (1.55)b		18.8 (0.721)b	<0.01	<0.01
3	N-Acetylneuraminic Acid	22.4 (2.28)a	18.1 (1.37)b		19.2 (6.14)ab	0.097	0.176
3	N-Cinnamylglycine	12.4 (1.44)a	12.7 (1.32)a		11 (0.47)b	<0.01	<0.01
3	N-Methylhistidine	15.7 (4.06)a	18.1 (2.98)b		15.1 (3.52)a	0.041	0.094
3	N?-Acetylhistamine	17.5 (2.93)a	18.2 (1.01)ab		19.6 (1.83)b	0.029	0.071
3	N?,N?,N?-Trimethyllysine	13.5 (1.74)a	16 (1.32)a		20.1 (2.08)b	<0.01	<0.01
3	N1,N12-Diacetylspermine	14.1 (1.63)a	13.8 (1.53)a		12.1 (3.4)b	0.031	0.074
3	Neopterin	16 (1.03)a	14.3 (1.35)b		14.5 (1.56)b	<0.01	<0.01
3	Nicotinamide	14.9 (3.07)a	15.4 (3.29)a		14.4 (2.46)a	0.696	0.766
3	Nicotinic Acid	23.3 (1.35)a	23.5 (1.89)a		23.7 (2.84)a	0.914	0.938
3	Oleic acid	14.8 (1.8)a	14.5 (2.26)a		16.2 (4.67)a	0.188	0.288
3	Ornithine	17.4 (1.52)a	17.1 (1.31)a		15.5 (1.54)b	0.01	0.032
3	p-Aminobenzoic Acid	14.7 (0.22)a	13.6 (2.14)b		13.6 (1.55)ab	0.033	0.079
3	Palmitoylcarnitine	19.1 (3.38)a	15.7 (2.22)b		15.7 (2.42)b	<0.01	0.031
3	Phenylacetic Acid	12.6 (0.677)a	13.3 (1.26)a		15.6 (0.523)b	<0.01	<0.01
3	Phenylacetylglycine	10.7 (0.765)a	15.6 (1.54)b		12.9 (2.96)c	<0.01	<0.01
3	Phloretic Acid	11.6 (0.975)ab	11.2 (1.21)a		11.8 (0.577)b	0.076	0.15
3	Piperine	8.42 (0.383)a	8.17 (0.666)a		8.99 (0.64)b	0.039	0.089
3	Proline	25.4 (1.92)a	24.9 (1.67)a		23.8 (1.49)b	<0.01	0.022
3	Propionic Acid	19.5 (1.69)a	22.1 (1.05)b		22.3 (1.47)b	<0.01	0.014
3	Protocatechuic Acid	12.6 (2.24)a	11.7 (0.584)a		14.8 (2.09)b	<0.01	<0.01

3	Putrescine	20.1 (2.53)a	20.4 (1.35)a		20 (1.52)a	0.796	0.852
3	Ralgin	11.6 (1.2)a	11.3 (0.202)ab		11.1 (0.511)b	<0.01	0.013
3	Riboflavin	18.6 (0.519)a	18.2 (0.553)a		17.6 (1.03)b	<0.01	0.012
3	sarcosine	24.5 (1.37)a	24 (0.589)a		22.5 (1.54)b	<0.01	<0.01
3	Sebacic Acid	14.4 (0.684)a	14.7 (0.487)a		15.8 (0.512)b	<0.01	<0.01
3	Serine	20.9 (1.19)a	20.6 (0.53)ab		19.6 (1.37)b	<0.01	0.02
3	Sinapinic Acid	11.4 (2.24)a	11.2 (0.889)a		12.4 (3.07)a	0.312	0.423
3	Skatole	9.26 (0.694)a	9.02 (0.27)a		10.5 (0.76)b	<0.01	0.019
3	Spermidine	18.1 (3.7)a	20 (2.72)a		18.7 (1.89)a	0.186	0.286
3	Spermine	12.3 (1.32)a	12.1 (0.756)a		12 (1.96)a	0.551	0.658
3	Stachydrine	15.1 (1.43)a	17.1 (2.47)b		16.2 (2.44)ab	0.039	0.089
3	Syringic Acid	10.9 (0.663)a	11.6 (0.946)a		17.6 (2.37)b	<0.01	<0.01
3	Taurine	21.4 (0.965)a	21.4 (0.914)a		22 (1.48)a	0.526	0.634
3	trans-4-Hydroxyproline	19.2 (1.5)a	18.3 (0.83)b		18.3 (1.06)b	0.013	0.037
3	trans-Cinnamic Acid	12 (0.93)a	12 (1.02)a		12.1 (1.46)a	0.5	0.608
3	Trigonelline	23.3 (0.947)a	19.9 (0.769)b		19.3 (2.09)b	<0.01	<0.01
3	Trimethylamine-N-oxide	17.5 (1.71)a	17.2 (1.34)a		14.9 (1.61)b	<0.01	0.029
3	Tyrosine	23.4 (1.8)a	23.7 (0.981)a		23.6 (1.32)a	0.991	0.995
3	Uracil	22.3 (1.45)a	21.9 (0.831)a		21.5 (1.33)a	0.266	0.38
3	Uric Acid	19.3 (5.13)a	14.6 (1.15)b		15.3 (2.26)b	<0.01	<0.01
3	Urobilin	23.2 (6.13)a	22.9 (1.31)a		24.2 (1.44)b	0.035	0.081
3	Urobilinogen	18.7 (8.81)a	20.8 (3.49)a		23 (1.83)b	<0.01	0.015
3	Valeric Acid	10.8 (2.08)a	13.2 (4.18)b		13.1 (1.17)b	<0.01	0.014
3	Valine	24.9 (2.24)a	24.8 (1.51)a		23.5 (1.32)a	0.175	0.276

3	y-Glutamylphenylalanine	15.5 (2.54)a	15.3 (1.01)a		15.6 (1.21)a	0.994	0.995
6	(-)-Epicatechin	10.6 (2.98)a	9.54 (1.7)a		8.96 (0.393)b	<0.01	0.026
6	1-Methylhydantoin	17.9 (4.01)a	17.4 (2)a		14.3 (3.69)b	<0.01	<0.01
6	1-Methyluric Acid	19.5 (1.81)a	15.7 (0.991)b		16.3 (1.92)c	<0.01	<0.01
6	2-Aminophenol	14.5 (0.714)a	16.9 (2.22)b		15.5 (1.15)c	<0.01	<0.01
6	2-Phenylacetamide	12.6 (0.698)a	12.9 (1.44)a		12.7 (1.03)a	0.815	0.861
6	3-Methylxanthine	15.7 (1.41)a	11.4 (0.628)b		10.7 (0.629)c	<0.01	<0.01
6	4-Hydroxyphenylpyruvic Acid	11.5 (2.6)a	11.1 (1.27)a		14.1 (3.18)b	<0.01	<0.01
6	4-Imidazoleacetic Acid	15.1 (1.79)a	15.2 (0.852)a		15.1 (1.13)a	0.538	0.647
6	4-Imidazoleacrylic Acid	21.1 (1.17)a	22.2 (1.28)b		22.1 (0.945)b	<0.01	0.02
6	4-Imidazolecarboxylic Acid	15.4 (0.875)a	14.6 (0.867)b		14.7 (1.69)b	0.01	0.031
6	4-Oxoproline	23.2 (1.22)ab	22.9 (0.56)a		23.3 (0.992)b	0.081	0.157
6	4-Pyridoxic acid	18.1 (1.12)a	20 (1.09)b		18.5 (0.698)a	<0.01	<0.01
6	5-Aminovaleric Acid	23.4 (5.05)a	23.9 (2.4)a		23.7 (2.32)a	0.97	0.982
6	5-Hydroxylysine	14.7 (0.875)a	15 (1.37)a		14.5 (0.906)a	0.626	0.718
6	5-Hydroxytryptamine	11.3 (3.27)a	13.9 (2.18)b		16.3 (1.97)c	<0.01	<0.01
6	6-Hydroxydopamine	18.5 (1.82)a	17.6 (1.99)a		17.6 (1.69)a	0.263	0.376
6	Acetic Acid	22 (1.48)a	23 (0.996)b		22.8 (1.05)b	0.028	0.071
6	Acetylmuramic Acid	19.5 (2.63)a	19.8 (1.93)a		19.7 (0.754)a	0.851	0.893
6	Arginine	17.7 (2.02)a	18 (2.64)a		18.7 (2.25)a	0.233	0.342
6	Asparagine	16.8 (2.23)a	15.5 (2.13)a		18.3 (1.13)b	<0.01	<0.01
6	Aspartic Acid	21 (1.49)a	20.1 (1.09)b		21 (1.17)a	<0.01	0.026
6	b-Alanine	17.3 (1.39)a	17.7 (2.65)a		17.2 (2.56)a	0.864	0.902
6	Betaine	23.5 (1.66)a	21.5 (2.64)b		20.9 (2.78)b	<0.01	<0.01

6	C18-Carnitine	15.6 (2.05)a	13.4 (2.04)b		11.5 (3.31)b	<0.01	<0.01
6	Caffeine	14.8 (2.07)a	10.3 (1.36)b		9.76 (1.03)b	<0.01	<0.01
6	cis-11,12-Methylene Pentadecanoylcarnitine	16.4 (2.92)a	15.2 (1.98)b		14.8 (1.62)b	0.06	0.127
6	Citrulline	21.5 (2.1)a	22.4 (1.18)ab		22.8 (1.05)b	0.08	0.154
6	Creatine	22.7 (1.84)a	19.7 (3.49)b		20.2 (2.03)b	<0.01	<0.01
6	Creatinine	19.2 (3.22)a	17.6 (1.74)ab		16.9 (3.99)b	0.072	0.144
6	Cyclohexanecarboxylic Acid	13.1 (1.45)a	13.5 (1.03)a		13.4 (2.8)a	0.195	0.296
6	Cystathionine	14.2 (0.837)a	13.5 (1.09)b		13.5 (1.12)b	0.066	0.134
6	Cystine	16.6 (1.1)a	14.7 (1.22)b		14.6 (0.959)b	<0.01	<0.01
6	D-2-Aminobutyric Acid	22 (2.19)a	21.2 (1.12)a		21 (0.653)a	0.351	0.462
6	D-Sphingosine	18.4 (1.2)a	16.9 (1.48)b		16.6 (1.27)b	<0.01	<0.01
6	D6-trans-Cinnamic Acid	16.3 (0.503)a	16.1 (0.265)a		15.7 (0.431)b	<0.01	<0.01
6	DL-3-aminoisobutryic acid	21.2 (3.57)a	19.9 (2.4)a		19.9 (0.976)a	0.236	0.344
6	DL-Tryptophan	23.9 (1.57)a	23 (1.67)a		23.9 (0.554)a	0.131	0.222
6	Dopamine	15.7 (0.92)a	17 (0.915)b		16.9 (0.516)b	<0.01	<0.01
6	Ectoine	14.3 (0.738)a	14.6 (1.53)a		14.5 (1.53)a	0.681	0.755
6	Equol	8.68 (0.845)a	8.65 (0.41)a		8.77 (0.413)a	0.952	0.966
6	Ergothioneine	14.8 (1.82)a	14 (0.756)b		13.3 (0.266)c	<0.01	<0.01
6	Ethanolamine	17 (2.27)a	17 (1.67)a		15.2 (1.97)b	<0.01	<0.01
6	Ferulic Acid	15.7 (4.42)a	16.8 (2.64)a		16.6 (2.51)a	0.13	0.22
6	Galactitol	18.9 (1.69)a	22.2 (1.73)b		16.8 (1.19)c	<0.01	<0.01
6	Genistein	9.51 (1.27)a	8.97 (0.5)a		13.1 (2.22)b	<0.01	<0.01
6	Glutamic Acid	24.8 (0.869)a	24.5 (0.679)a		25.2 (0.757)b	<0.01	0.031

6	Glutamine	20.8 (1.81)a	20 (0.865)b		21.4 (1.23)a	<0.01	<0.01
6	Glutaric Acid	14.7 (1.76)a	14.3 (1.69)a		14.7 (1.19)a	0.351	0.462
6	Glycine	21.7 (0.828)a	20.3 (0.864)b		20.1 (0.764)b	<0.01	<0.01
6	Glycitein	9.07 (0.831)a	8.81 (0.775)a		9.78 (4.4)b	<0.01	0.014
6	Hexanoic Acid	9.76 (2.97)a	11.8 (3.92)ab		11.7 (2.03)b	0.078	0.152
6	Histidine	19.7 (1.57)a	18.9 (1.53)b		18.8 (1.36)b	0.03	0.071
6	Imidazolepropionic Acid	22 (2.12)a	22.1 (1.43)a		22.3 (0.789)a	0.893	0.923
6	Indole-3-Acetic Acid	14.8 (2.06)a	16.8 (1.76)b		17.7 (1.83)b	0.029	0.071
6	Indole-3-Lactic Acid	22.6 (2.32)a	20.4 (3.13)b		17 (2.95)c	<0.01	<0.01
6	Indole-3-Propionic Acid	12.9 (2.9)a	14.6 (4.36)a		14.7 (5.58)a	0.258	0.371
6	Inosine	16.4 (3.15)a	15.5 (3.21)a		17.8 (2.4)b	<0.01	0.021
6	Isobutyric Acid	14.3 (5.07)a	19.4 (1.24)b		19.8 (1.06)b	<0.01	<0.01
6	Isovaleric Acid	12.1 (5.72)a	16.3 (0.801)b		17.3 (0.891)c	<0.01	<0.01
6	Jasmonic acid	14.9 (1.64)a	15.9 (1.37)a		17.3 (2.29)b	<0.01	<0.01
6	Kynurenic Acid	21.2 (1.21)a	19 (2.04)b		19.8 (1.41)b	<0.01	<0.01
6	L-Carnitine	21.7 (1.58)a	20.9 (1.28)b		20.1 (1.69)b	<0.01	<0.01
6	L-DOPA	14.2 (3.59)a	14.8 (1.15)a		14.9 (1.41)a	0.812	0.86
6	L-Kynurenine	15.9 (0.993)a	15.6 (0.709)a		16 (1.21)a	0.141	0.234
6	L-Phenylalanine	25.8 (1.5)a	25.5 (1.36)a		25.5 (1.41)a	0.343	0.455
6	L-Pipecolic Acid	23.5 (3.38)a	24.6 (2.16)b		22.9 (1)a	<0.01	0.023
6	L-Pyroglutamic Acid	22.4 (1.67)a	20.6 (2.27)b		20.6 (1.97)b	0.027	0.068
6	L-Saccharophine	15.8 (1.14)a	14.8 (0.608)b		14.9 (0.855)b	<0.01	0.022
6	Lysine	20.3 (0.983)a	21.2 (1.64)b		21.4 (1.55)b	0.038	0.087
6	m-Hydroxy-Hydrocinnamic Acid	13.2 (4.46)a	14.4 (3.41)a		15.5 (2.17)b	0.022	0.059

6	Methionine	23.8 (0.912)a	23.9 (0.958)a		23.7 (1.17)a	0.875	0.912
6	Myo-Inositol	20.8 (0.887)a	19.5 (1.79)b		18.9 (1.55)c	<0.01	<0.01
6	N-Acetylneuraminic Acid	22.3 (2.96)a	18 (2.01)b		19.1 (1.43)b	<0.01	<0.01
6	N-Cinnamylglycine	13 (1.19)a	12.5 (1.1)a		10.9 (1.24)b	<0.01	<0.01
6	N-Methylhistidine	15.7 (1.86)a	17.8 (3.86)a		15.6 (3.17)a	0.234	0.343
6	N?-Acetylhistamine	17.9 (2.18)a	18 (1.13)a		19 (0.978)b	0.024	0.063
6	N?,N?,N?-Trimethyllysine	16.5 (3.01)a	17.1 (2.59)a		18 (2.35)b	0.066	0.134
6	N1,N12-Diacetylspermine	14.9 (2.17)a	13.6 (1.91)b		13 (1.94)b	<0.01	0.026
6	Neopterin	16.7 (1.43)a	15 (1.32)b		14.3 (0.746)b	<0.01	<0.01
6	Nicotinamide	15.6 (4.06)a	14.4 (2.41)a		15.4 (1.39)a	0.206	0.309
6	Nicotinic Acid	22.9 (2)a	24.2 (1.16)b		24.4 (0.458)b	<0.01	0.019
6	Oleic acid	14.5 (1.66)a	12.9 (2.17)a		12.3 (4.54)a	0.137	0.23
6	Ornithine	18.1 (3.06)a	17.1 (1.59)ab		16.1 (2.4)b	0.064	0.131
6	p-Aminobenzoic Acid	14.7 (1.2)a	13.6 (1.98)a		13.8 (1.33)a	0.176	0.278
6	Palmitoylcarnitine	17.3 (1.74)a	16 (2.57)b		14.6 (2.57)b	<0.01	0.02
6	Phenylacetic Acid	13.2 (2.4)a	14 (1.54)a		15.4 (1.15)b	<0.01	<0.01
6	Phenylacetylglycine	12.6 (4.05)ab	15.1 (4.58)a		11.6 (1.61)b	<0.01	0.016
6	Phloretic Acid	12.3 (0.911)a	11.9 (1.76)a		12.8 (0.698)a	0.137	0.23
6	Piperine	7.99 (1.43)a	8.04 (0.724)a		8.41 (1.02)a	0.62	0.715
6	Proline	25.6 (2.01)a	24.6 (0.59)b		24 (1.52)c	<0.01	<0.01
6	Propionic Acid	20.4 (3.1)a	22.8 (1.16)b		22.3 (1.53)b	<0.01	<0.01
6	Protocatechuic Acid	13.9 (2.34)a	12.8 (1.26)b		14.3 (2.3)a	<0.01	0.031
6	Putrescine	20.9 (2.36)a	20.2 (2.58)a		20.2 (1.48)a	0.486	0.599
6	Ralgin	11.2 (0.457)a	11.2 (1.27)a		11.7 (1.76)a	0.68	0.755

6	Riboflavin	18.1 (1.11)a	18.2 (1.24)ab		17.5 (0.938)b	0.075	0.148
6	sarcosine	24.7 (1.18)a	23.8 (0.671)b		23.4 (0.685)c	<0.01	<0.01
6	Sebacic Acid	14.9 (1.22)a	15.1 (0.928)a		16.1 (0.799)b	<0.01	<0.01
6	Serine	20.7 (0.775)a	20.5 (0.727)a		20.4 (0.583)a	0.15	0.248
6	Sinapinic Acid	13.2 (2.85)a	13.5 (2.4)a		13.4 (1.77)a	0.588	0.69
6	Skatole	9.62 (1.02)a	8.81 (0.662)a		9.13 (0.831)a	0.198	0.3
6	Spermidine	18.1 (3.09)a	21 (2.3)b		19.8 (2.41)ab	0.05	0.108
6	Spermine	12.4 (1.43)a	12.1 (0.938)a		12 (1.48)a	0.341	0.454
6	Stachydrine	15 (1.11)a	17.7 (1.73)b		17.4 (4.8)b	<0.01	<0.01
6	Syringic Acid	12.5 (3.74)a	13.8 (2.68)a		16.9 (2.21)b	<0.01	<0.01
6	Taurine	21.7 (1.02)a	22.2 (1.45)a		21.9 (0.736)a	0.372	0.485
6	trans-4-Hydroxyproline	19 (0.709)a	18.3 (0.692)b		18.8 (1.14)a	0.02	0.054
6	trans-Cinnamic Acid	12 (1.84)a	12.1 (1.39)a		12.2 (0.818)a	0.983	0.991
6	Trigonelline	22.7 (1.37)a	19.9 (2.16)b		19.4 (1.48)b	<0.01	<0.01
6	Trimethylamine-N-oxide	16.1 (3.04)ab	16.7 (1.69)a		15 (1.31)b	0.021	0.057
6	Tyrosine	24 (1.43)a	24 (1.04)a		24.6 (0.774)b	0.01	0.031
6	Uracil	21.9 (2.16)a	21.9 (0.868)a		21.3 (0.792)a	0.094	0.173
6	Uric Acid	20.5 (6.74)a	14.5 (2.56)b		14.8 (2.51)b	<0.01	<0.01
6	Urobilin	19 (8.24)a	22.7 (2.22)a		24 (1.02)b	0.017	0.047
6	Urobilinogen	16.8 (6.04)a	18.5 (3.85)a		22.5 (1.35)b	<0.01	<0.01
6	Valeric Acid	10.5 (2.14)a	15.3 (2.21)b		13.2 (2.4)b	<0.01	<0.01
6	Valine	25.3 (1.73)a	24.4 (0.78)b		24.5 (0.972)b	<0.01	0.022
6	y-Glutamylphenylalanine	16.6 (2.55)a	14.8 (1.17)b		15.7 (1.63)ab	0.043	0.096
9	(-)-Epicatechin	10.5 (2.69)a	10.9 (2.18)a		9.04 (1.18)b	0.031	0.074

9	1-Methylhydantoin	18.2 (2.11)a	18 (2.96)a		14.3 (1.99)b	<0.01	<0.01
9	1-Methyluric Acid	17.2 (3.82)a	14.9 (2.92)b		16.7 (1.39)ab	0.018	0.05
9	2-Aminophenol	15.2 (2.6)a	17.1 (1.05)b		16.5 (1.22)b	<0.01	0.02
9	2-Phenylacetamide	12.4 (0.635)a	12.5 (1.52)a		12.9 (1.11)a	0.437	0.548
9	3-Methylxanthine	15.1 (2.97)a	11.2 (1.06)b		11.3 (0.863)b	<0.01	<0.01
9	4-Hydroxyphenylpyruvic Acid	12.1 (1.33)a	11.4 (0.629)a		13.6 (2.24)b	<0.01	<0.01
9	4-Imidazoleacetic Acid	16.3 (2.47)a	15.7 (1.03)a		16.1 (1.18)a	0.821	0.865
9	4-Imidazoleacrylic Acid	21 (1.53)ab	20.5 (2.67)a		22 (1.5)b	0.058	0.125
9	4-Imidazolecarboxylic Acid	15.4 (1.93)a	14.6 (0.975)a		14.8 (1.12)a	0.334	0.446
9	4-Oxoproline	23.4 (0.693)a	22.4 (0.728)b		22.9 (0.437)a	<0.01	0.017
9	4-Pyridoxic acid	19.1 (1.26)ab	19.9 (1.29)a		18.7 (1.46)b	0.049	0.106
9	5-Aminovaleric Acid	24.5 (2.05)a	22.8 (1.75)a		24.3 (2.27)a	0.122	0.21
9	5-Hydroxylysine	15.2 (0.919)a	15.1 (2.32)a		14.7 (1.85)a	0.498	0.608
9	5-Hydroxytryptamine	13.1 (2.29)a	12.7 (2.14)a		14.8 (2.99)a	0.109	0.191
9	6-Hydroxydopamine	18 (2.06)a	17.8 (1.41)a		17.5 (1.56)a	0.418	0.533
9	Acetic Acid	22.5 (1.89)a	22.7 (1.01)a		22.9 (0.415)a	0.114	0.196
9	Acetylmuramic Acid	19.7 (2.14)a	19.3 (1.32)a		19.6 (1.74)a	0.496	0.608
9	Arginine	17.5 (2.72)a	18.1 (1.05)a		19.2 (1.41)b	<0.01	0.022
9	Asparagine	16.6 (1.84)a	16.4 (1.47)a		18.2 (0.762)b	0.012	0.036
9	Aspartic Acid	21.3 (1.31)a	20.1 (0.682)b		20.7 (1.52)a	0.034	0.08
9	b-Alanine	17.1 (1.84)a	19 (3.45)a		18.3 (2.78)a	0.436	0.548
9	Betaine	23.3 (3.27)a	20.9 (2.14)b		18.7 (1.52)c	<0.01	<0.01
9	C18-Carnitine	15.4 (1.56)a	12.4 (2.23)b		11.1 (2.97)b	<0.01	<0.01
9	Caffeine	13 (3.53)a	9.48 (1.31)b		10.4 (1.45)b	<0.01	<0.01

9	cis-11,12-Methylene Pentadecanoylcarnitine	15.1 (2.34)a	14.8 (1.9)ab		13.6 (1.86)b	<0.01	0.026
9	Citrulline	22.3 (2.79)a	22.4 (2.9)a		22.4 (0.95)a	0.66	0.745
9	Creatine	21.1 (3.19)a	20 (3.3)b		19.5 (2.12)b	0.045	0.1
9	Creatinine	17.8 (4.67)a	17.6 (0.846)a		15.9 (4.31)a	0.468	0.581
9	Cyclohexanecarboxylic Acid	13.5 (1.43)a	14.5 (2.13)ab		15.2 (2.54)b	0.083	0.159
9	Cystathionine	14 (1.33)a	13.6 (0.592)a		13.4 (0.925)a	0.278	0.389
9	Cystine	16 (1.46)a	15.6 (1.84)ab		14.4 (1.03)b	<0.01	0.023
9	D-2-Aminobutyric Acid	21.2 (1.82)a	20.2 (1.2)a		20.6 (1.57)a	0.424	0.537
9	D-Sphingosine	17.9 (1.14)a	16.7 (1.06)b		15.8 (1.22)b	<0.01	<0.01
9	D6-trans-Cinnamic Acid	16.3 (0.343)a	15.9 (0.579)b		15.8 (0.342)b	<0.01	<0.01
9	DL-3-aminoisobutryic acid	20.5 (2.06)a	19.4 (1.62)a		20.6 (1.26)a	0.159	0.26
9	DL-Tryptophan	23.2 (1.33)a	22.6 (1.01)b		23.1 (0.903)a	0.013	0.038
9	Dopamine	16.9 (1.75)a	18.3 (1.21)b		17.1 (0.66)a	0.017	0.047
9	Ectoine	14.9 (1.68)a	15.1 (1.05)a		16.2 (1.58)a	0.086	0.163
9	Equol	8.7 (0.427)a	8.33 (0.228)b		8.7 (0.884)a	<0.01	0.026
9	Ergothioneine	14.6 (2.19)a	13.9 (1.13)a		13.7 (1.3)a	0.599	0.699
9	Ethanolamine	16.1 (1.04)a	15.5 (2.58)ab		14.9 (1.65)b	0.028	0.07
9	Ferulic Acid	18.4 (1.7)a	18.4 (1.33)a		15.8 (2.89)b	<0.01	0.02
9	Galactitol	18.9 (1.67)a	21.8 (0.926)b		16.7 (0.522)c	<0.01	<0.01
9	Genistein	8.95 (0.739)a	8.61 (0.59)a		12.6 (2.29)b	<0.01	<0.01
9	Glutamic Acid	25 (0.852)a	24.2 (0.79)b		24.1 (0.944)ab	0.037	0.086
9	Glutamine	20.7 (0.863)a	19.9 (0.841)b		20.7 (0.317)a	<0.01	0.016
9	Glutaric Acid	14.7 (1.27)a	14.6 (2.15)a		15.4 (0.921)a	0.17	0.269

9	Glycine	21.1 (1.68)a	19.8 (0.996)b		19.9 (0.854)b	<0.01	0.023
9	Glycitein	9.17 (0.779)a	8.74 (0.494)b		9.17 (3.16)a	<0.01	<0.01
9	Hexanoic Acid	11.5 (2.56)a	10.8 (1.53)a		11.8 (2.04)a	0.408	0.524
9	Histidine	19.4 (2.29)a	18.9 (1.33)ab		18 (2.3)b	0.061	0.128
9	Imidazolepropionic Acid	22.6 (2.73)a	22.5 (1.42)a		21.8 (1.37)a	0.433	0.546
9	Indole-3-Acetic Acid	17.2 (2.86)a	17.8 (2.72)a		18.2 (1.61)a	0.207	0.309
9	Indole-3-Lactic Acid	22.1 (2.67)a	20.1 (3.91)b		18.3 (3.01)c	<0.01	<0.01
9	Indole-3-Propionic Acid	12.8 (4.6)a	18.4 (4.62)a		16.4 (5.19)a	0.164	0.266
9	Inosine	15 (3.31)a	15.3 (3.04)a		17.6 (2.2)b	0.021	0.057
9	Isobutyric Acid	19.4 (3.09)a	19.1 (0.809)a		20.4 (0.756)b	<0.01	0.011
9	Isovaleric Acid	15.5 (3.83)a	16 (3.05)a		17.1 (1.73)b	0.029	0.071
9	Jasmonic acid	15.7 (1.16)a	15.4 (1.27)a		16.8 (1.47)b	<0.01	<0.01
9	Kynurenic Acid	21.1 (0.958)a	19.6 (1.61)b		18.6 (2.35)b	<0.01	<0.01
9	L-Carnitine	20.6 (1)a	20 (2.18)ab		19.9 (1.22)b	0.064	0.131
9	L-DOPA	14.9 (2.85)a	15.2 (1.38)a		15.1 (1.71)a	0.658	0.744
9	L-Kynurenine	14.7 (1.39)a	14.8 (1.5)a		15.9 (0.756)b	0.013	0.038
9	L-Phenylalanine	25.8 (1.29)a	24.9 (1.35)a		25.9 (0.37)a	0.109	0.191
9	L-Pipecolic Acid	24.5 (3.68)a	24.4 (2.28)a		23.6 (1.14)a	0.684	0.757
9	L-Pyroglutamic Acid	21.8 (3.35)a	20.1 (1.64)b		19.1 (1.31)b	0.019	0.053
9	L-Saccharophine	15.7 (0.779)a	15.4 (0.38)ab		15 (0.589)b	<0.01	0.011
9	Lysine	20.4 (2.33)a	21.8 (1.5)b		21.3 (0.86)b	<0.01	0.02
9	m-Hydroxy-Hydrocinnamic Acid	15.5 (1.85)a	13.8 (2.52)a		15.3 (1.44)a	0.166	0.267
9	Methionine	23.8 (1.43)ab	22.7 (1.33)a		24.3 (0.469)b	0.029	0.071
9	Myo-Inositol	20.8 (1.15)a	19.3 (2.54)a		19.8 (1.09)a	0.075	0.148

9	N-Acetylneuraminic Acid	20.6 (3.72)a	17.4 (1.72)b		17.7 (1.34)b	<0.01	<0.01
9	N-Cinnamylglycine	13.1 (1.2)a	11.8 (0.808)b		11.3 (1.03)b	<0.01	<0.01
9	N-Methylhistidine	14.4 (2.37)a	15.9 (2.98)a		14.6 (3.45)a	0.184	0.286
9	N?-Acetylhistamine	18.9 (1.88)a	18.8 (2.31)a		18.8 (1.05)a	0.552	0.658
9	N?,N?,N?-Trimethyllysine	16.4 (4.33)a	17.2 (3.05)a		17.9 (3.93)a	0.686	0.758
9	N1,N12-Diacetylspermine	13.2 (1.66)a	13.1 (1.49)a		12.8 (2.39)a	0.903	0.931
9	Neopterin	15.7 (1.03)a	14.4 (1.88)b		13.9 (0.755)b	<0.01	<0.01
9	Nicotinamide	15 (2.4)a	16.1 (1.2)a		15.3 (1.39)a	0.317	0.427
9	Nicotinic Acid	23.9 (1.35)a	23.2 (2.21)a		24.1 (2.7)a	0.743	0.811
9	Oleic acid	14 (1.72)a	13.2 (2.34)ab		11.6 (1.87)b	0.05	0.108
9	Ornithine	15.5 (4.82)a	17 (2.3)a		14.3 (2.19)a	0.299	0.409
9	p-Aminobenzoic Acid	15.1 (2.15)a	14.3 (3.02)a		14.7 (2.63)a	0.878	0.912
9	Palmitoylcarnitine	16.4 (1.48)a	15.7 (1.48)b		14.1 (0.975)c	<0.01	<0.01
9	Phenylacetic Acid	14.5 (1.59)a	14.2 (1.73)a		15.7 (1.15)b	<0.01	0.031
9	Phenylacetylglycine	13 (2.72)a	13.5 (4.44)a		11.9 (1.5)a	0.105	0.188
9	Phloretic Acid	13.3 (0.622)a	12.4 (1.26)b		12.5 (0.968)b	0.011	0.034
9	Piperine	8.76 (2.28)a	8.38 (1.22)a		8.45 (0.411)a	0.8	0.853
9	Proline	24.5 (2.56)a	24 (2.31)a		24.2 (0.982)a	0.298	0.409
9	Propionic Acid	22.5 (1.85)a	22.6 (0.504)a		22.6 (1.4)a	0.812	0.86
9	Protocatechuic Acid	17.1 (1.77)a	15.1 (1.87)b		14.4 (1.79)b	<0.01	<0.01
9	Putrescine	20 (1.94)a	20 (2.55)a		18.8 (2.1)a	0.268	0.381
9	Ralgin	12 (1.52)a	11.3 (0.885)a		11.1 (1.78)a	0.086	0.163
9	Riboflavin	18.3 (1.97)a	17.4 (1.86)a		17.8 (1.28)a	0.613	0.712
9	sarcosine	24 (0.866)a	23.1 (0.504)b		23.2 (0.793)b	0.035	0.081

9	Sebacic Acid	14.7 (0.823)a	14.6 (0.601)a		16.2 (1.22)b	<0.01	<0.01
9	Serine	20.8 (1.04)a	20 (1.12)a		20.2 (1.29)a	0.121	0.209
9	Sinapinic Acid	14.5 (1.34)a	14.1 (2.59)ab		13.8 (1.73)b	0.096	0.174
9	Skatole	9.25 (0.974)a	8.77 (0.598)b		9.6 (1.03)a	0.015	0.042
9	Spermidine	18.2 (3.47)a	21.4 (2.58)b		21.7 (3.05)b	<0.01	0.017
9	Spermine	11.4 (1.04)a	12 (1.31)a		11.9 (2.51)a	0.106	0.189
9	Stachydrine	18 (2.41)a	17.1 (2.75)a		17.9 (1.96)a	0.907	0.933
9	Syringic Acid	15.8 (1.62)a	14.9 (3.4)b		16.4 (2.8)a	0.023	0.06
9	Taurine	21.6 (1.23)a	21.4 (1.8)a		21.6 (0.332)a	0.707	0.775
9	trans-4-Hydroxyproline	20 (1.46)a	20.7 (1.61)a		18.7 (0.691)b	<0.01	<0.01
9	trans-Cinnamic Acid	12.5 (1.58)a	12.2 (1.21)a		12.6 (1.04)a	0.525	0.634
9	Trigonelline	21.3 (1.58)a	17.2 (3.06)b		18.2 (2.55)b	<0.01	<0.01
9	Trimethylamine-N-oxide	15.3 (1.93)a	16.3 (3.81)a		14.2 (0.893)b	0.059	0.125
9	Tyrosine	24.3 (1.33)ab	23.4 (1.37)a		24.4 (0.753)b	0.066	0.134
9	Uracil	22 (1.28)a	21.4 (0.928)a		21.2 (1.54)a	0.239	0.347
9	Uric Acid	15.7 (1.64)a	15.2 (2.95)a		14.4 (2.37)a	0.09	0.168
9	Urobilin	23.2 (4.6)a	23 (2.85)a		23.6 (0.582)a	0.285	0.396
9	Urobilinogen	15.4 (6.7)a	17.5 (5.14)a		21.1 (1.68)b	0.022	0.058
9	Valeric Acid	13.3 (2.51)a	13.1 (1.81)ab		14.6 (3.25)b	0.068	0.136
9	Valine	24.7 (1.48)a	23.9 (1.45)a		24.6 (0.717)a	0.212	0.314
9	y-Glutamylphenylalanine	15.3 (1.06)a	14.4 (1.06)b		15.3 (1.05)a	0.039	0.089
12	(-)-Epicatechin	10.8 (1.97)a	9.45 (1.27)b	9.85 (2.02)ab	9.74 (1.44)b	0.059	0.125
12	1-Methylhydantoin	17.7 (2.98)a	17.3 (2.11)a	16.8 (3.31)a	14 (2.37)b	0.014	0.041
12	1-Methyluric Acid	17.1 (1.77)a	17.9 (2.9)a	15.8 (0.518)a	16.7 (1.58)a	0.128	0.218

12	2-Aminophenol	16.5 (1.72)a	16.3 (1.29)a	15.8 (1.39)a	15.8 (1.5)a	0.674	0.751
12	2-Phenylacetamide	13 (1.03)a	13.2 (1.04)a	11.8 (2.65)a	13 (0.604)a	0.207	0.309
12	3-Methylxanthine	13.9 (3.16)a	14.2 (5.12)a	11.6 (2.06)a	11.8 (1.81)a	0.088	0.165
12	4-Hydroxyphenylpyruvic Acid	12 (1.04)a	11.7 (0.909)a	12.5 (1.1)a	12.7 (1.87)a	0.123	0.211
12	4-Imidazoleacetic Acid	15.2 (1.07)a	15.3 (0.87)a	15.7 (1.74)a	16 (0.999)a	0.185	0.286
12	4-Imidazoleacrylic Acid	20.5 (2.66)a	22.3 (2.97)a	21.6 (2.93)a	22 (2.07)a	0.29	0.4
12	4-Imidazolecarboxylic Acid	15.4 (1.86)a	15.6 (1.22)a	15.6 (2.3)a	15.9 (1.98)a	0.577	0.682
12	4-Oxoproline	22.9 (1.4)a	23 (1.05)a	22.9 (0.462)a	23.2 (1.28)a	0.995	0.995
12	4-Pyridoxic acid	20.3 (2.43)a	20.8 (1.84)a	20.4 (1.39)a	19.8 (1.14)a	0.472	0.583
12	5-Aminovaleric Acid	24.1 (2.02)a	22.3 (4.07)a	24.6 (2.03)a	23.1 (1.07)a	0.085	0.162
12	5-Hydroxylysine	14.6 (1.23)a	14.9 (0.969)a	15.1 (0.933)a	15.3 (2.36)a	0.419	0.533
12	5-Hydroxytryptamine	13.2 (3.71)a	13 (2.02)a	13.6 (2.02)a	13.6 (1.43)a	0.623	0.717
12	6-Hydroxydopamine	18.5 (1.23)a	18.5 (2.09)a	18.2 (1.63)a	17.2 (1.38)b	0.028	0.07
12	Acetic Acid	23 (0.887)ab	23 (0.902)ab	23.4 (0.686)a	22.6 (1.71)b	0.044	0.098
12	Acetylmuramic Acid	19.3 (1.21)a	19.5 (1.66)a	19.8 (1.53)a	19.6 (1.66)a	0.371	0.485
12	Arginine	18.4 (1.95)a	19.8 (1.55)a	19 (1.36)a	19.6 (1.06)a	0.375	0.488
12	Asparagine	16.6 (1.85)a	16.9 (2.7)ab	17.9 (1.68)ab	18.3 (2.06)b	0.062	0.129
12	Aspartic Acid	20.7 (1.42)a	19.8 (1.75)a	20.2 (1.87)a	20.9 (1.06)a	0.379	0.492
12	b-Alanine	17.8 (1.88)a	16.9 (1.77)a	17.5 (2.62)a	17.6 (3.12)a	0.419	0.533
12	Betaine	20.8 (3.17)a	22.2 (2.06)a	19.6 (3.43)a	21 (1.85)a	0.616	0.713
12	C18-Carnitine	14.9 (3.43)a	13.7 (4.53)a	13.3 (4.94)a	13.2 (3.91)a	0.224	0.331
12	Caffeine	13.4 (3.63)a	11.6 (2.69)a	11.3 (1.82)a	10.9 (3.31)a	0.136	0.228
12	cis-11,12-Methylene Pentadecanoylcarnitine	15.3 (2.25)a	14.7 (1.31)ab	14 (2.93)ab	13.7 (0.609)b	0.028	0.071
12	Citrulline	22.5 (1.41)a	22.5 (1.05)a	22.5 (1.08)a	22.9 (0.953)a	0.269	0.381
12	Creatine	20.5 (2.41)a	19.4 (4.1)a	21.6 (2.06)a	21 (2.04)a	0.278	0.389

12	Creatinine	16.2 (1.58)a	15.7 (2.41)a	15 (2.76)a	14.9 (3.13)a	0.608	0.708
12	Cyclohexanecarboxylic Acid	14.7 (3.5)ab	13.7 (1.81)a	15.9 (1.92)b	15.3 (1.97)ab	0.056	0.121
12	Cystathionine	13.2 (0.623)a	13.6 (0.807)a	13 (1.16)a	13.5 (1.19)a	0.274	0.386
12	Cystine	14.7 (1.28)a	14.8 (1.75)a	14.6 (0.934)a	14.1 (0.84)a	0.257	0.37
12	D-2-Aminobutyric Acid	20.7 (1.5)ab	21.3 (0.886)a	20.7 (0.94)ab	20.4 (0.747)b	0.109	0.191
12	D-Sphingosine	19.6 (3.36)a	17.7 (1.8)ab	18.3 (2.55)ab	16.8 (0.987)b	0.094	0.173
12	D6-trans-Cinnamic Acid	16 (0.327)ab	16.2 (0.377)a	16.2 (0.38)a	15.8 (0.401)b	0.029	0.071
12	DL-3-aminoisobutryic acid	21.1 (1.67)a	18.8 (1.21)b	20.3 (0.63)a	20.1 (1.44)a	<0.01	<0.01
12	DL-Tryptophan	23.1 (2.28)a	23.8 (1)a	23.5 (1.39)a	23.7 (1.98)a	0.579	0.683
12	Dopamine	16.3 (1.45)a	16.9 (1.21)a	17.1 (0.735)a	16.8 (0.312)a	0.448	0.559
12	Ectoine	15.2 (1.82)a	15 (1.68)a	15.5 (1.32)a	14.9 (1.47)a	0.857	0.897
12	Equol	8.5 (0.868)a	8.45 (0.398)a	8.53 (0.402)a	8.49 (0.801)a	0.794	0.852
12	Ergothioneine	14.7 (2.12)a	13.7 (1.06)a	13.6 (1.07)a	14 (0.444)a	0.143	0.236
12	Ethanolamine	15.5 (1.07)a	16.5 (1.16)a	15.7 (1.25)a	15.8 (1.63)a	0.18	0.281
12	Ferulic Acid	18.1 (0.95)a	18.1 (2.11)a	18.3 (2.44)a	16.9 (1.76)a	0.31	0.421
12	Galactitol	18.1 (1.57)a	19 (3.81)a	17.8 (4.03)a	17 (1.31)a	0.215	0.319
12	Genistein	9.43 (3.22)ab	8.84 (1.44)a	8.78 (2.1)ab	11.1 (1.85)b	0.06	0.127
12	Glutamic Acid	24.2 (1.16)a	24.1 (1.06)a	24.3 (1.33)a	24.5 (0.805)a	0.595	0.696
12	Glutamine	20.7 (1.2)a	21.1 (1.1)a	21.1 (1.36)a	20.8 (1.87)a	0.669	0.748
12	Glutaric Acid	14.6 (1.09)a	14.5 (0.914)a	14.9 (0.703)a	15.1 (0.896)a	0.112	0.195
12	Glycine	19.3 (0.933)a	20.2 (1.18)b	20.5 (0.944)b	20 (0.502)ab	0.046	0.1
12	Glycitein	8.83 (1.02)a	8.97 (0.721)ab	8.75 (0.821)ab	9.37 (2.09)b	0.083	0.158
12	Hexanoic Acid	10.6 (4.2)a	10.2 (1.89)a	11.4 (1.94)a	10.9 (1.07)a	0.347	0.46
12	Histidine	18.2 (2.15)a	18.8 (1.51)a	17.9 (1.31)a	18.1 (1.32)a	0.751	0.817
12	Imidazolepropionic Acid	22.5 (0.824)a	21.8 (1.85)a	22.5 (1.12)a	22.6 (1.42)a	0.184	0.286
12	Indole-3-Acetic Acid	16.8 (2.21)a	15.9 (2.42)a	17.2 (1.47)a	17.1 (2.22)a	0.32	0.43

12	Indole-3-Lactic Acid	19.7 (5.76)a	18.5 (3.6)a	18 (3.11)a	17.3 (3.36)a	0.467	0.581
12	Indole-3-Propionic Acid	15.9 (6.14)a	18.6 (1.17)ab	19.9 (1.61)b	17.8 (3.09)a	0.022	0.058
12	Inosine	15.4 (2.06)a	17.7 (2.82)ab	16.7 (3.21)a	18.3 (1.8)b	<0.01	0.022
12	Isobutyric Acid	20.8 (2.15)a	20.1 (0.873)a	20.9 (1.5)a	20 (1.16)a	0.284	0.396
12	Isovaleric Acid	16.2 (2.2)a	16.9 (1.53)a	16.9 (1.82)a	17.3 (2.4)a	0.811	0.86
12	Jasmonic acid	16.8 (2.26)a	15.4 (1.37)a	16.1 (1.75)a	16.9 (2.62)a	0.186	0.286
12	Kynurenic Acid	20.5 (0.56)a	18.8 (2.05)b	20.2 (2.41)b	19.5 (2.02)b	<0.01	<0.01
12	L-Carnitine	19.8 (1.11)a	19.7 (2.08)a	19.8 (1.34)a	19.6 (0.937)a	0.946	0.962
12	L-DOPA	14.4 (2.53)a	14.1 (0.944)a	14.9 (0.982)a	14.5 (1.61)a	0.236	0.344
12	L-Kynurenine	15 (0.97)a	15.2 (0.978)a	15 (0.62)a	15.8 (1.21)a	0.107	0.19
12	L-Phenylalanine	25.4 (0.862)a	26.4 (1.38)a	25.9 (1.58)a	26.2 (1.48)a	0.165	0.267
12	L-Pipecolic Acid	23.8 (1.3)a	23.8 (2.3)a	23.4 (1.26)a	23.5 (1.13)a	0.975	0.986
12	L-Pyroglutamic Acid	19.2 (1.05)a	20 (1.58)a	19.6 (0.781)a	19.9 (1.86)a	0.203	0.307
12	L-Saccharophine	15.1 (2.19)a	15.1 (1.98)a	15.2 (1.53)a	15.3 (1.4)a	0.636	0.724
12	Lysine	19.9 (2.03)a	21.4 (1.14)b	20.8 (0.795)ab	21.3 (0.914)b	0.019	0.053
12	m-Hydroxy-Hydrocinnamic Acid	14.8 (2.65)a	14.3 (2.29)a	14.9 (2.82)a	14.9 (1.33)a	0.762	0.825
12	Methionine	23.9 (0.807)a	24.4 (1.12)a	24.1 (1.79)a	24.1 (1.32)a	0.421	0.534
12	Myo-Inositol	20.1 (1.6)a	20.6 (1.11)a	21.2 (2.05)a	19.8 (1.41)a	0.256	0.37
12	N-Acetylneuraminic Acid	18.8 (1.04)a	18.5 (2.88)a	17.9 (2.19)a	17.7 (1.54)a	0.271	0.384
12	N-Cinnamylglycine	12.4 (1.96)ab	12.7 (1.9)a	11.4 (1.48)ab	11.3 (0.668)b	0.015	0.041
12	N-Methylhistidine	15 (2.2)a	14 (2.16)a	14.4 (3.6)a	15.2 (2.61)a	0.499	0.608
12	N?-Acetylhistamine	19.2 (1.52)a	18.6 (2.52)a	18.6 (1.65)a	18.7 (1.12)a	0.669	0.748
12	N?,N?,N?-Trimethyllysine	17.9 (2.54)a	16.1 (3.64)a	17.6 (2.61)a	16.6 (3.2)a	0.389	0.503
12	N1,N12-Diacetylspermine	12.7 (1.71)a	12.3 (1.52)a	13.2 (1.63)a	13 (2.27)a	0.189	0.289
12	Neopterin	14.6 (2.22)a	14.3 (1.34)a	14.1 (0.895)a	15 (1.13)a	0.631	0.722
12	Nicotinamide	14.9 (3.49)a	16.5 (3.74)a	15.5 (1.02)a	16.1 (2.6)a	0.768	0.826

12	Nicotinic Acid	24.2 (2.51)a	23.7 (1.24)a	24.1 (1.05)a	24.5 (0.789)a	0.539	0.647
12	Oleic acid	14.9 (2.11)a	14.5 (3.8)a	15.3 (2.49)a	12.8 (3.05)a	0.286	0.396
12	Ornithine	15.1 (1.65)a	15.3 (1.83)a	15 (1.98)a	15.9 (1.18)a	0.444	0.555
12	p-Aminobenzoic Acid	14.4 (2.03)a	15.1 (1.14)a	14.5 (1.29)a	15.2 (1.48)a	0.414	0.531
12	Palmitoylcarnitine	16.5 (2.78)a	16 (3.12)a	14.9 (3.13)a	15.3 (2.36)a	0.167	0.267
12	Phenylacetic Acid	15.2 (1.61)a	14.6 (1.54)a	14.7 (1.47)a	15.2 (1.27)a	0.493	0.605
12	Phenylacetylglycine	12.6 (2.41)ab	12.9 (3.12)ab	14.7 (2.8)a	11.9 (2.92)b	0.062	0.13
12	Phloretic Acid	13.9 (1.64)a	12.4 (0.8)b	13.1 (1.37)ab	13 (1.39)ab	0.043	0.096
12	Piperine	9.51 (1.3)a	8.87 (1.75)a	9.47 (6.25)a	9.12 (1.81)a	0.924	0.946
12	Proline	23.7 (1.46)ab	24.9 (1.2)a	24.1 (1.5)ab	23.6 (1.88)b	0.028	0.071
12	Propionic Acid	22.3 (1.14)a	23.1 (1.85)a	23 (1.09)a	22.9 (1.71)a	0.351	0.462
12	Protocatechuic Acid	16.8 (1.7)a	14.2 (2.18)b	16.6 (3.32)ab	14.3 (2.5)b	0.022	0.058
12	Putrescine	19.7 (2.15)a	18.6 (1.05)a	19.7 (2.01)a	20.5 (3.41)a	0.307	0.418
12	Ralgin	11.5 (1.56)a	11 (0.422)a	11.4 (1.11)a	11.3 (1.78)a	0.185	0.286
12	Riboflavin	18.5 (1.02)a	18.5 (1.18)a	18.4 (0.903)a	18.2 (0.991)a	0.766	0.826
12	sarcosine	23.5 (1.04)a	23.7 (0.513)a	23.6 (0.902)a	23.3 (0.936)a	0.156	0.256
12	Sebacic Acid	15.8 (1.52)a	14.8 (1.08)a	15 (0.735)a	15.8 (0.76)a	0.079	0.154
12	Serine	20.5 (1.15)a	20.7 (0.871)a	20.8 (0.713)a	20.8 (1.23)a	0.581	0.683
12	Sinapinic Acid	15.1 (2.02)a	14 (1.67)a	15.3 (1.32)a	13.3 (2.23)a	0.088	0.165
12	Skatole	8.86 (0.557)a	9.23 (0.237)a	9.26 (0.413)a	9.32 (1.53)a	0.162	0.264
12	Spermidine	18.7 (5.76)a	20.7 (1.4)b	20.7 (2.59)b	21.2 (2.39)b	0.026	0.067
12	Spermine	11 (0.636)a	11.6 (1.34)ab	12.3 (2.22)b	12.1 (2.56)ab	0.066	0.134
12	Stachydrine	20.1 (4.17)a	17.8 (1.29)a	19 (5.61)a	18.3 (3.2)a	0.14	0.233
12	Syringic Acid	16.4 (2.55)a	13.5 (2.09)b	16.1 (2.68)a	16.7 (2.95)a	0.012	0.035
12	Taurine	21.8 (1.04)a	22.5 (1.08)a	22.1 (0.991)a	21.8 (0.642)a	0.102	0.184
12	trans-4-Hydroxyproline	19.2 (1.42)a	19.2 (1.56)a	19.3 (0.921)a	19.4 (1.56)a	0.833	0.876

12	trans-Cinnamic Acid	12.9 (1.21)a	12.7 (0.719)a	12.8 (0.737)a	12.3 (0.67)a	0.371	0.485
12	Trigonelline	20 (1.71)a	19.6 (1.17)a	18.7 (2.68)a	19.5 (1.48)a	0.503	0.61
12	Trimethylamine-N-oxide	14.9 (2.32)a	14.3 (2.05)a	14.4 (1.27)a	15 (1.72)a	0.239	0.347
12	Tyrosine	24.3 (0.809)a	24.7 (1.09)a	24.4 (0.968)a	24.6 (1.63)a	0.636	0.724
12	Uracil	22 (0.751)a	21.8 (0.613)a	22 (0.925)a	22 (1.81)a	0.76	0.825
12	Uric Acid	14.6 (1.15)a	17 (2.21)b	15.9 (1.01)ab	15.3 (2.6)ab	0.079	0.154
12	Urobilin	23.4 (1.39)a	23.3 (1.27)a	23.4 (1.6)a	23.5 (1.5)a	0.987	0.994
12	Urobilinogen	20.6 (3.16)a	20.6 (2.56)a	21.6 (1.57)a	22 (3.17)a	0.294	0.404
12	Valeric Acid	13.9 (2.54)a	16.4 (3.65)a	14.9 (2.64)a	16 (3.3)a	0.393	0.506
12	Valine	24.6 (1.41)a	24.9 (1.15)a	24.6 (1.24)a	24.1 (1.34)a	0.47	0.582
12	y-Glutamylphenylalanine	15.1 (1.88)a	15 (2)a	15.3 (1.77)a	15.4 (1.56)a	0.881	0.912

[1] Data are log transformed peak areas and presented as median (25^{th} quartile, 75^{th} quartile). Differences in diet were assessed by Kruskal-Wallis test on percent abundances. Post-hoc analysis of pairwise differences in diet were assessed by Dunn's test. Medians without a common letter differ. FDR calculated by Benjamini and Hochberg false discovery rate procedure. BF = Breast-fed, MF = milk formula fed, NLB = no longer breastfeeding, SF = soy formula fed.

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Supplementary Table 6: Fecal alpha-diversity indices at three, six, nine, and 12 months of age in infants fed with breastmilk or formula diets[1]

Diversity indices	Age	Diet	Time:Diet Interaction	Sex	Birth Weight
Observed	**	**			
Chao1		*			
Shannon		**		*	
Simpson		**		*	

[1]Differences in dietary intake assessed by two-way ANCOVA, blocked for gender, and birth weight as covariate. *P*-value provided for main effects of Age and Diet, interaction, blocking variable (Sex), and covariate (Birth weight). * P <0.05, ** P <0.01. Sample sizes range from 10 to 20 per diet group at three, six, nine and 12 months of age.

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Supplementary Table 7: Beta-diversity was altered by infant age and diet.[1]

Coefficients	Degrees of Freedom	Time	Index	F-model	R2	P_{adj}
Age	3	2.378	0.793	4.266	0.061	0.013
Diet	3	2.970	0.990	5.329	0.076	0.013
Gender	1	0.506	0.506	2.725	0.013	0.050
Birth Weight	1	0.245	0.245	1.319	0.006	0.478
Time:Diet	6	1.365	0.227	1.224	0.035	0.409
Residuals	169	31.402	0.186		0.808	
Total	183	38.867			1	

[1] Permutational Multivariate ANOVA (PERMANOVA) table output using the adonis() function from the R vegan package. Beta-diversity estimated using Bray-Curtis Dissimilarities. PERMANOVA tested main effects of age and diet, covariate (Birth weight), and blocking variable (Gender). P-values represented adjusted p-values based on Benjamini and Hochberg's false discovery rate correction.

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Supplementary Table 8: Principal component analysis of metabolites at three, six, nine and 12 months in infants fed with breastmilk, milk or soy formula diets[1].

Diet	diff	lwr	upr	p adj	Age	PC1	PC2
MF vs BF	5.718	3.511	7.926	<0.001	month 3	<0.001	0.020
SF vs BF	15.0312	13.157	16.904	<0.001	month 3	<0.001	0.020
SF vs MF	9.312	7.194	11.429	<0.001	month 3	<0.001	0.020
MF vs BF	-7.999	-11.135	-4.862	<0.001	month 6	<0.001	0.027
SF vs BF	-13.039	-16.326	-9.753	<0.001	month 6	<0.001	0.027
SF vs MF	-5.040	-8.067	-2.014	<0.001	month 6	<0.001	0.027
MF vs BF	-2.591	-6.569	1.385	0.262	month 9	<0.001	<0.001
SF vs BF	-8.978	-12.956	-5.001	<0.001	month 9	<0.001	<0.001
SF vs MF	-6.386	-10.564	-2.208	0.001	month 9	<0.001	<0.001
MF vs BF	4.978	-0.164	10.121	0.061	month 12	0.086	0.130
NLB vs BF	2.601	-3.032	8.235	0.611	month 12	0.086	0.130
SF vs BF	3.427	-1.715	8.570	0.298	month 12	0.086	0.130
NLB vs MF	-2.376	-8.010	3.256	0.677	month 12	0.086	0.130
SF vs MF	-1.551	-6.694	3.591	0.852	month 12	0.086	0.130
SF vs NLB	0.825	-4.808	6.459	0.979	month 12	0.086	0.130

[1]The column titled diff is the difference in means, lwr/upr are the 95th interval bounds, padj is the adjusted *P* value for the pairwise comparison, PC1 and PC2 are *P* values of the overall ANOVA. BF = Breast-fed, MF = milk formula fed, NLB = no longer breastfeeding, SF = soy formula fed.

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Supplementary Table 9: Significant Pearson's correlations between fecal genera level taxa and metabolites at three, six, nine and twelve months of age.[1]

3-Months				
Genus	**Metabolite**	**Coef**	**P**	**FDR**
Streptococcus	2-Phenylacetic Acid	0.685	<0.001	0.023
Streptococcus	3-Methylthiopropionic Acid	0.697	<0.001	0.020
SMB53	Azelaic Acid	0.649	<0.001	0.049
f__Ruminococcaceae	Azelaic Acid	0.648	<0.001	0.049
f__Clostridiaceae	Dihydroferulic Acid	0.672	<0.001	0.032
SMB53	Gentisic acid	0.702	<0.001	0.019
f__Ruminococcaceae	Gentisic acid	0.644	<0.001	0.049
f__Ruminococcaceae	Isocitric Acid	0.645	<0.001	0.049
Streptococcus	3-Methylxanthine	-0.814	<0.001	0.001
Veillonella	3-Methylxanthine	-0.705	<0.001	0.019
f__Ruminococcaceae	3-Methylxanthine	-0.743	<0.001	0.015
f__Clostridiaceae	3-Methylxanthine	-0.687	<0.001	0.023
Streptococcus	Caffeine	-0.727	<0.001	0.015
Veillonella	Caffeine	-0.642	<0.001	0.049
f__Peptostreptococcaceae	D6-trans-Cinnamic Acid	-0.662	<0.001	0.036
Streptococcus	D6-trans-Cinnamic Acid	-0.663	<0.001	0.036
SMB53	D6-trans-Cinnamic Acid	-0.728	<0.001	0.015
Streptococcus	Ethanolamine	-0.705	<0.001	0.019
SMB53	Ethanolamine	-0.726	<0.001	0.015
Streptococcus	Isovaleric Acid	0.669	<0.001	0.032
SMB53	Jasmonic acid	0.686	<0.001	0.023
Streptococcus	Phenylacetic Acid	0.681	<0.001	0.025
SMB53	Sebacic Acid	0.710	<0.001	0.019
f__Ruminococcaceae	Sebacic Acid	0.700	<0.001	0.019
f__Ruminococcaceae	Syringic Acid	0.642	<0.001	0.049
6-Months				
Genus	**Metabolite**	**Coef**	**P**	**FDR**
Oscillospira	(S)-3,4-Dihydroxybutyric Acid	-0.514	<0.001	0.011
Enterococcus	2-Hydroxy-3-methylbutyric Acid	0.431	0.003	0.040
f__Peptostreptococcaceae	2-Hydroxy-3-methylbutyric Acid	-0.457	0.002	0.029
f__Enterobacteriaceae	2-Hydroxy-3-methylbutyric Acid	0.446	0.002	0.033
SMB53	2-Hydroxy-3-methylbutyric Acid	-0.493	0.001	0.016
f__Clostridiaceae	2-Hydroxy-3-methylbutyric Acid	-0.423	0.004	0.045
f__Lachnospiraceae	2-Hydroxy-3-methylbutyric Acid	-0.451	0.002	0.031
Oscillospira	2-Hydroxy-3-methylbutyric Acid	-0.509	<0.001	0.013

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Coprococcus	2-Hydroxyadipic Acid	-0.508	<0.001	0.013
f__Peptostreptococcaceae	2-Hydroxyadipic Acid	-0.433	0.003	0.039
[Clostridium]	2-Hydroxyadipic Acid	-0.489	0.001	0.017
SMB53	2-Hydroxyadipic Acid	-0.488	0.001	0.018
f__Erysipelotrichaceae	2-Hydroxyadipic Acid	-0.471	0.001	0.024
f__Lachnospiraceae	2-Hydroxyadipic Acid	-0.528	<0.001	0.009
Oscillospira	2-Hydroxyadipic Acid	-0.650	<0.001	0.001
[Ruminococcus]	2-Oxoglutaric Acid	-0.451	0.002	0.031
f__Erysipelotrichaceae	2-Oxoglutaric Acid	-0.518	<0.001	0.011
f__Lachnospiraceae	2-Oxoglutaric Acid	-0.515	<0.001	0.011
f__Peptostreptococcaceae	2-Phenylacetic Acid	0.493	0.001	0.016
SMB53	2-Phenylacetic Acid	0.424	0.004	0.044
[Eubacterium]	2-Phenylacetic Acid	0.617	<0.001	0.001
f__Lachnospiraceae	2-Phenylacetic Acid	0.599	<0.001	0.002
Oscillospira	2-Phenylacetic Acid	0.520	<0.001	0.010
Oscillospira	3-Dehydroshikimic acid	-0.638	<0.001	0.001
f__Peptostreptococcaceae	3-Hydroxybutyric Acid	-0.459	0.002	0.028
f__Erysipelotrichaceae	3-Hydroxybutyric Acid	-0.460	0.002	0.028
[Eubacterium]	3-Hydroxybutyric Acid	-0.494	0.001	0.016
Oscillospira	3-Hydroxybutyric Acid	-0.606	<0.001	0.001
o__Clostridiales	3-Methyl-2-oxobutyric Acid	-0.497	0.001	0.016
f__Peptostreptococcaceae	3-Methyl-2-oxobutyric Acid	-0.449	0.002	0.031
SMB53	3-Methyl-2-oxobutyric Acid	-0.459	0.002	0.028
Bifidobacterium	3-Methyl-2-oxobutyric Acid	0.441	0.003	0.035
f__Ruminococcaceae	3-Methyl-2-oxobutyric Acid	-0.466	0.001	0.026
f__Erysipelotrichaceae	3-Methyl-2-oxobutyric Acid	-0.426	0.004	0.042
Blautia	3-Methyl-2-oxobutyric Acid	-0.513	<0.001	0.011
f__Lachnospiraceae	3-Methyl-2-oxobutyric Acid	-0.544	<0.001	0.006
f__Peptostreptococcaceae	3-Methylthiopropionic Acid	0.559	<0.001	0.004
[Ruminococcus]	3-Methylthiopropionic Acid	0.455	0.002	0.030
SMB53	3-Methylthiopropionic Acid	0.523	<0.001	0.010
f__Erysipelotrichaceae	3-Methylthiopropionic Acid	0.517	<0.001	0.011
[Eubacterium]	3-Methylthiopropionic Acid	0.604	<0.001	0.002
f__Lachnospiraceae	3-Methylthiopropionic Acid	0.567	<0.001	0.004
Oscillospira	3-Methylthiopropionic Acid	0.584	<0.001	0.003
Enterococcus	3-O-Methyl-Gallic Acid	-0.444	0.003	0.034
o__Clostridiales	3-O-Methyl-Gallic Acid	0.524	<0.001	0.010
Roseburia	3-O-Methyl-Gallic Acid	0.427	0.004	0.042
Blautia	3-O-Methyl-Gallic Acid	0.434	0.003	0.038
f__Erysipelotrichaceae	4-Hydroxybenzoic Acid	0.448	0.002	0.032

f__Peptostreptococcaceae	4-Hydroxyphenylacetic Acid	0.504	<0.001	0.014
[Clostridium]	4-Hydroxyphenylacetic Acid	0.479	0.001	0.021
SMB53	4-Hydroxyphenylacetic Acid	0.482	0.001	0.020
f__Lachnospiraceae	4-Hydroxyphenylacetic Acid	0.460	0.002	0.028
f__Peptostreptococcaceae	a-hydroxyisocaproic acid	-0.419	0.005	0.046
SMB53	a-hydroxyisocaproic acid	-0.490	0.001	0.017
f__Clostridiaceae	a-hydroxyisocaproic acid	-0.434	0.003	0.039
f__Peptostreptococcaceae	Adenine	-0.555	<0.001	0.005
SMB53	Adenine	-0.484	0.001	0.019
Enterococcus	Azelaic Acid	-0.441	0.003	0.035
o__Clostridiales	Azelaic Acid	0.547	<0.001	0.006
f__Peptostreptococcaceae	Azelaic Acid	0.586	<0.001	0.002
SMB53	Azelaic Acid	0.561	<0.001	0.004
Bifidobacterium	Azelaic Acid	-0.483	0.001	0.019
f__Erysipelotrichaceae	Azelaic Acid	0.427	0.004	0.042
Blautia	Azelaic Acid	0.453	0.002	0.030
f__Lachnospiraceae	Azelaic Acid	0.439	0.003	0.036
Oscillospira	Azelaic Acid	0.442	0.003	0.035
f__Peptostreptococcaceae	Citric Acid	-0.458	0.002	0.028
[Clostridium]	Citric Acid	-0.439	0.003	0.036
f__Erysipelotrichaceae	Citric Acid	-0.449	0.002	0.031
[Eubacterium]	Citric Acid	-0.542	<0.001	0.007
f__Lachnospiraceae	Citric Acid	-0.585	<0.001	0.002
Oscillospira	Citric Acid	-0.717	<0.001	<0.001
f__Peptostreptococcaceae	Cysteine	-0.434	0.003	0.039
SMB53	Cysteine	-0.446	0.002	0.033
f__Erysipelotrichaceae	Cysteine	-0.454	0.002	0.030
[Eubacterium]	Cysteine	-0.502	0.001	0.014
f__Lachnospiraceae	Cysteine	-0.609	<0.001	0.001
Oscillospira	Cysteine	-0.647	<0.001	0.001
f__Erysipelotrichaceae	Dihydro-Isoferulic acid-glucuronide	0.461	0.002	0.028
Enterococcus	Dihydrocaffeic acid	-0.450	0.002	0.031
Bifidobacterium	Dihydrocaffeic acid	-0.528	<0.001	0.009
[Eubacterium]	Dihydroferulic Acid	0.537	<0.001	0.007
Oscillospira	Dihydroferulic Acid	0.427	0.004	0.042
f__Peptostreptococcaceae	Dihydroferulic Acid-4-Sulfate	-0.423	0.004	0.045
SMB53	Dihydroferulic Acid-4-Sulfate	-0.446	0.002	0.033
[Eubacterium]	Dihydroferulic Acid-4-Sulfate	-0.451	0.002	0.031
f__Lachnospiraceae	Dihydroferulic Acid-4-Sulfate	-0.437	0.003	0.037
Oscillospira	Dihydroferulic Acid-4-Sulfate	-0.662	<0.001	<0.001

o__Clostridiales	Gentisic acid	0.422	0.004	0.045
f__Peptostreptococcaceae	Gentisic acid	0.432	0.003	0.039
[Ruminococcus]	Gentisic acid	0.431	0.004	0.040
SMB53	Gentisic acid	0.431	0.003	0.040
f__Erysipelotrichaceae	Gentisic acid	0.525	<0.001	0.010
f__Lachnospiraceae	Gentisic acid	0.513	<0.001	0.011
Oscillospira	Gluconic Acid	-0.468	0.001	0.025
Coprococcus	glucose	-0.458	0.002	0.028
[Clostridium]	glucose	-0.464	0.002	0.027
f__Erysipelotrichaceae	glucose	-0.530	<0.001	0.009
Blautia	glucose	-0.456	0.002	0.029
f__Lachnospiraceae	glucose	-0.576	<0.001	0.003
Oscillospira	glucose	-0.527	<0.001	0.009
f__Peptostreptococcaceae	GUDCA	0.438	0.003	0.036
[Ruminococcus]	GUDCA	0.488	0.001	0.018
[Eubacterium]	GUDCA	0.592	<0.001	0.002
Oscillospira	GUDCA	0.505	<0.001	0.014
o__Clostridiales	Hydroxyphenyllactic Acid	-0.469	0.001	0.025
f__Peptostreptococcaceae	Hydroxyphenyllactic Acid	-0.486	0.001	0.018
SMB53	Hydroxyphenyllactic Acid	-0.511	<0.001	0.012
f__Lachnospiraceae	Hydroxyphenyllactic Acid	-0.441	0.003	0.035
Oscillospira	Hydroxyphenyllactic Acid	-0.663	<0.001	<0.001
o__Clostridiales	Isocitric Acid	0.435	0.003	0.038
f__Bifidobacteriaceae	Isocitric Acid	-0.436	0.003	0.037
Bifidobacterium	Isocitric Acid	-0.445	0.002	0.033
f__Erysipelotrichaceae	Isoleucine	0.455	0.002	0.030
[Eubacterium]	Isoleucine	0.504	<0.001	0.014
f__Lachnospiraceae	Isoleucine	0.432	0.003	0.039
Oscillospira	Isoleucine	0.427	0.004	0.042
o__Clostridiales	Lactic Acid	-0.466	0.001	0.026
f__Peptostreptococcaceae	Lactic Acid	-0.540	<0.001	0.007
SMB53	Lactic Acid	-0.591	<0.001	0.002
f__Erysipelotrichaceae	Lactic Acid	-0.501	0.001	0.014
[Eubacterium]	Lactic Acid	-0.426	0.004	0.043
Blautia	Lactic Acid	-0.469	0.001	0.025
f__Lachnospiraceae	Lactic Acid	-0.663	<0.001	<0.001
Oscillospira	Lactic Acid	-0.637	<0.001	0.001
o__Clostridiales	m-hydroxy-hydrocinnamic acid	-0.537	<0.001	0.007
f__Peptostreptococcaceae	m-hydroxy-hydrocinnamic acid	-0.559	<0.001	0.004
f__Enterobacteriaceae	m-hydroxy-hydrocinnamic acid	0.517	<0.001	0.011
Roseburia	m-hydroxy-hydrocinnamic acid	-0.493	0.001	0.016

SMB53	m-hydroxy-hydrocinnamic acid	-0.566	<0.001	0.004
f__Lachnospiraceae	m-hydroxy-hydrocinnamic acid	-0.594	<0.001	0.002
Oscillospira	m-hydroxy-hydrocinnamic acid	-0.639	<0.001	0.001
Bifidobacterium	Methyl-2-oxovaleric Acid	0.441	0.003	0.035
f__Ruminococcaceae	Methyl-2-oxovaleric Acid	-0.417	0.005	0.048
Blautia	Methyl-2-oxovaleric Acid	-0.432	0.003	0.039
Coprococcus	Methylmalonic Acid	-0.619	<0.001	0.001
SMB53	Methylmalonic Acid	-0.461	0.002	0.028
Dorea	Methylmalonic Acid	-0.580	<0.001	0.003
f__Clostridiaceae	Methylmalonic Acid	-0.424	0.004	0.044
f__Lachnospiraceae	Methylmalonic Acid	-0.454	0.002	0.030
o__Clostridiales	o-Hydroxyhippuric acid	-0.432	0.003	0.039
[Ruminococcus]	o-Hydroxyhippuric acid	-0.462	0.002	0.028
SMB53	o-Hydroxyhippuric acid	-0.436	0.003	0.037
f__Ruminococcaceae	o-Hydroxyhippuric acid	-0.439	0.003	0.036
f__Erysipelotrichaceae	o-Hydroxyhippuric acid	-0.435	0.003	0.038
Blautia	o-Hydroxyhippuric acid	-0.432	0.003	0.039
f__Lachnospiraceae	o-Hydroxyhippuric acid	-0.670	<0.001	<0.001
Oscillospira	o-Hydroxyhippuric acid	-0.670	<0.001	<0.001
f__Peptostreptococcaceae	O-Phospho-L-serine	-0.465	0.001	0.026
Streptococcus	O-Phospho-L-serine	0.498	0.001	0.016
[Ruminococcus]	O-Phospho-L-serine	-0.552	<0.001	0.005
f__Erysipelotrichaceae	O-Phospho-L-serine	-0.441	0.003	0.035
[Eubacterium]	O-Phospho-L-serine	-0.496	0.001	0.016
f__Lachnospiraceae	O-Phospho-L-serine	-0.511	<0.001	0.012
Oscillospira	O-Phospho-L-serine	-0.685	<0.001	<0.001
f__Erysipelotrichaceae	Octadecanedioic Acid	0.434	0.003	0.038
Oscillospira	Orotic Acid	-0.495	0.001	0.016
Faecalibacterium	p-Coumaric acid	0.429	0.004	0.041
o__Clostridiales	Pyrocatechol	0.452	0.002	0.031
f__Peptostreptococcaceae	Pyrocatechol	0.507	<0.001	0.013
[Ruminococcus]	Pyrocatechol	0.482	0.001	0.019
Roseburia	Pyrocatechol	0.444	0.003	0.034
SMB53	Pyrocatechol	0.514	<0.001	0.011
f__Lachnospiraceae	Pyrocatechol	0.560	<0.001	0.004
o__Clostridiales	Pyruvic acid	-0.438	0.003	0.037
Coprococcus	Pyruvic acid	-0.457	0.002	0.029
f__Peptostreptococcaceae	Pyruvic acid	-0.539	<0.001	0.007
[Ruminococcus]	Pyruvic acid	-0.433	0.003	0.039
SMB53	Pyruvic acid	-0.566	<0.001	0.004
f__Ruminococcaceae	Pyruvic acid	-0.489	0.001	0.017

f__Erysipelotrichaceae	Pyruvic acid	-0.622	<0.001	0.001
[Eubacterium]	Pyruvic acid	-0.426	0.004	0.043
f__Lachnospiraceae	Pyruvic acid	-0.568	<0.001	0.004
Oscillospira	Pyruvic acid	-0.673	<0.001	<0.001
Coprococcus	Rutin	-0.424	0.004	0.044
Coprococcus	Shikimic Acid	-0.503	<0.001	0.014
f__Peptostreptococcaceae	Shikimic Acid	-0.439	0.003	0.036
[Clostridium]	Shikimic Acid	-0.421	0.004	0.045
Oscillospira	Shikimic Acid	-0.609	<0.001	0.001
[Eubacterium]	Sucrose	0.420	0.005	0.046
f__Peptostreptococcaceae	TCDCA	0.493	0.001	0.016
[Ruminococcus]	TCDCA	0.426	0.004	0.043
[Ruminococcus]	TDCA	0.453	0.002	0.030
Blautia	TDCA	0.491	0.001	0.017
Enterococcus	Tyrosol	-0.421	0.004	0.045
Coprococcus	Tyrosol	0.497	0.001	0.016
f__Peptostreptococcaceae	Tyrosol	0.443	0.003	0.034
Roseburia	Tyrosol	0.417	0.005	0.048
SMB53	Tyrosol	0.440	0.003	0.036
[Ruminococcus]	Uric Acid	-0.476	0.001	0.022
Enterococcus	(-)-Epicatechin	0.601	<0.001	0.002
[Ruminococcus]	1-Methylhydantoin	-0.507	<0.001	0.013
SMB53	1-Methylhydantoin	-0.440	0.003	0.036
Bifidobacterium	1-Methylhydantoin	0.620	<0.001	0.001
f__Erysipelotrichaceae	1-Methylhydantoin	-0.497	0.001	0.016
Oscillospira	1-Methylhydantoin	-0.607	<0.001	0.001
[Eubacterium]	1-Methyluric Acid	-0.452	0.002	0.031
Oscillospira	1-Methyluric Acid	-0.490	0.001	0.017
Faecalibacterium	2-Aminophenol	0.437	0.003	0.037
o__Clostridiales	3-Methylxanthine	-0.431	0.004	0.040
Coprococcus	3-Methylxanthine	-0.526	<0.001	0.009
f__Peptostreptococcaceae	3-Methylxanthine	-0.457	0.002	0.029
SMB53	3-Methylxanthine	-0.459	0.002	0.028
f__Erysipelotrichaceae	3-Methylxanthine	-0.593	<0.001	0.002
Blautia	3-Methylxanthine	-0.426	0.004	0.043
f__Lachnospiraceae	3-Methylxanthine	-0.612	<0.001	0.001
Oscillospira	3-Methylxanthine	-0.532	<0.001	0.008
o__Clostridiales	4-Hydroxyphenylpyruvic Acid	0.491	0.001	0.017
f__Peptostreptococcaceae	4-Hydroxyphenylpyruvic Acid	0.445	0.002	0.034
[Ruminococcus]	4-Hydroxyphenylpyruvic Acid	0.474	0.001	0.023
SMB53	4-Hydroxyphenylpyruvic Acid	0.443	0.003	0.035

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Bifidobacterium	4-Hydroxyphenylpyruvic Acid	-0.593	<0.001	0.002
f__Erysipelotrichaceae	4-Hydroxyphenylpyruvic Acid	0.447	0.002	0.033
Blautia	4-Hydroxyphenylpyruvic Acid	0.431	0.004	0.040
f__Lachnospiraceae	4-Hydroxyphenylpyruvic Acid	0.435	0.003	0.038
Coprococcus	4-Imidazoleacrylic Acid	0.421	0.004	0.045
f__Clostridiaceae	4-Imidazoleacrylic Acid	0.453	0.002	0.030
Oscillospira	4-Imidazoleacrylic Acid	0.463	0.002	0.028
Blautia	4-Imidazolecarboxylic Acid	-0.416	0.005	0.050
f__Lachnospiraceae	4-Imidazolecarboxylic Acid	-0.495	0.001	0.016
f__Peptostreptococcaceae	5-Hydroxytryptamine	0.423	0.004	0.045
[Ruminococcus]	5-Hydroxytryptamine	0.614	<0.001	0.001
[Clostridium]	5-Hydroxytryptamine	0.444	0.003	0.034
SMB53	5-Hydroxytryptamine	0.442	0.003	0.035
Bifidobacterium	5-Hydroxytryptamine	-0.591	<0.001	0.002
f__Erysipelotrichaceae	5-Hydroxytryptamine	0.522	<0.001	0.010
f__Lachnospiraceae	5-Hydroxytryptamine	0.531	<0.001	0.008
Oscillospira	5-Hydroxytryptamine	0.488	0.001	0.018
Parabacteroides	5-Hydroxytryptamine	-0.450	0.002	0.031
Roseburia	Asparagine	0.464	0.001	0.027
Blautia	Aspartic Acid	0.494	0.001	0.016
f__Lachnospiraceae	Aspartic Acid	0.480	0.001	0.020
Faecalibacterium	Aspartic Acid	0.469	0.001	0.025
[Eubacterium]	Betaine	-0.497	0.001	0.016
Oscillospira	Betaine	-0.568	<0.001	0.004
Dorea	C18-Carnitine	-0.428	0.004	0.042
f__Erysipelotrichaceae	C18-Carnitine	-0.422	0.004	0.045
f__Lachnospiraceae	C18-Carnitine	-0.478	0.001	0.021
Oscillospira	C18-Carnitine	-0.582	<0.001	0.003
f__Erysipelotrichaceae	Caffeine	-0.539	<0.001	0.007
Blautia	Caffeine	-0.461	0.002	0.028
f__Lachnospiraceae	Caffeine	-0.526	<0.001	0.009
Oscillospira	Caffeine	-0.460	0.002	0.028
Coprococcus	Creatine	-0.468	0.001	0.025
[Eubacterium]	Creatine	-0.455	0.002	0.030
f__Lachnospiraceae	Creatine	-0.460	0.002	0.028
Oscillospira	Creatine	-0.625	<0.001	0.001
Roseburia	Cystine	-0.421	0.004	0.045
f__Lachnospiraceae	Cystine	-0.587	<0.001	0.002
Oscillospira	D-Sphingosine	-0.493	0.001	0.016
o__Clostridiales	D6-trans-Cinnamic Acid	-0.437	0.003	0.037
Bifidobacterium	D6-trans-Cinnamic Acid	0.568	<0.001	0.004

Blautia	D6-trans-Cinnamic Acid	-0.481	0.001	0.020
Oscillospira	D6-trans-Cinnamic Acid	-0.437	0.003	0.037
[Ruminococcus]	Dopamine	0.472	0.001	0.024
f__Erysipelotrichaceae	Dopamine	0.459	0.002	0.028
f__Lachnospiraceae	Dopamine	0.571	<0.001	0.004
Coprococcus	Ergothioneine	-0.431	0.003	0.040
f__Lachnospiraceae	Ergothioneine	-0.432	0.003	0.039
Coprococcus	Ethanolamine	-0.445	0.002	0.033
f__Peptostreptococcaceae	Ethanolamine	-0.476	0.001	0.022
Bacteroides	Ethanolamine	0.631	<0.001	0.001
SMB53	Ethanolamine	-0.525	<0.001	0.009
f__Clostridiaceae	Ethanolamine	-0.492	0.001	0.017
Blautia	Ethanolamine	-0.484	0.001	0.019
f__Lachnospiraceae	Ethanolamine	-0.460	0.002	0.028
o__Clostridiales	Galactitol	-0.504	<0.001	0.014
SMB53	Galactitol	-0.469	0.001	0.025
o__Clostridiales	Genistein	0.488	0.001	0.018
f__Lachnospiraceae	Glutamic Acid	0.451	0.002	0.031
SMB53	Glutamine	0.424	0.004	0.044
o__Clostridiales	Glycine	-0.457	0.002	0.029
[Ruminococcus]	Glycine	-0.432	0.003	0.039
SMB53	Glycine	-0.423	0.004	0.044
f__Erysipelotrichaceae	Glycine	-0.472	0.001	0.024
Blautia	Glycine	-0.576	<0.001	0.003
f__Lachnospiraceae	Glycine	-0.619	<0.001	0.001
Oscillospira	Glycine	-0.449	0.002	0.031
Bifidobacterium	Glycitein	-0.461	0.002	0.028
Coprococcus	Indole-3-Acetic Acid	0.481	0.001	0.020
f__Peptostreptococcaceae	Indole-3-Acetic Acid	0.486	0.001	0.018
[Clostridium]	Indole-3-Acetic Acid	0.629	<0.001	0.001
SMB53	Indole-3-Acetic Acid	0.447	0.002	0.033
[Eubacterium]	Indole-3-Acetic Acid	0.436	0.003	0.037
f__Clostridiaceae	Indole-3-Acetic Acid	0.455	0.002	0.030
Oscillospira	Indole-3-Acetic Acid	0.427	0.004	0.042
o__Clostridiales	Indole-3-Lactic Acid	-0.450	0.002	0.031
f__Peptostreptococcaceae	Indole-3-Lactic Acid	-0.418	0.005	0.047
SMB53	Indole-3-Lactic Acid	-0.466	0.001	0.026
Bifidobacterium	Indole-3-Lactic Acid	0.487	0.001	0.018
f__Lachnospiraceae	Indole-3-Lactic Acid	-0.466	0.001	0.026
Oscillospira	Indole-3-Lactic Acid	-0.612	<0.001	0.001
Bifidobacterium	Inosine	-0.612	<0.001	0.001

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Coprococcus	Isobutyric Acid	0.456	0.002	0.029
f__Peptostreptococcaceae	Isobutyric Acid	0.459	0.002	0.028
[Ruminococcus]	Isobutyric Acid	0.458	0.002	0.028
Roseburia	Isobutyric Acid	0.457	0.002	0.029
SMB53	Isobutyric Acid	0.424	0.004	0.044
f__Ruminococcaceae	Isobutyric Acid	0.422	0.004	0.045
f__Erysipelotrichaceae	Isobutyric Acid	0.569	<0.001	0.004
[Eubacterium]	Isobutyric Acid	0.501	0.001	0.014
Blautia	Isobutyric Acid	0.473	0.001	0.023
f__Lachnospiraceae	Isobutyric Acid	0.635	<0.001	0.001
Oscillospira	Isobutyric Acid	0.558	<0.001	0.005
o__Clostridiales	Isovaleric Acid	0.431	0.004	0.040
Coprococcus	Isovaleric Acid	0.432	0.003	0.039
f__Peptostreptococcaceae	Isovaleric Acid	0.543	<0.001	0.007
[Ruminococcus]	Isovaleric Acid	0.440	0.003	0.036
Roseburia	Isovaleric Acid	0.444	0.003	0.034
SMB53	Isovaleric Acid	0.534	<0.001	0.008
f__Erysipelotrichaceae	Isovaleric Acid	0.552	<0.001	0.005
[Eubacterium]	Isovaleric Acid	0.553	<0.001	0.005
Blautia	Isovaleric Acid	0.449	0.002	0.032
f__Lachnospiraceae	Isovaleric Acid	0.649	<0.001	0.001
Oscillospira	Isovaleric Acid	0.609	<0.001	0.001
Bifidobacterium	Jasmonic acid	-0.447	0.002	0.033
Coprococcus	Kynurenic Acid	-0.420	0.005	0.046
Roseburia	L-Carnitine	-0.425	0.004	0.044
Blautia	L-Carnitine	-0.460	0.002	0.028
o__Clostridiales	Myo-Inositol	-0.431	0.004	0.040
f__Erysipelotrichaceae	Myo-Inositol	-0.446	0.002	0.033
f__Lachnospiraceae	Myo-Inositol	-0.570	<0.001	0.004
Oscillospira	Myo-Inositol	-0.520	<0.001	0.010
Coprococcus	N-Acetylneuraminic Acid	-0.538	<0.001	0.007
f__Erysipelotrichaceae	N-Acetylneuraminic Acid	-0.504	<0.001	0.014
f__Lachnospiraceae	N-Acetylneuraminic Acid	-0.504	<0.001	0.014
Oscillospira	N-Acetylneuraminic Acid	-0.488	0.001	0.018
o__Clostridiales	N-Cinnamylglycine	-0.445	0.002	0.033
Blautia	N-Cinnamylglycine	-0.451	0.002	0.031
f__Lachnospiraceae	N-Cinnamylglycine	-0.454	0.002	0.030
Oscillospira	N-Cinnamylglycine	-0.579	<0.001	0.003
Oscillospira	N1,N12-Diacetylspermine	-0.421	0.004	0.045
o__Clostridiales	Neopterin	-0.438	0.003	0.036
f__Erysipelotrichaceae	Neopterin	-0.501	0.001	0.015

Blautia	Neopterin	-0.485	0.001	0.018
f__Lachnospiraceae	Neopterin	-0.505	<0.001	0.014
Oscillospira	Neopterin	-0.473	0.001	0.023
f__Lachnospiraceae	Palmitoylcarnitine	-0.469	0.001	0.025
Oscillospira	Palmitoylcarnitine	-0.626	<0.001	0.001
f__Peptostreptococcaceae	Phenylacetic Acid	0.565	<0.001	0.004
[Ruminococcus]	Phenylacetic Acid	0.515	<0.001	0.011
Roseburia	Phenylacetic Acid	0.423	0.004	0.045
SMB53	Phenylacetic Acid	0.569	<0.001	0.004
f__Erysipelotrichaceae	Phenylacetic Acid	0.458	0.002	0.029
[Eubacterium]	Phenylacetic Acid	0.571	<0.001	0.004
f__Clostridiaceae	Phenylacetic Acid	0.457	0.002	0.029
f__Lachnospiraceae	Phenylacetic Acid	0.633	<0.001	0.001
Oscillospira	Phenylacetic Acid	0.645	<0.001	0.001
o__Clostridiales	Proline	-0.437	0.003	0.037
Coprococcus	Proline	-0.494	0.001	0.016
f__Peptostreptococcaceae	Proline	-0.494	0.001	0.016
Bacteroides	Proline	0.420	0.005	0.046
[Clostridium]	Proline	-0.421	0.004	0.045
SMB53	Proline	-0.514	<0.001	0.011
f__Ruminococcaceae	Proline	-0.551	<0.001	0.005
f__Erysipelotrichaceae	Proline	-0.428	0.004	0.042
f__Clostridiaceae	Proline	-0.472	0.001	0.024
Oscillospira	Proline	-0.472	0.001	0.024
Bacteroides	Propionic Acid	0.438	0.003	0.037
[Eubacterium]	Propionic Acid	0.486	0.001	0.018
f__Lachnospiraceae	Propionic Acid	0.422	0.004	0.045
Oscillospira	Propionic Acid	0.441	0.003	0.035
o__Clostridiales	sarcosine	-0.518	<0.001	0.011
Coprococcus	sarcosine	-0.522	<0.001	0.010
f__Peptostreptococcaceae	sarcosine	-0.531	<0.001	0.008
Roseburia	sarcosine	-0.451	0.002	0.031
SMB53	sarcosine	-0.535	<0.001	0.008
f__Ruminococcaceae	sarcosine	-0.494	0.001	0.016
f__Erysipelotrichaceae	sarcosine	-0.484	0.001	0.019
f__Clostridiaceae	sarcosine	-0.438	0.003	0.036
Blautia	sarcosine	-0.540	<0.001	0.007
f__Lachnospiraceae	sarcosine	-0.517	<0.001	0.011
Oscillospira	sarcosine	-0.484	0.001	0.019
o__Clostridiales	Sebacic Acid	0.419	0.005	0.046
f__Peptostreptococcaceae	Sebacic Acid	0.577	<0.001	0.003

SMB53	Sebacic Acid	0.554	<0.001	0.005
Oscillospira	Sebacic Acid	0.418	0.005	0.048
Bifidobacterium	Syringic Acid	-0.427	0.004	0.042
Oscillospira	Syringic Acid	0.464	0.001	0.027
o__Clostridiales	Trigonelline	-0.448	0.002	0.032
Coprococcus	Trigonelline	-0.468	0.001	0.025
Roseburia	Trigonelline	-0.454	0.002	0.030
f__Erysipelotrichaceae	Trigonelline	-0.491	0.001	0.017
Blautia	Trigonelline	-0.501	0.001	0.014
f__Lachnospiraceae	Trigonelline	-0.558	<0.001	0.005
Oscillospira	Trigonelline	-0.422	0.004	0.045
f__Peptostreptococcaceae	Tyrosine	0.508	<0.001	0.013
SMB53	Tyrosine	0.458	0.002	0.028
[Ruminococcus]	Uric Acid	-0.459	0.002	0.028
f__Erysipelotrichaceae	Uric Acid	-0.452	0.002	0.031
f__Lachnospiraceae	Uric Acid	-0.451	0.002	0.031
Oscillospira	Uric Acid	-0.467	0.001	0.026
[Ruminococcus]	Urobilin	0.607	<0.001	0.001
f__Erysipelotrichaceae	Urobilin	0.514	<0.001	0.011
f__Lachnospiraceae	Urobilin	0.471	0.001	0.024
Oscillospira	Urobilin	0.588	<0.001	0.002
[Ruminococcus]	Urobilinogen	0.529	<0.001	0.009
f__Erysipelotrichaceae	Urobilinogen	0.601	<0.001	0.002
f__Lachnospiraceae	Urobilinogen	0.427	0.004	0.042
Oscillospira	Urobilinogen	0.516	<0.001	0.011
[Eubacterium]	Valeric Acid	0.550	<0.001	0.005
f__Lachnospiraceae	Valeric Acid	0.462	0.002	0.028
Oscillospira	Valeric Acid	0.437	0.003	0.037
f__Ruminococcaceae	Valine	-0.523	<0.001	0.010
9-Months				
Genus	**Metabolite**	**Coef**	**P**	**FDR**
[Ruminococcus]	Hexadecanoic acid	-0.684	<0.001	0.037
f__Lachnospiraceae	Hexadecanoic acid	-0.678	<0.001	0.037
f__Lachnospiraceae	L-Saccharophine	-0.783	<0.001	0.001
12-Months				
Genus	**Metabolite**	**Coef**	**P**	**FDR**
f__Peptostreptococcaceae	Hydroxyphenyllactic Acid	-0.540	<0.001	0.033
f__Lachnospiraceae	Hydroxyphenyllactic Acid	-0.554	<0.001	0.030
f__Peptostreptococcaceae	Methyl-a-D-Glucopyranoside	-0.657	<0.001	0.001

SMB53	Methyl-a-D-Glucopyranoside	-0.545	<0.001	0.033
f__Peptostreptococcaceae	cis-11,12-Methylene Pentadecanoylcarnitine	-0.554	<0.001	0.030
Bacteroides	Lysine	-0.682	<0.001	<0.001

[1]Genera counts were transformed using a centered-log ratio transformation prior to correlation. Zeros were imputed using the geometric Bayesian multiplicative method. Metabolomics data were log transformed. False discovery rate correction was used to adjust P-values for multiple comparisons. Abbreviations: Coef: Pearson's r coefficient; FDR: False discovery rate.