Supplementary Table S1. Modulation of EA.hy926 cell metabolome by shRNA silencing and I3MT-3 treatment. Numbers represent fold changes in metabolite concentrations; **Red** and **green** shaded cells indicate p ≤ 0.05 (**red** indicates that the mean values are significantly higher for that comparison; **green** indicates values that are significantly lower). Light red and light green shaded cells indicate 0.05 < p< 0.10 (light red indicates that the mean values trend higher for that comparison; light green values trend lower).* indicates compounds that have not been officially confirmed based on a standard, but the Metabolon company is confident in its identity.

Super Pathway	Sub Pathway	Biochemical Name	sh3-MST *vs.* sh NT	p-value	I3MT-3 *vs.* sh NT	p-value
Amino Acid	Glycine, Serine and Threonine Metabolism	glycine	1.13	0.1647	1.37	0.0010
		N-acetylglycine	1.37	0.0547	2.20	<0,0001
		sarcosine	1.19	0.7732	4.03	0.0089
		dimethylglycine	1.04	0.7011	1.24	0.0124
		betaine	1.05	0.5948	0.90	0.1992
		serine	1.41	0.0006	1.12	0.1816
		N-acetylserine	1.15	0.1669	0.98	0.8150
		threonine	1.10	0.2627	1.12	0.1677
		N-acetylthreonine	1.13	0.1985	0.94	0.4999
	Alanine and Aspartate Metabolism	alanine	0.96	0.6149	1.11	0.4070
		N-acetylalanine	1.03	0.7222	1.59	0.0001
		aspartate	1.11	0.2617	0.91	0.2745
		N-acetylaspartate (NAA)	0.69	0.0011	1.03	0.7408
		asparagine	1.31	0.0033	1.21	0.0291
		N-acetylasparagine	1.17	0.2052	1.01	0.9313
	Glutamate Metabolism	glutamate	1.11	0.2034	0.93	0.3526
		glutamine	1.03	0.7180	1.06	0.4786
		N-acetylglutamate	1.04	0.7117	1.43	0.0002
		N-acetylglutamine	1.24	0.0466	0.93	0.5620
		4-hydroxyglutamate	0.99	0.9539	0.98	0.9034
		glutamate, gamma-methyl ester	0.86	0.2713	0.71	0.0169
		pyroglutamine*	1.31	0.0059	1.27	0.0142
		N-acetyl-aspartyl-glutamate (NAAG)	0.78	0.0091	1.24	0.0128
		beta-citrylglutamate	1.17	0.1078	1.26	0.0190
		carboxyethyl-GABA	1.01	0.8830	0.86	0.0239
		S-1-pyrroline-5-carboxylate	2.37	0.0003	1.13	0.3498
	Histidine Metabolism	histidine	1.06	0.5407	1.29	0.0073
		1-methylhistidine	0.72	0.0706	1.12	0.4018
		3-methylhistidine	0.85	0.4403	1.51	0.0497
		N-acetylhistidine	1.16	0.0994	1.16	0.1185
		imidazole propionate	1.12	0.4010	2.88	<0,0001
		imidazole lactate	1.15	0.2219	1.82	<0,0001
		carnosine	0.74	0.0229	0.94	0.5689
		1-methyl-4-imidazoleacetate	1.28	0.0431	1.64	0.0005
		1-ribosyl-imidazoleacetate*	1.41	0.1950	10.13	<0,0001
		4-imidazoleacetate	1.49	0.0285	2.09	0.0002
		histidine methyl ester	0.95	0.5459	1.03	0.8842
	Lysine Metabolism	lysine	1.35	0.0032	1.02	0.7837
		N6-acetyllysine	1.63	<0,0001	1.21	0.0286
		N6,N6,N6-trimethyllysine	1.20	0.1565	1.12	0.3667
		5-hydroxylysine	1.09	0.7613	0.99	0.9869
		5-(galactosylhydroxy)-L-lysine	1.72	<0,0001	1.15	0.1288
		2-aminoadipate	0.85	0.0744	1.06	0.4613
		pipecolate	0.99	0.8160	1.12	0.2041
		6-oxopiperidine-2-carboxylate	0.68	0.0039	1.18	0.2158
		cadaverine	0.97	0.6821	0.69	0.0552
		N-acetyl-cadaverine	0.79	0.1733	0.78	0.2508
		5-aminovalerate	1.10	0.2646	1.07	0.3692

	N-trimethyl 5-aminovalerate	1.55	0.0007	1.07	0.6011
Phenylalanine Metabolism	phenylalanine	1.17	0.0563	1.18	0.0328
	N-acetylphenylalanine	0.91	0.3131	1.19	0.0761
	phenyllactate (PLA)	0.76	0.0094	1.06	0.5588
Tyrosine Metabolism	tyrosine	1.07	0.5237	1.12	0.3027
	3-(4-hydroxyphenyl)lactate	0.80	0.0479	1.17	0.1325
	phenol sulfate	2.09	0.0003	0.47	0.0003
	3-methoxytyrosine	0.58	0.0352	1.08	0.6678
	O-methyltyrosine	1.00	0.8346	0.92	0.3776
	tyramine O-sulfate	1.35	0.0296	1.03	0.7656
	N-formylphenylalanine	1.01	0.8817	0.68	0.5189
Tryptophan Metabolism	tryptophan	1.04	0.6226	1.19	0.0516
	C-glycosyltryptophan	2.01	<0,0001	0.99	0.9191
	kynurenine	1.00	0.9947	1.40	0.0014
	serotonin	1.05	0.6486	1.28	0.1577
	5-hydroxyindoleacetate	1.67	0.2369	1.80	0.1276
	indolelactate	0.89	0.2300	1.20	0.0509
	indoleacetate	1.47	0.0541	0.71	0.1588
Leucine, Isoleucine and Valine Metabolism	leucine	1.15	0.0884	1.17	0.0511
	N-acetylleucine	1.01	0.8607	1.39	0.0038
	4-methyl-2-oxopentanoate	0.64	0.1040	0.64	0.2055
	alpha-hydroxyisocaproate	1.00	1.0000	1.12	0.0961
	isovalerylcarnitine (C5)	1.95	<0,0001	0.49	<0,0001
	beta-hydroxyisovalerate	1.37	0.0082	0.89	0.3418
	3-methylglutaconate	0.80	0.0671	0.72	0.0102
	isoleucine	0.98	0.7981	1.25	0.0156
	N-acetylisoleucine	0.89	0.3344	1.40	0.0450
	3-methyl-2-oxovalerate	0.50	0.0267	0.64	0.2678
	alpha-hydroxyisovalerate	0.69	0.1241	1.13	0.3924
	2-methylbutyrylcarnitine (C5)	1.39	0.0066	0.32	<0,0001
	2-methylbutyrylglycine	1.50	0.0828	0.72	0.3227
	tiglylcarnitine (C5:1-DC)	1.15	0.3991	0.47	<0,0001
	3-hydroxy-2-ethylpropionate	1.06	0.8298	1.00	0.9654
	ethylmalonate	0.65	0.0069	2.97	<0,0001
	methylsuccinate	0.70	0.0035	0.78	0.0340
	valine	1.12	0.2697	1.26	0.0256
	N-acetylvaline	0.94	0.6025	1.11	0.3228
	3-methyl-2-oxobutyrate	0.57	0.0123	0.75	0.2086
	isobutyrylcarnitine (C4)	1.23	0.3005	0.38	<0,0001
	3-hydroxyisobutyrate	1.07	0.6640	0.72	0.0125
	2,3-dihydroxy-2-methylbutyrate	1.92	0.0020	10.52	<0,0001
Methionine, Cysteine, SAM and Taurine Metabolism	methionine	1.29	0.0034	1.16	0.0685
	N-acetylmethionine	1.13	0.2070	1.03	0.8037
	N-formylmethionine	0.81	0.0380	0.95	0.6315
	methionine sulfone	1.06	0.6525	1.18	0.1184
	methionine sulfoxide	1.36	0.0093	1.34	0.0223
	N-acetylmethionine sulfoxide	1.23	0.2245	1.37	0.1242
	S-adenosylmethionine (SAM)	1.02	0.9618	1.02	0.8416
	S-adenosylhomocysteine (SAH)	0.64	0.0042	0.64	0.0049
	homocysteine	2.39	0.0000	1.12	0.2173
	cystathionine	1.12	0.1308	1.36	0.0003
	cysteine	1.14	0.1627	1.23	0.0321
	N-acetylcysteine	1.15	0.4433	1.92	0.0019
	S-methylcysteine	0.86	0.2984	1.64	0.0194
	cystine	0.78	0.4122	1.65	0.2222

		lanthionine	0.64	0.0322	4.10	<0,0001
		cysteine sulfinic acid	1.15	0.2330	1.29	0.0361
		hypotaurine	1.65	0.0002	1.26	0.0406
		taurine	1.79	0.0004	1.13	0.3888
		N-acetyltaurine	1.30	0.0676	0.91	0.4647
		3-sulfo-L-alanine	1.09	0.4399	1.34	0.0089
	Urea cycle; Arginine and Proline Metabolism	arginine	1.45	0.0005	1.03	0.7668
		argininosuccinate	1.28	0.3211	0.89	0.6453
		ornithine	1.43	0.0050	1.21	0.1018
		2-oxoarginine*	1.42	0.0854	2.72	<0,0001
		citrulline	1.00	0.8598	0.94	0.6779
		homoarginine	1.05	0.7557	1.12	0.5781
		homocitrulline	0.73	0.0661	1.32	0.1260
		proline	1.10	0.3261	1.21	0.0473
		dimethylarginine (SDMA + ADMA)	1.34	0.1131	0.91	0.7013
		N-acetylarginine	1.16	0.0857	1.30	0.0042
		N-delta-acetylornithine	0.93	0.5712	1.13	0.5058
		trans-4-hydroxyproline	1.15	0.1308	0.99	0.8530
		pro-hydroxy-pro	1.20	0.8429	2.17	0.1013
		N-methylproline	0.98	0.8046	1.00	0.8801
		N-monomethylarginine	1.53	0.0026	1.04	0.7129
	Creatine Metabolism	creatine	1.30	0.0044	0.94	0.4546
		creatinine	1.10	0.3249	0.95	0.5501
	Polyamine Metabolism	putrescine	1.06	0.8233	0.82	0.1645
		spermidine	1.30	0.0305	1.02	0.8105
		N('1)-acetylspermidine	1.08	0.9046	1.76	0.0005
		N(1)-acetylspermine	0.97	0.8119	2.50	0.0010
		N1,N12-diacetylspermine	1.00	1.0000	1.11	0.0961
		5-methylthioadenosine (MTA)	0.93	0.4336	0.78	0.0192
		N-acetylputrescine	0.89	0.2441	0.93	0.5812
		4-acetamidobutanoate	0.76	0.1273	1.74	0.0032
		N(8)-acetylspermidine	0.99	0.6856	0.95	0.7542
	Guanidino and Acetamido Metabolism	1-methylguanidine	1.00	1.0000	1.00	1.0000
		4-guanidinobutanoate	1.43	0.0426	1.63	0.0063
	Glutathione Metabolism	glutathione, reduced (GSH)	1.06	0.7378	0.92	0.7240
		glutathione, oxidized (GSSG)	1.18	0.2432	1.01	0.9201
		cysteine-glutathione disulfide	1.24	0.0870	1.49	0.0025
		S-methylglutathione	1.54	0.0538	1.10	0.5388
		cysteinylglycine	1.09	0.3680	0.78	0.0108
		5-oxoproline	1.00	0.9433	1.05	0.6431
		2-hydroxybutyrate/2-hydroxyisobutyrate	0.79	0.1779	0.92	0.7335
		ophthalmate	1.59	0.0001	0.67	0.0002
		S-nitrosoglutathione (GSNO)	0.81	0.1596	1.02	0.8452
		4-hydroxy-nonenal-glutathione	1.27	0.4776	0.74	0.1294
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamylcysteine	0.63	0.0019	0.61	0.0013
		gamma-glutamylglutamate	0.77	0.0521	0.92	0.5635
		gamma-glutamylglutamine	0.76	0.0570	1.07	0.5272
		gamma-glutamylglycine	0.81	0.3847	0.99	0.8668
		gamma-glutamylhistidine	0.65	0.1302	0.62	0.1423
		gamma-glutamylisoleucine*	0.77	0.0020	1.19	0.0360
		gamma-glutamylleucine	0.81	0.0522	0.90	0.3641
		gamma-glutamyl-epsilon-lysine	0.93	0.4292	0.71	0.0007
		gamma-glutamylmethionine	0.87	0.4318	1.00	0.8734
		gamma-glutamylphenylalanine	0.68	0.0055	1.00	0.9397
		gamma-glutamylthreonine	1.09	0.5878	0.48	<0,0001

		gamma-glutamyltryptophan	0.70	0.0024	1.34	0.0085
		gamma-glutamyltyrosine	0.87	0.4630	1.26	0.0843
		gamma-glutamylvaline	0.69	0.0013	0.92	0.4397
	Dipeptide	alanylleucine	2.17	0.0166	0.69	0.0890
		glycylisoleucine	2.64	<0,0001	2.18	0.0004
		glycylleucine	3.72	<0,0001	1.87	0.0003
		glycylvaline	2.93	<0,0001	1.55	0.0031
		isoleucylglycine	2.26	<0,0001	1.21	0.1456
		leucylglycine	2.46	0.0002	1.19	0.4027
		phenylalanylalanine	4.39	<0,0001	1.90	0.0139
		phenylalanylglycine	3.35	<0,0001	1.58	0.0109
		prolylglycine	2.26	<0,0001	1.38	0.0030
		threonylphenylalanine	2.64	0.0005	0.97	0.6897
		tryptophylglycine	3.62	<0,0001	1.76	0.0030
		tyrosylglycine	3.49	<0,0001	1.62	0.0043
		valylglutamine	1.72	0.0015	0.85	0.2869
		valylglycine	3.36	<0,0001	1.74	0.0069
		valylleucine	1.29	0.5135	0.62	0.0817
		leucylglutamine*	1.11	0.4701	0.58	0.0002
	Acetylated Peptides	phenylacetylglycine	1.00	0.9421	1.04	0.9300
Carbo-hydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	glucose	1.73	0.2798	0.56	0.2298
		glucose 6-phosphate	1.58	0.1613	1.12	0.7279
		glucose 1-phosphate	6.25	0.0268	0.93	0.9511
		fructose 1,6-diphosphate/glucose 1,6-diphosphate	16.99	<0,0001	1.63	0.2990
		dihydroxyacetone phosphate (DHAP)	2.56	0.0011	1.19	0.5170
		3-phosphoglycerate	2.22	0.0049	1.27	0.2902
		phosphoenolpyruvate (PEP)	1.24	0.3663	0.61	0.0337
		pyruvate	0.65	0.0170	0.83	0.3321
		lactate	1.24	0.0770	0.83	0.2044
		glycerate	1.11	0.5255	1.75	0.0568
	Pentose Phosphate Pathway	6-phosphogluconate	4.91	0.0193	0.96	0.2765
		ribose 1-phosphate	0.72	0.0382	0.93	0.6777
		sedoheptulose-7-phosphate	2.02	0.0111	2.54	0.0021
	Pentose Metabolism	ribose	0.91	0.3895	0.87	0.1868
		ribitol	0.71	0.0004	1.05	0.5700
		ribonate	0.86	0.1557	0.85	0.1321
		arabonate/xylonate	1.03	0.6383	0.53	0.0006
		ribulonate/xylulonate*	0.85	0.1707	0.70	0.0035
	Disaccharides and Oligosaccharides	lactose	1.16	0.3517	0.77	0.1820
	Fructose, Mannose and Galactose Metabolism	fructose	1.31	0.2920	0.83	0.3737
		mannitol/sorbitol	1.14	0.3096	0.83	0.1138
		galactitol (dulcitol)	1.12	0.1950	1.08	0.3656
		galactose 1-phosphate	2.10	0.0509	0.95	0.9437
		galactonate	0.77	0.0853	1.02	0.8464
	Nucleotide Sugar	UDP-glucose	4.09	0.0186	1.48	0.7596
		UDP-galactose	1.73	0.0259	1.09	0.8980
		UDP-glucuronate	1.30	0.0402	1.03	0.7428
		guanosine 5'-diphospho-fucose	1.45	0.0033	1.30	0.0284
		UDP-N-acetylglucosamine/galactosamine	1.02	0.8260	1.22	0.0218
		cytidine 5'-monophospho-N-acetylneuraminic acid	1.23	0.2080	0.92	0.4928
	Aminosugar Metabolism	glucuronate	1.69	0.0006	1.00	0.8573
		N-acetylglucosamine 6-phosphate	1.07	0.8413	1.09	0.7146
		N-acetyl-glucosamine 1-phosphate	0.77	0.2242	1.13	0.9505
		N-acetylneuraminate	1.50	0.0012	0.92	0.5376
		N-acetylglucosaminylasparagine	1.27	0.0046	1.17	0.0386

		erythronate*	0.73	0.0035	1.49	0.0004
		N-acetylglucosamine/N-acetylgalactosamine	0.79	0.1207	1.29	0.0743
Energy	TCA Cycle	citrate	1.36	0.1065	1.19	0.3472
		aconitate [cis or trans]	1.83	0.0187	1.28	0.2834
		alpha-ketoglutarate	0.93	0.5305	0.85	0.1825
		succinylcarnitine (C4-DC)	1.39	0.0047	0.55	<0,0001
		succinate	0.92	0.3696	1.19	0.0805
		fumarate	0.85	0.2776	0.73	0.0549
		malate	1.20	0.0699	1.14	0.1529
		2-methylcitrate/homocitrate	0.93	0.5051	1.06	0.5498
	Oxidative Phosphorylation	phosphate	1.03	0.8519	1.03	0.7423
Lipid	Fatty Acid Metabolism	arachidonoyl CoA	3.91	0.0003	2.35	0.0071
	Medium Chain Fatty Acid	caprylate (8:0)	1.47	0.4519	0.48	0.3224
		laurate (12:0)	1.16	0.2759	1.00	0.9715
		5-dodecenoate (12:1n7)	1.61	0.2769	1.36	0.4715
	Long Chain Fatty Acid	myristate (14:0)	0.88	0.9419	0.57	0.1378
		myristoleate (14:1n5)	1.20	0.2207	0.64	0.0137
		pentadecanoate (15:0)	1.07	0.6439	0.69	0.4046
		palmitate (16:0)	0.99	0.8167	0.73	0.3568
		palmitoleate (16:1n7)	0.90	0.9859	0.55	0.2348
		margarate (17:0)	0.96	0.8238	0.69	0.3767
		10-heptadecenoate (17:1n7)	0.90	0.9694	0.55	0.2769
		stearate (18:0)	1.07	0.5479	0.85	0.6265
		oleate/vaccenate (18:1)	0.93	0.9673	0.63	0.2702
		nonadecanoate (19:0)	0.98	0.7420	0.83	0.6542
		10-nonadecenoate (19:1n9)	0.98	0.8152	0.68	0.3732
		arachidate (20:0)	0.97	0.8060	0.86	0.7281
		eicosenoate (20:1)	0.92	0.9696	0.63	0.1858
		erucate (22:1n9)	0.87	0.7549	0.49	0.0267
	Polyunsaturated Fatty Acid (n3 and n6)	eicosapentaenoate (EPA; 20:5n3)	1.87	0.3519	1.48	0.4014
		docosapentaenoate (n3 DPA; 22:5n3)	2.23	0.2478	1.61	0.3569
		docosahexaenoate (DHA; 22:6n3)	2.13	0.2541	1.63	0.3091
		docosatrienoate (22:3n3)	1.54	0.3238	1.25	0.5108
		nisinate (24:6n3)	1.32	0.4855	0.72	0.4799
		linoleate (18:2n6)	1.02	0.8849	0.59	0.3321
		linolenate [alpha or gamma; (18:3n3 or 6)]	1.21	0.6335	0.55	0.2410
		dihomo-linolenate (20:3n3 or n6)	1.87	0.2594	1.70	0.2313
		arachidonate (20:4n6)	1.92	0.3766	1.53	0.4187
		adrenate (22:4n6)	2.92	0.2735	1.72	0.4737
		docosapentaenoate (n6 DPA; 22:5n6)	2.22	0.2307	1.71	0.2589
		docosadienoate (22:2n6)	1.05	0.7720	0.71	0.3326
		dihomo-linoleate (20:2n6)	1.20	0.5472	0.82	0.7332
		mead acid (20:3n9)	2.00	0.2573	1.51	0.3458
		docosatrienoate (22:3n6)*	1.76	0.3546	1.03	0.8570
	Fatty Acid, Branched	13-methylmyristate (i15:0)	1.29	0.3500	0.70	0.2870
		15-methylpalmitate (i17:0)	0.94	0.8339	0.66	0.3095
		17-methylstearate (i19:0)	0.87	0.8712	0.76	0.6175
	Fatty Acid, Dicarboxylate	dimethylmalonic acid	1.00	1.0000	1.00	1.0000
		glutarate (C5-DC)	0.93	0.5689	1.95	<0,0001
		2-hydroxyglutarate	0.82	0.0629	0.71	0.0034
		2-hydroxyadipate	0.75	0.2074	0.87	0.4948
		maleate	0.52	0.0016	0.51	0.0011
		azelate (C9-DC)	1.47	0.0264	0.98	0.9932
		dodecadienoate (12:2)*	1.23	0.7411	0.21	0.0767
	Fatty Acid Metabolism (also BCAA Metabolism)	butyrylcarnitine (C4)	1.83	0.0032	1.17	0.2621

(also BCAA Metabolism)	propionylcarnitine (C3)	4.35	<0,0001	0.88	0.8993
Fatty Acid, Acyl Glycine	N-palmitoylglycine	1.29	0.2887	1.25	0.3009
	3-hydroxybutyroylglycine**	0.91	0.4265	0.92	0.6546
Fatty Acid, Acyl Carnitine	acetylcarnitine (C2)	2.30	0.0001	1.23	0.1585
	3-hydroxybutyrylcarnitine (1)	0.65	0.2570	1.76	0.2238
	3-hydroxybutyrylcarnitine (2)	1.20	0.0378	1.89	<0,0001
	hexanoylcarnitine (C6)	0.76	0.0100	0.76	0.0100
	octanoylcarnitine (C8)	3.20	0.0961	1.00	1.0000
	laurylcarnitine (C12)	1.91	0.0961	1.00	1.0000
	myristoylcarnitine (C14)	2.20	0.0003	0.91	0.6843
	palmitoylcarnitine (C16)	1.45	0.0375	0.94	0.8387
	palmitoleoylcarnitine (C16:1)*	2.90	<0,0001	1.06	0.7216
	stearoylcarnitine (C18)	1.21	0.0824	1.08	0.4665
	linoleoylcarnitine (C18:2)*	4.32	<0,0001	1.25	0.3206
	linolenoylcarnitine (C18:3)*	6.18	<0,0001	0.86	0.7125
	oleoylcarnitine (C18:1)	2.54	0.0001	1.16	0.4557
	myristoleoylcarnitine (C14:1)*	1.61	0.0961	1.00	1.0000
	arachidoylcarnitine (C20)*	1.20	0.0312	1.14	0.1097
	arachidonoylcarnitine (C20:4)	3.76	0.0007	1.27	0.4112
	behenoylcarnitine (C22)*	1.00	1.0000	1.00	1.0000
	dihomo-linolenoylcarnitine (C20:3n3 or 6)*	3.06	0.0001	1.62	0.0412
	dihomo-linoleoylcarnitine (C20:2)*	2.21	0.0191	1.34	0.3680
	eicosenoylcarnitine (C20:1)*	1.39	0.0032	1.21	0.0703
	docosapentaenoylcarnitine (C22:5n3)*	4.00	0.0001	1.19	0.5507
	docosahexaenoylcarnitine (C22:6)*	3.83	<0,0001	1.11	0.6078
	lignoceroylcarnitine (C24)*	1.00	1.0000	1.06	0.1540
	margaroylcarnitine (C17)*	1.28	0.0733	1.02	0.8951
	cerotoylcarnitine (C26)*	1.00	1.0000	1.00	1.0000
	ximenoylcarnitine (C26:1)*	1.00	1.0000	1.00	1.0000
	3-hydroxypalmitoylcarnitine	1.31	0.1327	1.02	0.8314
Carnitine Metabolism	deoxycarnitine	1.29	0.0028	0.95	0.4750
	carnitine	1.19	0.0693	0.86	0.0993
Ketone Bodies	3-hydroxybutyrate (BHBA)	0.89	0.5912	1.10	0.4836
Fatty Acid Metabolism (Acyl Choline)	palmitoylcholine	1.22	0.5573	2.09	0.0046
	docosahexaenoylcholine	1.21	0.1860	1.18	0.1622
Fatty Acid, Monohydroxy	4-hydroxybutyrate (GHB)	1.14	0.2692	1.35	0.0205
	2-hydroxydecanoate	1.31	0.5919	1.43	0.2513
	2-hydroxypalmitate	0.95	0.9896	0.91	0.9433
	2-hydroxystearate	0.91	0.9913	0.88	0.8000
	3-hydroxylaurate	1.86	0.0001	1.16	0.1858
	3-hydroxymyristate	1.42	0.2321	0.64	0.2503
	13-HODE + 9-HODE	0.87	0.5350	0.39	0.0197
	3-hydroxystearate	0.81	0.8621	0.87	0.9134
Endocannabinoid	oleoyl ethanolamide	0.97	0.9556	0.59	0.0731
	docosahexaenoyl ethanolamide	0.88	0.4033	0.83	0.2550
	arachidonoyl ethanolamide	1.50	0.0228	0.78	0.1437
	N-myristoyltaurine*	1.43	0.1542	0.91	0.8087
	N-arachidonoyltaurine	1.25	0.3510	1.10	0.6136
	N-oleoyltaurine	1.19	0.4261	0.91	0.7684
	N-stearoyltaurine	1.67	0.0831	0.81	0.5585
	N-palmitoyltaurine	1.44	0.1715	0.83	0.5891
	linoleoyl ethanolamide	0.84	0.7226	0.71	0.5004
	palmitoleoyl ethanolamide*	0.70	0.0188	0.81	0.1447
	N-oleoylserine	1.11	0.6230	0.60	0.1117
Inositol Metabolism	myo-inositol	0.96	0.6238	1.18	0.1264

	inositol 1-phosphate (I1P)	1.58	0.0033	1.33	0.0501
Phospholipid Metabolism	choline	0.95	0.6508	1.09	0.3566
	choline phosphate	0.94	0.4588	0.63	<0,0001
	cytidine 5'-diphosphocholine	1.51	0.0021	1.30	0.0311
	glycerophosphorylcholine (GPC)	1.20	0.2414	1.03	0.8519
	phosphoethanolamine	2.01	0.1187	3.45	0.0019
	cytidine-5'-diphosphoethanolamine	1.17	0.6447	1.44	0.0538
	glycerophosphoethanolamine	0.96	0.7075	0.98	0.8518
	glycerophosphoserine*	1.24	0.0253	0.89	0.2052
	glycerophosphoinositol*	1.82	0.1053	1.31	0.4609
	trimethylamine N-oxide	1.15	0.0964	0.99	0.8216
Phosphatidylcholine (PC)	1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	1.23	0.0205	0.97	0.7011
	1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)*	1.14	0.1116	1.11	0.1990
	1,2-dipalmitoyl-GPC (16:0/16:0)	1.48	0.0062	1.32	0.0376
	1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	1.10	0.2476	1.01	0.9138
	1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	1.37	0.0042	1.30	0.0111
	1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	1.14	0.0928	1.03	0.7456
	1-palmitoyl-2-dihomo-linolenoyl-GPC (16:0/20:3n3 or 6)*	1.34	0.0040	1.62	<0,0001
	1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	1.29	0.0015	1.15	0.0546
	1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)	1.17	0.0890	1.23	0.0276
	1-palmitoleoyl-2-linoleoyl-GPC (16:1/18:2)*	1.26	0.0388	1.36	0.0031
	1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)*	1.06	0.5099	1.31	0.0143
	1,2-distearoyl-GPC (18:0/18:0)	0.87	0.2551	1.14	0.5336
	1-stearoyl-2-oleoyl-GPC (18:0/18:1)	1.09	0.3189	1.05	0.5673
	1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	0.97	0.4800	1.05	0.7967
	1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	1.21	0.0751	1.09	0.3417
	1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)	0.99	0.8632	1.17	0.0740
	1,2-dioleoyl-GPC (18:1/18:1)	0.87	0.1948	0.83	0.1372
	1-oleoyl-2-linoleoyl-GPC (18:1/18:2)*	1.01	0.8850	0.80	0.0716
	1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)*	1.14	0.1919	1.31	0.0073
	1,2-dilinoleoyl-GPC (18:2/18:2)	1.12	0.4826	1.04	0.7588
Phosphatidylethanolamine (PE)	1,2-dipalmitoyl-GPE (16:0/16:0)*	1.44	0.3243	1.30	0.3123
	1-palmitoyl-2-oleoyl-GPE (16:0/18:1)	1.17	0.0665	0.95	0.5124
	1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	1.24	0.0106	0.75	0.0008
	1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*	1.28	0.0062	1.03	0.6652
	1-palmitoyl-2-docosahexaenoyl-GPE (16:0/22:6)*	1.23	0.0166	1.18	0.0429
	1-palmitoleoyl-2-oleoyl-GPE (16:1/18:1)*	1.00	1.0000	1.00	1.0000
	1-stearoyl-2-oleoyl-GPE (18:0/18:1)	1.15	0.1221	1.03	0.7586
	1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	1.37	0.0187	1.01	0.8857
	1-stearoyl-2-docosahexaenoyl-GPE (18:0/22:6)*	1.06	0.5625	1.01	0.8420
	1,2-dioleoyl-GPE (18:1/18:1)	1.18	0.1544	0.81	0.0458
	1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*	1.29	0.1451	0.76	0.0669
	1-oleoyl-2-arachidonoyl-GPE (18:1/20:4)*	1.27	0.1325	0.88	0.3496
	1-oleoyl-2-docosahexaenoyl-GPE (18:1/22:6)*	1.24	0.0685	0.96	0.7667
Phosphatidylserine (PS)	1-palmitoyl-2-oleoyl-GPS (16:0/18:1)	1.19	0.0157	1.09	0.1798
	1-stearoyl-2-oleoyl-GPS (18:0/18:1)	1.11	0.1351	1.03	0.6092
	1-stearoyl-2-arachidonoyl-GPS (18:0/20:4)	1.76	0.0006	1.38	0.0255
Phosphatidylglycerol (PG)	1-palmitoyl-2-oleoyl-GPG (16:0/18:1)	0.99	0.9277	0.86	0.3141
	1,2-distearoyl-GPG (18:0/18:0)	1.14	0.3343	1.17	0.1784
	1-stearoyl-2-oleoyl-GPG (18:0/18:1)	1.01	0.9785	1.02	0.9476
	1,2-dioleoyl-GPG (18:1/18:1)	1.10	0.3996	1.15	0.2473
Phosphatidylinositol (PI)	1,2-dipalmitoyl-GPI (16:0/16:0)*	0.54	0.0078	0.56	0.0228
	1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*	0.95	0.6707	0.86	0.2950
	1-palmitoleoyl-2-oleoyl-GPI (16:1/18:1)*	1.17	0.0999	1.07	0.4483
	1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*	1.22	0.0139	1.07	0.3811

	1-stearoyl-2-oleoyl-GPI (18:0/18:1)*	0.92	0.4943	1.07	0.6007
	1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	1.06	0.4896	0.91	0.2949
	1,2-dioleoyl-GPI (18:1/18:1)	1.12	0.3187	1.13	0.2420
	1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	1.15	0.1142	1.07	0.3978
	1-oleoyl-2-arachidonoyl-GPI (18:1/20:4) *	1.31	0.0309	1.25	0.0504
Lysophospholipid	1-palmitoyl-GPC (16:0)	0.93	0.4061	0.73	0.1799
	2-palmitoyl-GPC (16:0)*	0.84	0.8159	0.64	0.2440
	1-palmitoleoyl-GPC (16:1)*	0.62	0.0214	0.54	0.0091
	2-palmitoleoyl-GPC (16:1)*	0.45	0.0001	0.43	0.0001
	1-stearoyl-GPC (18:0)	0.99	0.6728	1.00	0.9771
	1-oleoyl-GPC (18:1)	0.73	0.0611	0.56	0.0098
	1-linoleoyl-GPC (18:2)	2.44	0.7972	0.64	0.2499
	1-arachidonoyl-GPC (20:4n6)*	0.53	0.0948	0.38	0.0091
	1-lignoceroyl-GPC (24:0)	1.03	0.9444	1.46	0.0588
	1-cerotoyl-GPC (26:0)*	0.93	0.6663	1.28	0.1980
	1-palmitoyl-GPE (16:0)	0.84	0.2362	0.82	0.2384
	1-stearoyl-GPE (18:0)	0.82	0.1267	0.80	0.1225
	2-stearoyl-GPE (18:0)*	1.26	0.8308	0.86	0.7180
	1-oleoyl-GPE (18:1)	0.71	0.1075	0.43	0.0003
	1-linoleoyl-GPE (18:2)*	0.93	0.8237	0.50	0.0837
	1-arachidonoyl-GPE (20:4n6)*	1.16	0.4689	0.66	0.3216
	1-palmitoyl-GPS (16:0)*	1.27	0.2966	0.90	0.7888
	1-stearoyl-GPS (18:0)*	1.40	0.2448	0.77	0.5440
	1-oleoyl-GPS (18:1)	0.79	0.7154	0.77	0.4175
	1-palmitoyl-GPG (16:0)*	0.86	0.6758	0.90	0.7877
	1-stearoyl-GPG (18:0)	1.03	0.8290	0.91	0.8680
	1-oleoyl-GPG (18:1)*	0.69	0.1642	0.87	0.8961
	1-linoleoyl-GPG (18:2)*	0.95	0.8463	0.94	0.9882
	1-palmitoyl-GPI (16:0)	0.50	0.0909	0.56	0.1885
	1-stearoyl-GPI (18:0)	0.54	0.0957	0.60	0.1695
	1-oleoyl-GPI (18:1)*	0.47	0.0534	0.61	0.2470
	1-linoleoyl-GPI (18:2)*	0.35	0.0152	0.64	0.2728
	1-arachidonoyl-GPI (20:4)*	0.32	0.0033	0.85	0.7148
Plasmalogen	1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*	1.07	0.3404	1.01	0.9463
	1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*	0.89	0.3034	1.01	0.9603
	1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	1.04	0.6006	1.19	0.0383
	1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*	0.84	0.0569	0.98	0.8465
	1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	1.17	0.0327	0.97	0.7028
	1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	0.87	0.1066	1.10	0.2731
	1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	0.83	0.0909	0.99	0.9178
	1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*	0.92	0.4592	0.97	0.7995
	1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	1.16	0.2589	1.12	0.3173
	1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	0.81	0.0471	0.96	0.7586
	1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	1.11	0.1614	1.04	0.5300
Lysoplasmalogen	1-(1-enyl-palmitoyl)-GPE (P-16:0)*	0.80	0.1816	0.79	0.2241
	1-(1-enyl-oleoyl)-GPE (P-18:1)*	0.86	0.1949	0.74	0.0118
	1-(1-enyl-stearoyl)-GPE (P-18:0)*	0.91	0.3866	0.94	0.7641
	1-(1-enyl-oleoyl)-2-oleoyl-GPE (P-18:1/18:1)*	0.89	0.3699	1.14	0.3458
Glycerolipid Metabolism	glycerol	0.87	0.4477	0.83	0.2901
	glycerol 3-phosphate	0.44	0.0010	1.22	0.2520
	glycerophosphoglycerol	0.85	0.1104	1.04	0.7189
Monoacylglycerol	1-myristoylglycerol (14:0)	0.83	0.7614	0.70	0.9536
	1-pentadecanoylglycerol (15:0)	1.10	0.7935	0.59	0.3093
	1-palmitoylglycerol (16:0)	0.77	0.7779	0.67	0.9339
	1-palmitoleoylglycerol (16:1)*	0.86	0.7639	0.71	0.7790

	1-margaroylglycerol (17:0)	1.37	0.4736	0.90	0.6599
	1-oleoylglycerol (18:1)	1.40	0.3739	0.88	0.9332
	1-linoleoylglycerol (18:2)	2.08	0.1885	1.31	0.5105
	1-dihomo-linolenylglycerol (20:3)	1.48	0.4325	1.44	0.3520
	1-arachidonylglycerol (20:4)	1.34	0.3046	0.75	0.4608
	1-docosahexaenoylglycerol (22:6)	1.18	0.8120	0.72	0.4998
	2-myristoylglycerol (14:0)	0.98	0.8813	0.39	0.0977
	2-palmitoylglycerol (16:0)	0.87	0.9196	0.83	0.6086
	2-palmitoleoylglycerol (16:1)*	1.01	0.9952	0.75	0.8963
	2-oleoylglycerol (18:1)	1.24	0.6923	0.82	0.7501
	2-linoleoylglycerol (18:2)	1.37	0.5625	0.82	0.8120
	2-arachidonoylglycerol (20:4)	1.32	0.4670	0.83	0.5139
	1-heptadecenoylglycerol (17:1)*	2.04	0.1730	1.06	0.8958
	2-heptadecenoylglycerol (17:1)*	1.51	0.4104	0.66	0.2646
	1-dihomo-linoleoylglycerol (20:2)	1.61	0.3214	0.69	0.2897
Diacylglycerol	diacylglycerol (12:0/18:1, 14:0/16:1, 16:0/14:1) [2]*	1.04	0.8149	0.70	0.0829
	diacylglycerol (14:0/18:1, 16:0/16:1) [1]*	0.59	0.0753	0.41	0.0281
	diacylglycerol (14:0/18:1, 16:0/16:1) [2]*	0.82	0.2443	0.68	0.0219
	diacylglycerol (16:1/18:2 [2], 16:0/18:3 [1])*	1.02	0.9104	1.06	0.6991
	palmitoyl-myristoyl-glycerol (16:0/14:0) [2]	0.86	0.4605	0.49	0.0007
	palmitoyl-palmitoyl-glycerol (16:0/16:0) [2]*	0.79	0.1734	0.61	0.0066
	palmitoleoyl-palmitoleoyl-glycerol (16:1/16:1) [2]*	0.54	0.0196	0.64	0.0550
	palmitoyl-oleoyl-glycerol (16:0/18:1) [1]*	0.66	0.0512	0.70	0.1950
	palmitoyl-oleoyl-glycerol (16:0/18:1) [2]*	0.80	0.1153	0.71	0.0162
	palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*	0.81	0.0610	0.81	0.0672
	palmitoleoyl-oleoyl-glycerol (16:1/18:1) [2]*	1.17	0.6825	0.86	0.5673
	palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]*	0.64	0.1038	0.90	0.9970
	palmitoyl-dihomo-linolenoyl-glycerol (16:0/20:3n3 or 6) [2]*	0.98	0.9872	1.12	0.3680
	palmitoyl-arachidonoyl-glycerol (16:0/20:4) [1]*	0.65	0.0079	0.83	0.3080
	palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]*	0.78	0.0361	0.83	0.1410
	palmitoyl-docosahexaenoyl-glycerol (16:0/22:6) [1]*	1.07	0.7051	1.08	0.5343
	palmitoyl-docosahexaenoyl-glycerol (16:0/22:6) [2]*	0.88	0.6767	1.14	0.6176
	stearoyl-linoleoyl-glycerol (18:0/18:2) [2]*	0.97	0.8712	0.72	0.0128
	oleoyl-oleoyl-glycerol (18:1/18:1) [1]*	0.33	0.0686	0.64	0.5065
	oleoyl-oleoyl-glycerol (18:1/18:1) [2]*	0.66	0.0065	0.69	0.0092
	oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	0.78	0.4189	0.62	0.1259
	oleoyl-linoleoyl-glycerol (18:1/18:2) [2]	0.80	0.0803	0.82	0.1447
	stearoyl-arachidonoyl-glycerol (18:0/20:4) [1]*	0.96	0.8018	0.52	0.0219
	stearoyl-arachidonoyl-glycerol (18:0/20:4) [2]*	0.95	0.7316	0.67	0.0030
	oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]*	0.87	0.2990	0.90	0.5676
	linoleoyl-arachidonoyl-glycerol (18:2/20:4) [1]*	1.02	0.9459	1.63	0.1544
	linoleoyl-arachidonoyl-glycerol (18:2/20:4) [2]*	1.17	0.6995	1.57	0.1046
	stearoyl-docosahexaenoyl-glycerol (18:0/22:6) [1]*	0.79	0.1461	0.71	0.0613
	stearoyl-docosahexaenoyl-glycerol (18:0/22:6) [2]*	0.92	0.6103	0.69	0.0137
Sphingolipid Synthesis	sphinganine	1.35	0.0050	0.74	0.0031
	sphingadienine	1.40	0.1528	0.65	0.1004
	phytosphingosine	1.22	0.0299	1.01	0.8716
Dihydroceramides	N-palmitoyl-sphinganine (d18:0/16:0)	1.14	0.2081	0.97	0.7562
	N-stearoyl-sphinganine (d18:0/18:0)*	0.96	0.6547	0.96	0.6244
Ceramides	N-palmitoyl-sphingosine (d18:1/16:0)	1.15	0.1581	0.93	0.4569
	N-(2-hydroxypalmitoyl)-sphingosine (d18:1/16:0(2OH))	1.09	0.5092	1.01	0.9819
	N-stearoyl-sphingosine (d18:1/18:0)*	0.99	0.8630	0.90	0.2818
	N-palmitoyl-sphingadienine (d18:2/16:0)*	1.20	0.1679	0.98	0.9437
	N-stearoyl-sphingadienine (d18:2/18:0)*	1.09	0.3747	0.91	0.3943
	N-behenoyl-sphingadienine (d18:2/22:0)*	1.66	0.5738	1.05	0.9640

	N-palmitoyl-heptadecasphingosine (d17:1/16:0)*	1.19	0.0359	1.08	0.2921
	ceramide (d18:1/14:0, d16:1/16:0)*	1.00	0.9531	0.94	0.6209
	ceramide (d18:1/17:0, d17:1/18:0)*	1.10	0.3591	0.89	0.2375
	ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)*	0.94	0.5173	0.79	0.0450
	ceramide (d16:1/24:1, d18:1/22:1)*	0.80	0.0561	1.02	0.8772
	ceramide (d18:2/24:1, d18:1/24:2)*	1.16	0.0639	0.95	0.5070
Hexosylceramides (HCER)	glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	1.20	0.0908	0.55	<0,0001
	glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	0.97	0.7746	0.54	<0,0001
	glycosyl-N-behenoyl-sphingadienine (d18:2/22:0)*	1.03	0.9148	0.36	0.0016
	glycosyl ceramide (d18:1/20:0, d16:1/22:0)*	0.73	0.0588	0.31	<0,0001
	glycosyl ceramide (d18:1/23:1, d17:1/24:1)*	0.99	0.8514	0.61	0.0102
	glycosyl ceramide (d18:2/24:1, d18:1/24:2)*	1.05	0.7135	0.61	0.0002
Lactosylceramides (LCER)	lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)	1.25	0.0792	0.77	0.0432
	lactosyl-N-behenoyl-sphingosine (d18:1/22:0)*	1.08	0.6792	1.05	0.7713
	lactosyl-N-nervonoyl-sphingosine (d18:1/24:1)*	0.99	0.8165	0.73	0.0034
Dihydrosphingomyelins	myristoyl dihydrosphingomyelin (d18:0/14:0)*	1.11	0.6339	0.88	0.5789
	palmitoyl dihydrosphingomyelin (d18:0/16:0)*	1.10	0.6365	1.07	0.6252
	behenoyl dihydrosphingomyelin (d18:0/22:0)*	0.84	0.0980	1.15	0.2411
	sphingomyelin (d18:0/18:0, d19:0/17:0)*	0.81	0.1120	0.98	0.9609
	sphingomyelin (d18:0/20:0, d16:0/22:0)*	0.85	0.0909	1.05	0.7029
Sphingomyelins	palmitoyl sphingomyelin (d18:1/16:0)	1.29	0.0672	1.07	0.5652
	stearoyl sphingomyelin (d18:1/18:0)	1.07	0.5417	1.02	0.8145
	behenoyl sphingomyelin (d18:1/22:0)*	0.62	0.0278	0.93	0.6514
	tricosanoyl sphingomyelin (d18:1/23:0)*	1.13	0.2520	1.36	0.0035
	lignoceroyl sphingomyelin (d18:1/24:0)	0.93	0.3916	1.29	0.0096
	sphingomyelin (d18:2/23:1)*	1.41	0.0669	1.00	0.9620
	sphingomyelin (d18:2/24:2)*	1.06	0.9995	0.94	0.8107
	sphingomyelin (d17:1/14:0, d16:1/15:0)*	1.34	0.0212	1.07	0.4485
	sphingomyelin (d18:1/14:0, d16:1/16:0)*	1.23	0.1209	0.95	0.7365
	sphingomyelin (d18:2/14:0, d18:1/14:1)*	1.39	0.0040	0.82	0.0605
	sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*	1.22	0.0719	1.13	0.2234
	sphingomyelin (d17:2/16:0, d18:2/15:0)*	1.43	0.0084	1.28	0.0772
	sphingomyelin (d18:2/16:0, d18:1/16:1)*	1.44	0.0028	1.05	0.6217
	sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	1.27	0.1395	1.10	0.4592
	sphingomyelin (d18:1/18:1, d18:2/18:0)	1.31	0.0055	1.01	0.9568
	sphingomyelin (d18:1/20:0, d16:1/22:0)*	1.08	0.4423	0.99	0.9999
	sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*	0.97	0.7940	1.15	0.2688
	sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*	1.31	0.0044	1.07	0.3958
	sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:2)*	1.28	0.3546	1.00	0.9614
	sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*	1.03	0.8291	1.06	0.5616
	sphingomyelin (d18:1/24:1, d18:2/24:0)*	0.79	0.1101	1.05	0.8751
	sphingomyelin (d18:2/24:1, d18:1/24:2)*	1.36	0.0275	1.12	0.3314
	sphingomyelin (d18:1/25:0, d19:0/24:1, d19:1/24:0)*	1.28	0.1042	1.13	0.3834
Sphingosines	sphingosine	1.29	0.1498	0.86	0.4456
	hexadecasphingosine (d16:1)*	1.31	0.2824	0.96	0.9343
	heptadecasphingosine (d17:1)	1.33	0.2376	0.79	0.3361
Mevalonate Metabolism	3-hydroxy-3-methylglutarate	1.14	0.4111	2.22	<0,0001
Sterol	cholesterol	1.02	0.8293	1.06	0.4566
	7-hydroxycholesterol (alpha or beta)	1.22	0.9625	1.34	0.2146
Primary Bile Acid Metabolism	cholate	1.00	1.0000	1.00	1.0000
	glycocholate	1.00	1.0000	1.00	1.0000
	taurocholate	1.03	0.7378	0.82	0.0992
	chenodeoxycholate	1.01	0.8759	0.87	0.4040
	glycochenodeoxycholate	1.34	0.2017	0.79	0.3126
	taurochenodeoxycholate	1.07	0.4635	1.27	0.0545

	Secondary Bile Acid Metabolism	deoxycholate	1.00	1.0000	1.00	1.0000
		glycodeoxycholate	1.00	1.0000	1.00	1.0000
		taurodeoxycholate	1.03	0.7766	0.87	0.3372
Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	AICA ribonucleotide	1.00	1.0000	1.00	1.0000
		inosine 5'-monophosphate (IMP)	0.86	0.2483	1.42	0.0170
		inosine	0.66	0.0058	1.01	0.8824
		hypoxanthine	0.62	0.0032	0.93	0.7498
		xanthine	1.15	0.4348	1.01	0.9532
		xanthosine 5'-monophosphate (xmp)	1.00	1.0000	1.00	1.0000
		xanthosine	1.20	0.2786	1.15	0.5288
		N1-methylinosine	2.80	0.0004	0.86	0.7759
		2'-deoxyinosine	0.71	0.0801	0.51	0.0033
		urate	0.96	0.6495	1.52	0.0002
		allantoin	0.86	0.0844	0.97	0.6848
		allantoic acid	0.68	0.0343	0.53	0.0036
	Purine Metabolism, Adenine containing	adenosine 5'-diphosphate (ADP)	2.93	0.0002	1.74	0.0174
		adenosine 5'-monophosphate (AMP)	0.90	0.3353	1.06	0.6515
		adenosine 3'-monophosphate (3'-AMP)	2.11	0.0021	1.20	0.4024
		adenosine 2'-monophosphate (2'-AMP)	1.87	0.0110	1.36	0.2275
		adenosine 3',5'-cyclic monophosphate (cAMP)	1.15	0.1313	1.00	0.9737
		adenylosuccinate	0.51	0.0176	1.20	0.4797
		adenosine	0.23	0.0021	0.16	0.0013
		adenine	1.10	0.5595	0.91	0.5097
		N1-methyladenosine	0.99	0.9965	0.89	0.6280
		N6-methyladenosine	0.25	0.0005	0.25	0.0005
		N6-carbamoylthreonyladenosine	1.01	0.9899	1.83	<0,0001
		2'-deoxyadenosine 5'-monophosphate	0.55	0.0005	0.42	<0,0001
		2'-deoxyadenosine	0.44	0.0013	0.44	0.0013
		diadenosine triphosphate	0.84	0.0766	1.32	0.0114
		N6-succinyladenosine	0.45	0.0001	1.34	0.0903
	Purine Metabolism, Guanine containing	guanosine 5'- monophosphate (5'-GMP)	0.79	0.0491	0.94	0.6797
		guanosine	0.39	<0,0001	0.68	0.0572
		guanine	0.53	0.0016	0.70	0.1064
		7-methylguanine	1.42	0.0032	1.25	0.0428
		N2-methylguanosine	1.03	0.7534	0.71	0.0717
		N2,N2-dimethylguanosine	1.01	0.9491	0.71	0.0621
		2'-deoxyguanosine	0.68	0.1900	0.42	0.0059
	Pyrimidine Metabolism, Orotate containing	N-carbamoylaspartate	0.90	0.8874	1.46	0.5655
		orotate	1.16	0.1293	0.67	0.4152
		orotidine	0.82	0.0863	0.60	0.0001
	Pyrimidine Metabolism, Uracil containing	uridine 5'-triphosphate (UTP)	10.66	<0,0001	2.41	0.0120
		uridine 5'-diphosphate (UDP)	2.90	0.0001	1.45	0.0809
		uridine 5'-monophosphate (UMP)	0.90	0.2395	1.00	0.9800
		uridine 3'-monophosphate (3'-UMP)	2.72	0.0009	1.39	0.1104
		uridine	0.76	0.0894	0.79	0.2018
		uracil	0.30	0.0007	0.63	0.2299
		pseudouridine	0.90	0.4775	0.76	0.0505
		5,6-dihydrouridine	0.99	0.8366	0.69	0.0436
		2'-O-methyluridine	0.74	0.1991	0.65	0.0541
		5-methyluridine (ribothymidine)	1.08	0.5094	0.53	0.0246
		2'-deoxyuridine	0.80	0.0961	0.80	0.0961
		3-ureidopropionate	1.19	0.2665	0.59	0.0020
		beta-alanine	1.40	0.0034	1.60	0.0001
	Pyrimidine Metabolism, Cytidine containing	cytidine diphosphate	2.58	0.0003	1.64	0.0247
		cytidine 5'-monophosphate (5'-CMP)	0.85	0.1254	0.87	0.2344

		cytidine	0.60	0.0021	0.84	0.3623
		cytosine	0.59	0.0016	0.84	0.3453
		3-methylcytidine	1.09	0.5846	1.05	0.7135
		5-methylcytidine	1.04	0.8669	0.72	0.0242
		2'-deoxycytidine	0.46	0.0992	0.45	0.1349
		2'-O-methylcytidine	0.73	0.1472	0.69	0.0914
	Pyrimidine Metabolism, Thymine containing	thymidine 5'-monophosphate	0.47	0.0001	0.51	0.0006
		thymidine	0.15	<0,0001	0.12	<0,0001
		thymine	0.21	0.0007	0.35	0.0312
		3-aminoisobutyrate	1.06	0.7488	0.92	0.7888
	Purine and Pyrimidine Metabolism	methylphosphate	0.28	0.0002	0.19	0.0000
Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	nicotinate ribonucleoside	1.00	1.0000	1.00	1.0000
		nicotinamide	0.82	0.0346	0.85	0.0686
		nicotinamide ribonucleotide (NMN)	0.30	0.0004	0.64	0.2605
		nicotinamide riboside	1.12	0.4956	1.55	0.0096
		nicotinamide adenine dinucleotide (NAD+)	1.42	0.0020	1.45	0.0011
		nicotinamide adenine dinucleotide reduced (NADH)	1.17	0.2728	1.27	0.1168
		nicotinate adenine dinucleotide (NAAD+)	1.00	1.0000	1.00	1.0000
		1-methylnicotinamide	1.43	0.0007	1.20	0.0638
		trigonelline (N'-methylnicotinate)	1.34	0.0043	1.21	0.0527
		adenosine 5'-diphosphoribose (ADP-ribose)	1.77	0.0332	1.54	0.0616
	Riboflavin Metabolism	riboflavin (Vitamin B2)	1.06	0.4850	1.18	0.0554
		flavin adenine dinucleotide (FAD)	1.14	0.1734	1.17	0.0955
		flavin mononucleotide (FMN)	1.16	0.3342	1.29	0.0598
	Pantothenate and CoA Metabolism	pantothenate	0.79	0.0387	0.75	0.0161
		phosphopantetheine	0.42	0.0047	0.32	0.0005
		3'-dephosphocoenzyme A	0.16	0.0001	0.43	0.0577
		coenzyme A	0.73	0.0684	1.05	0.7679
		pantetheine	1.27	0.1525	1.39	0.0459
	Ascorbate and Aldarate Metabolism	gulonate*	0.87	0.1625	0.96	0.6380
	Tocopherol Metabolism	alpha-tocopherol	1.44	0.0042	1.13	0.2609
	Biotin Metabolism	biotin	1.00	1.0000	1.00	1.0000
	Folate Metabolism	5-methyltetrahydrofolate (5MeTHF)	1.09	0.6441	1.28	0.2271
	Tetrahydrobiopterin Metabolism	dihydrobiopterin	1.00	1.0000	1.00	1.0000
	Pterin Metabolism	pterin	1.57	0.1050	1.11	0.7323
	Hemoglobin and Porphyrin Metabolism	bilirubin (Z,Z)	1.27	0.6535	0.62	0.1639
	Thiamine Metabolism	thiamin (Vitamin B1)	0.95	0.4347	1.19	0.1608
		thiamin monophosphate	0.69	0.0796	2.98	0.0000
	Vitamin A Metabolism	retinol (Vitamin A)	1.20	0.1433	2.03	0.0000
	Vitamin B6 Metabolism	pyridoxine (Vitamin B6)	0.94	0.6984	0.99	0.9944
		pyridoxamine	1.13	0.5496	0.95	0.7435
		pyridoxamine phosphate	0.70	0.2063	1.10	0.6453
		pyridoxal phosphate	1.09	0.5392	1.15	0.2255
		pyridoxal	1.09	0.2575	1.00	0.9568
		pyridoxate	0.90	0.6450	1.47	0.0362
Xeno-biotics	Benzoate Metabolism	hippurate	1.04	0.7556	2.04	<0,0001
		3-hydroxyhippurate	1.05	0.8758	2.49	0.0007
		benzoate	1.35	0.0563	1.04	0.4708
		catechol sulfate	0.84	0.2588	0.82	0.1876
		guaiacol sulfate	1.44	0.1393	0.86	0.5585
		4-methylcatechol sulfate	0.79	0.0913	0.96	0.7402
		p-cresol sulfate	1.00	0.9641	1.19	0.0935
	Food Component/Plant	gluconate	0.95	0.5119	0.75	0.8650

	beta-guanidinopropanoate	2.03	0.0451	2.05	0.0294
	ergothioneine	1.94	<0,0001	1.15	0.1672
	erythritol	0.94	0.5374	0.87	0.1232
	homostachydrine*	0.76	0.1774	1.11	0.6085
	N-glycolylneuraminate	1.16	0.2267	0.97	0.9653
	stachydrine	1.13	0.4313	1.04	0.8711
	methyl glucopyranoside (alpha + beta)	0.80	0.4125	0.33	0.0002
Drug - Antibiotic	penicillin G	0.83	0.4051	0.89	0.5525
Drug - Other	S-carboxymethyl-L-cysteine	0.95	0.6718	0.79	0.1563
	benfotiamine	1.01	0.6840	0.73	0.4984
Chemical	sulfate*	1.04	0.6861	0.79	0.1059
	O-sulfo-L-tyrosine	0.93	0.4184	1.08	0.4830
	2-aminophenol sulfate	3.22	<0,0001	0.14	<0,0001
	glycerol 2-phosphate	0.61	0.0034	0.94	0.6182
	phenol red	0.96	0.7620	1.02	0.8259
	succinimide	1.24	0.2102	1.27	0.1166
	4-acetamidobenzoate	1.81	0.2726	2.63	0.0093
	thioproline	1.28	0.0482	1.16	0.1970