Supplementary Table 1. A comprehensive list of all metabolites screen for in this study.

mz_rt	EmpiricalCompound	Input m/z	Retention time	ion	mz_diff	Statistic	Significant
195.0496_0.43	C00800, L-Gulonate	195.0496	0.43	M-H[-]	-0.0014	-3.29	yes
407.2792_5.05	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	407.2792	5.05	M-H[-]	-0.0011	2.46	yes
408.2827_5.05	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	408.2827	5.05	M(C13)-H[-]	-0.001	2.45	yes
391.2844_5.87	C02528, Chenodeoxycholate	391.2844	5.87	M-H[-]	-0.001	2.34	yes
543.3872_8.84	C05200, 3-Hexaprenyl-4,5-dihydroxybenzoate	543.3872	8.84	M-H2O-H[-]	0.0029	-2.68	yes
83.0131_0.44	C00232, Succinate semialdehyde	83.0131	0.44	M-H2O-H[-]	-0.0007	-3.15	yes
392.0442_0.47	C16620, 6-Methylthioguanosine monophosphate	392.0442	0.47	M-H[-]	0.0007	-2.58	yes
86.025_0.46	C00740, D-Serine	86.025	0.46	M-H2O-H[-]	0.0003	-3.45	yes
140.0105_0.45	C00740, D-Serine	140.0105	0.45	M+Cl[-]	-0.001	-5.02	yes
183.961_0.41	C00740, D-Serine	183.961	0.41	M+Br[-]	0.0001	-2.91	yes
68.0501_0.46	CE1944, 1-pyrroline	68.0501	0.46	M-H[-]	-0.0005	-2.45	yes
652.079_0.51	C00203, UDP-N-acetyl-D-galactosamine	652.079	0.51	M+HCOO[-]	-0.0002	-4.14	yes
606.0744_0.49	C00203, UDP-N-acetyl-D-galactosamine	606.0744	0.49	M-H[-]	0.0001	-3.91	yes
607.0792_0.49	C00203, UDP-N-acetyl-D-galactosamine	607.0792	0.49	M(C13)-H[-]	0.0015	-3.57	yes
785.1558_2.32	C00016, FAD	785.1558	2.32	M(C13)-H[-]	0.0026	-3.38	yes
784.1517_2.32	C00016, FAD	784.1517	2.32	M-H[-]	0.0019	-3.22	yes
1069.4723_11.82	C05860, beta-D-Mannosyldiacetylchitobiosyldiphosphodolichol	1069.4723	11.82	M-H2O-H[-]	0.0067	-3.74	yes
325.025_0.45	C04242, 5-Fluorodeoxyuridine monophosphate	325.025	0.45	M-H[-]	0.0008	-2.5	yes
588.0781_0.5	C00325, GDP-L-fucose	588.0781	0.5	M-H[-]	0.0032	-4.34	yes
565.0473_0.51	C00052, UDP-D-galactose	565.0473	0.51	M-H[-]	-0.0004	-3.6	yes
566.0488_0.51	C00052, UDP-D-galactose	566.0488	0.51	M(C13)-H[-]	-0.0023	-4.49	yes
112.0393_0.47	C01110, 5-Amino-2-oxopentanoic acid	112.0393	0.47	M-H2O-H[-]	-0.001	-2.85	yes
151.0247_0.45	C01110, 5-Amino-2-oxopentanoic acid	151.0247	0.45	M+Na-2H[-]	-0.0009	-2.62	yes
267.0721_0.46	C00760, Cellulose	267.0721	0.46	M-2H[2-]	-0.0001	-6.92	yes
280.2349_8.06	C01595, Linoleate	280.2349	8.06	M(C13)-H[-]	-0.0014	-2.8	yes
279.2319_8.06	C01595, Linoleate	279.2319	8.06	M-H[-]	-0.001	-2.79	yes
363.2152_6.43	C05470, Urocortisone	363.2152	6.43	M-H[-]	-0.0025	-2.88	yes
516.2852_4.32	C15516, Taurohyocholate	516.2852	4.32	M(S34)-H[-]	0.005	-5.07	yes
515.287_4.33	C15516, Taurohyocholate	515.287	4.33	M(C13)-H[-]	-0.0008	-4.94	yes
514.2839_4.33	C15516, Taurohyocholate	514.2839	4.33	M-H[-]	-0.0005	-4.9	yes
496.273_4.58	C15516, Taurohyocholate	496.273	4.58	M-H2O-H[-]	-0.0008	-3.18	yes
295.2267_6.43	C14826, 12(13)-EpOME	295.2267	6.43	M-H[-]	-0.0011	-2.81	yes
296.2302_6.43	C14826, 12(13)-EpOME	296.2302	6.43	M(C13)-H[-]	-0.001	-2.81	yes
368.2626_7.78	C06429, (4Z,7Z,10Z,13Z,16Z,19Z)-Docosahexaenoic acid	368.2626	7.78	M+ACN-H[-]	0.0031	-2.89	yes
449.3095_5.21	C05466,	449.3095	5.21	M(C13)-H[-]	-0.0007	-3.3	yes
448.306_5.22	C05466,	448.306	5.22	M-H[-]	-0.0008	-3.24	yes
311.2215_5.74	C04717, (9Z,11E)-(13S)-13-Hydroperoxyoctadeca-9,11-dienoic acid	311.2215	5.74	M-H[-]	-0.0013	-2.41	yes
278.2181_7.65	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	278.2181	7.65	M(C13)-H[-]	-0.0026	-3.38	yes
277.2154_7.65	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	277.2154	7.65	M-H[-]	-0.0019	-3.29	yes
364.2188_6.43	C05474, 3alpha,11beta,21-Trihydroxy-20-oxo-5beta-pregnan-18-al	364.2188	6.43	M(C13)-H[-]	-0.0023	-2.81	yes
305.2463_8.27	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	305.2463	8.27	M-H[-]	-0.0023	-2.47	yes
306.2511_8.29	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	306.2511	8.29	M(C13)-H[-]	-0.0009	-2.39	yes
303.232_7.97	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	303.232	7.97	M-H[-]	-0.0009	-2.33	yes
304.2355_7.97	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	304.2355	7.97	M(C13)-H[-]	-0.0008	-2.32	yes
464.3008_4.57	C01921, Glycocholate	464.3008	4.57	M-H[-]	-0.0009	-4.57	yes

335.2205_6.18	C04849, (5Z,9E,14Z)-(8xi,11R,12S)-11,12-Epoxy-8-hydroxyicosa-5,9,14-trienoic acid	335.2205	6.18	M-H[-]	-0.0023	-2.48	yes
317.2112_6.3	C04849, (5Z,9E,14Z)-(8xi,11R,12S)-11,12-Epoxy-8-hydroxyicosa-5,9,14-trienoic acid	317.2112	6.3	M-H2O-H[-]	-0.001	-2.45	yes
318.2128_6.3	C00909, Leukotriene A4	318.2128	6.3	M(C13)-H[-]	-0.0028	-2.41	yes
499.2922_4.9	C05465, Taurochenodeoxycholate	499.2922	4.9	M(C13)-H[-]	-0.0007	-3.32	yes
498.2889_4.9	C05465, Taurochenodeoxycholate	498.2889	4.9	M-H[-]	-0.0006	-3.28	yes
187.0964_3.31	C08261,	187.0964	3.31	M-H[-]	-0.0012	-2.48	yes
446.29_4.88	C01921, Glycocholate	446.29	4.88	M-H2O-H[-]	-0.0011	-2.6	yes
121.0271_2.3	C00299, Uridine	121.0271	2.3	M-2H[2-]	-0.0004	-3.3	yes
392.2879_5.87	C02528, Chenodeoxycholate	392.2879	5.87	M(C13)-H[-]	-0.0009	2.56	yes
463.2304_4.35	tststeroneglc, testosterone glucuronide	463.2304	4.35	M-H[-]	-0.0034	2.42	yes
168.0233_0.43	C04677, 1-(5'-Phosphoribosyl)-5-amino-4-imidazolecarboxamide	168.0233	0.43	M-2H[2-]	-0.0008	-2.48	yes
164.0704_0.66	CE2172,	164.0704	0.66	M-H[-]	-0.0013	-2.89	yes
283.0686_0.47	C00294, Inosine	283.0686	0.47	M-H+O[-]	0.0002	-3.97	yes
224.0664_3.49	C00475, Cytidine	224.0664	3.49	M-H2O-H[-]	-0.0012	3.65	yes
336.0443_0.45	C03492, D-4'-Phosphopantothenate	336.0443	0.45	M+Cl37[-]	0.0014	-3.43	yes
299.0717_0.56	C03492, D-4'-Phosphopantothenate	299.0717	0.56	M(C13)-H[-]	-0.0014	-2.82	yes
298.0687_0.48	C03492, D-4'-Phosphopantothenate	298.0687	0.48	M-H[-]	-0.001	-2.42	yes
74.0198_0.41	C00121, D-Ribose	74.0198	0.41	M-2H[2-]	0.0007	-2.95	yes
263.1021_2.07	C04148, alpha-N-Phenylacetyl-L-glutamine	263.1021	2.07	M-H[-]	-0.0016	-4.09	yes
145.0614_0.41	C00740, D-Serine	145.0614	0.41	M+ACN-H[-]	-0.0005	-2.37	yes
167.0197_0.44	C00366, Urate	167.0197	0.44	M-H[-]	-0.0013	-2.6	yes
149.0112_0.45	C00366, Urate	149.0112	0.45	M-H2O-H[-]	0.0008	-2.28	yes
146.0597_1.5	CE2172,	146.0597	1.5	M-H2O-H[-]	-0.0014	-2.6	yes
255.2317_8.44	C00249, Hexadecanoic acid	255.2317	8.44	M-H[-]	-0.0012	-3.52	yes
256.2341_8.44	C00249, Hexadecanoic acid	256.2341	8.44	M(C13)-H[-]	-0.0022	-3.46	yes
204.0845_1.05	C00525, D-Tryptophan	204.0845	1.05	M(C13)-H[-]	-0.0015	-3.12	yes
203.0813_1.05	C00525, D-Tryptophan	203.0813	1.05	M-H[-]	-0.0013	-2.94	yes
187.0958_0.47	C08261,	187.0958	0.47	M-H[-]	-0.0018	-3.06	yes
227.2001_7.74	C06424, Tetradecanoic acid	227.2001	7.74	M-H[-]	-0.0015	-2.56	yes
308.079_0.44	C01169, S-Succinyldihydrolipoamide	308.079	0.44	M(S34)-H[-]	-0.0007	-2.56	yes
159.0912_1.06	C00398, Tryptamine	159.0912	1.06	M-H[-]	-0.0015	-2.69	yes
148.0417_0.5	C05578, 5,6-Dihydroxyindole	148.0417	0.5	M-H[-]	0.0013	-2.58	yes
368.161_4.47	C04555, 3beta-Hydroxyandrost-5-en-17-one 3-sulfate	368.161	4.47	M(C13)-H[-]	-0.0008	3.88	yes
367.1577_4.46	C04555, 3beta-Hydroxyandrost-5-en-17-one 3-sulfate	367.1577	4.46	M-H[-]	-0.0007	3.26	yes
133.0129_0.45	C00149, (S)-Malate	133.0129	0.45	M-H[-]	-0.0013	-3.84	yes
134.0175_0.44	C00149, (S)-Malate	134.0175	0.44	M(C13)-H[-]	-0.0001	-3.29	yes
346.0545_0.47	C00020, AMP	346.0545	0.47	M-H[-]	-0.0013	-5.04	yes
338.2622_7.78	CE4839, 6,9,12,15,18-all-cis-tetracosapentaenoate	338.2622	7.78	M-H2O-H[-]	0.0007	-4.77	yes
324.1938_5.37	CE6504,	324.1938	5.37	M-H2O-H[-]	-0.0004	-2.21	yes
218.1021_0.67	C00864, Pantothenate	218.1021	0.67	M-H[-]	-0.0013	-4.05	yes
237.096_3.03	C11132, 2-Methoxyestrone 3-glucuronide	237.096	3.03	M-2H[2-]	0.001	-3.52	yes
131.055_0.42	C01110, 5-Amino-2-oxopentanoic acid	131.055	0.42	M(C13)-H[-]	0.0007	-3.54	yes
281.2476_8.53	C01712, (9E)-Octadecenoic acid	281.2476	8.53	M-H[-]	-0.001	-3.07	yes
264.1034_2.07	C00378, Thiamin	264.1034	2.07	M-H[-]	-0.0016	2.17	yes
257.247_8.47	C00249, Hexadecanoic acid	257.247	8.47	M+H[1+]	-0.0005	-2.54	yes
300.2894_5.76	ttdcrn, tetradecanoyl carnitine	300.2894	5.76	M-C3H4O2+H[1+]	-0.0003	2.7	yes
414.3596_6.57	hpdcacrn, heptadecanoyl carnitine	414.3596	6.57	M+H[1+]	0.0018	3.36	yes

319.3008_5.6	C12144, Phytosphingosine	319.3008	5.6	M(C13)+H[1+]	-0.0029	3.6	yes
318.3_5.6	C12144, Phytosphingosine	318.3	5.6	M+H[1+]	-0.0003	3.18	yes
858.5241_12.03	C02737, Phosphatidylserine	858.5241	12.03	M+Na[1+]	-0.0015	2.43	yes
400.3413_6.34	C02990, L-Palmitoylcarnitine	400.3413	6.34	M+H[1+]	-0.0009	2.72	yes
282.2788_5.77	C12144, Phytosphingosine	282.2788	5.77	M-H4O2+H[1+]	-0.0003	2.75	yes
279.2311_7.66	C00249, Hexadecanoic acid	279.2311	7.66	M+Na[1+]	0.0016	-4.1	yes
429.3765_6.81	stcrn, stearoylcarnitine	429.3765	6.81	M(C13)+H[1+]	-0.0003	2.58	yes
428.3733_6.82	stcrn, stearoylcarnitine	428.3733	6.82	M+H[1+]	-0.0001	2.58	yes
322.0574_0.44	C00364, dTMP	322.0574	0.44	M[1+]	0.0008	-2.82	yes
341.0711_0.44	C00364, dTMP	341.0711	0.44	M+H2O+H[1+]	-0.0034	-2.63	yes
305.0553_0.44	C00364, dTMP	305.0553	0.44	M-H2O+H[1+]	0.002	-2.45	yes
431.3859_7.87	CE5021,	431.3859	7.87	M-H2O+H[1+]	-0.0024	-2.7	yes
180.0673_1.86	CE5536, adrenochrome	180.0673	1.86	M+H[1+]	0.0018	-2.75	yes
296.0649_0.4	C04640, 2-(Formamido)-N1-(5'-phosphoribosyl)acetamidine	296.0649	0.4	M-H2O+H[1+]	0.0007	-5.71	yes
516.3028_6.17	C15516, Taurohyocholate	516.3028	6.17	M+H[1+]	0.0038	-3.53	yes
148.0604_0.47	C00025, L-Glutamate	148.0604	0.47	M+H[1+]	-0.0001	-3.42	yes
399.3286_5.99	CE2201, 23S,25-dihydroxyvitamin D3	399.3286	5.99	M-H2O+H[1+]	0.0029	-2.6	yes
85.0286_0.45	C06144, 3-Butynoate	85.0286	0.45	M+H[1+]	0.0002	-3.36	yes
372.3094_5.83	ttdcrn, tetradecanoyl carnitine	372.3094	5.83	M+H[1+]	-0.0014	-2.62	yes
472.3036_5.21	C05466,	472.3036	5.21	M+Na[1+]	0.0002	-2.68	yes
432.3109_5.22	C05466,	432.3109	5.22	M-H2O+H[1+]	0.0001	-2.62	yes
414.3007_5.22	C05466,	414.3007	5.22	M-H4O2+H[1+]	0.0005	-2.61	yes
225.0892_2.47	C00214, Thymidine	225.0892	2.47	M-H2O+H[1+]	0.0022	-3.14	yes
517.3021_2.77	C15516, Taurohyocholate	517.3021	2.77	M(C13)+H[1+]	-0.0003	-3.51	yes
504.271_4.57	C01921, Glycocholate	504.271	4.57	M+K[1+]	-0.0008	-2.92	yes
430.2955_4.57	C01921, Glycocholate	430.2955	4.57	M-H4O2+H[1+]	0.0004	-2.77	yes
488.2981_4.57	C01921, Glycocholate	488.2981	4.57	M+Na[1+]	-0.0002	-2.75	yes
448.3059_4.59	C01921, Glycocholate	448.3059	4.59	M-H2O+H[1+]	0.0002	-2.53	yes
424.3421_6.14	lneldccrn, Linoelaidyl carnitine	424.3421	6.14	M+H[1+]	-0.0	-2.79	yes
425.3448_6.14	lneldccrn, Linoelaidyl carnitine	425.3448	6.14	M(C13)+H[1+]	-0.0007	-2.69	yes
451.3633_6.3	dlnlcgcrn, dihomo-gamma-linolenyl carnitine	451.3633	6.3	M(C13)+H[1+]	0.0021	-3.16	yes
450.3585_6.3	dlnlcgcrn, dihomo-gamma-linolenyl carnitine	450.3585	6.3	M+H[1+]	0.0007	-2.74	yes
309.0443_0.43	C03838, 5'-Phosphoribosylglycinamide	309.0443	0.43	M+Na[1+]	-0.0016	-3.93	yes
226.0825_2.46	C00475, Cytidine	226.0825	2.46	M-H2O+H[1+]	0.0003	-3.23	yes
417.3743_9.21	CE1924, (+)-gama-tocopherol	417.3743	9.21	M+H[1+]	0.0016	-3.53	yes
494.3244_6.17	c226crn, cervonyl carnitine	494.3244	6.17	M+Na[1+]	0.0003	-3.95	yes
195.049_0.57	C00191, D-Glucuronate	195.049	0.57	M+H[1+]	-0.001	-4.02	yes
118.0862_0.44	C00183, L-Valine	118.0862	0.44	M+H[1+]	-0.0001	-2.63	yes
401.344_6.34	C02990, L-Palmitoylcarnitine	401.344	6.34	M(C13)+H[1+]	-0.0016	-2.8	yes
845.6751_10.13	C11378,	845.6751	10.13	M-H2O+H[1+]	-0.0055	2.99	yes
347.2914_9.18	C02528, Chenodeoxycholate	347.2914	9.18	M-HCOOH+H[1+]	-0.0032	-2.66	yes
321.2815_9.04	C02528, Chenodeoxycholate	321.2815	9.04	M-C3H4O2+H[1+]	0.0026	-2.6	yes
207.0252_0.4	C05580, 3,4-Dihydroxymandelate	207.0252	0.4	M+Na[1+]	-0.0013	2.93	yes
218.1392_0.45	pcrn, propionyl-carnitine	218.1392	0.45	M+H[1+]	0.0005	-2.89	yes
450.9581_0.45	CE2875, 3'-monoiodo-L-thyronine 4'-O-sulfate	450.9581	0.45	M-CO+H[1+]	0.0001	-4.45	yes
409.2954_6.41	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	409.2954	6.41	M+H[1+]	0.0005	-2.66	yes
137.0458_0.46	C00262, Hypoxanthine	137.0458	0.46	M+H[1+]	0.0	-4.95	yes

138.0493_0.45	C00262, Hypoxanthine	138.0493	0.45	M(C13)+H[1+]	0.0001	-6.52	yes
433.3146_5.23	CE5560, glycolithocholate	433.3146	5.23	M+H[1+]	-0.0041	-2.58	yes
415.304_5.21	CE5560, glycolithocholate	415.304	5.21	M-H2O+H[1+]	-0.0041	-2.57	yes
402.3433_6.34	C01561, Calcidiol	402.3433	6.34	M(C13)+H[1+]	-0.0015	-3.59	yes
198.1123_1.52	C05588, L-Metanephrine	198.1123	1.52	M+H[1+]	-0.0002	-2.74	yes
630.0721_0.5	C00203, UDP-N-acetyl-D-galactosamine	630.0721	0.5	M+Na[1+]	0.0012	-3.38	yes
526.3875_10.19	tettet6crn, Tetracosatetraenoyl carnitine	526.3875	10.19	M+Na[1+]	0.0008	-3.5	yes
214.0491_1.35	C02712, N-Acetylmethionine	214.0491	1.35	M+Na[1+]	-0.0018	-3.31	yes
163.0287_2.52	CE1310, N-acetyl-L-cysteine	163.0287	2.52	M+H[1+]	-0.0011	-2.53	yes
263.2367_8.08	C00517, Hexadecanal	263.2367	8.08	M+Na[1+]	0.0021	-2.35	yes
280.2356_7.65	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	280.2356	7.65	M(C13)+H[1+]	0.0003	-4.96	yes
508.3748_7.01	C04230, 1-Acyl-sn-glycero-3-phosphocholine	508.3748	7.01	M+H[1+]	-0.0014	-2.34	yes
509.3767_7.0	C04230, 1-Acyl-sn-glycero-3-phosphocholine	509.3767	7.0	M(C13)+H[1+]	-0.0029	-2.33	yes
450.3216_5.26	C05466,	450.3216	5.26	M+H[1+]	0.0002	-3.34	yes
451.3247_5.26	C05466,	451.3247	5.26	M(C13)+H[1+]	-0.0001	-3.09	yes
319.227_4.51	C14826, 12(13)-EpOME	319.227	4.51	M+Na[1+]	0.0026	-2.7	yes
223.1691_6.45	C02679, Dodecanoic acid	223.1691	6.45	M+Na[1+]	0.0022	-2.58	yes
155.1067_8.07	CE2576,	155.1067	8.07	M-H2O+H[1+]	0.0001	-3.02	yes
307.2629_8.28	C01530, Octadecanoic acid	307.2629	8.28	M+Na[1+]	0.0021	-2.73	yes
314.2709_6.61	dmnoncrn, 4,8 dimethylnonanoyl carnitine	314.2709	6.61	M-H2O+H[1+]	0.002	-2.48	yes
354.2597_8.04	dmnoncrn, 4,8 dimethylnonanoyl carnitine	354.2597	8.04	M+Na[1+]	-0.0018	-3.49	yes
282.2561_8.07	C01712, (9E)-Octadecenoic acid	282.2561	8.07	M[1+]	0.0002	-4.76	yes
279.2317_6.45	C14826, 12(13)-EpOME	279.2317	6.45	M-H2O+H[1+]	-0.0001	-2.44	yes
319.2216_6.43	C14826, 12(13)-EpOME	319.2216	6.43	M+Na[1+]	-0.0028	-2.35	yes
538.2807_4.32	C15516, Taurohyocholate	538.2807	4.32	M+Na[1+]	-0.0003	-5.41	yes
516.2955_4.31	C15516, Taurohyocholate	516.2955	4.31	M+H[1+]	-0.0035	-3.21	yes
498.2887_4.34	C15516, Taurohyocholate	498.2887	4.34	M-H2O+H[1+]	0.0003	-5.39	yes
554.2496_4.33	C15516, Taurohyocholate	554.2496	4.33	M+K[1+]	-0.0049	-5.05	yes
480.2781_4.33	C15516, Taurohyocholate	480.2781	4.33	M-H4O2+H[1+]	0.0003	-5.74	yes
281.2475_8.08	ocdcea, octadecenoate (n-C18:1)	281.2475	8.08	M[1+]	-0.0005	-3.29	yes
455.2987_6.66	CE5560, glycolithocholate	455.2987	6.66	M+Na[1+]	-0.002	-2.67	yes
119.0854_8.02	CE2577,	119.0854	8.02	M-H4O2+H[1+]	-0.0001	-2.87	yes
111.1158_8.07	CE2577,	111.1158	8.07	M-CO2+H[1+]	-0.0011	-2.81	yes
83.0854_8.06	CE2577,	83.0854	8.06	M-C3H4O2+H[1+]	-0.0002	-2.58	yes
522.2883_4.91	C05465, Taurochenodeoxycholate	522.2883	4.91	M+Na[1+]	0.0022	-3.88	yes
500.3043_4.98	C05465, Taurochenodeoxycholate	500.3043	4.98	M+H[1+]	0.0002	-3.7	yes
464.2832_4.89	C05465, Taurochenodeoxycholate	464.2832	4.89	M-H4O2+H[1+]	0.0003	-3.62	yes
501.3056_4.98	C05465, Taurochenodeoxycholate	501.3056	4.98	M(C13)+H[1+]	-0.0019	-3.41	yes
261.2186_7.66	C14826, 12(13)-EpOME	261.2186	7.66	M-H4O2+H[1+]	-0.0026	-2.42	yes
325.0861_0.45	C14853, Benzo[a]pyrene-7,8-dihydrodiol-9,10-oxide	325.0861	0.45	M+Na[1+]	0.0025	-3.14	yes
308.2665_8.28	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	308.2665	8.28	M(C13)+H[1+]	-0.0001	-2.82	yes
289.2519_8.3	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	289.2519	8.3	M-H2O+H[1+]	-0.0007	-2.46	yes
324.2856_7.2	C00836, Sphinganine	324.2856	7.2	M+Na[1+]	-0.0018	-2.42	yes
169.121_8.07	CE2061,	169.121	8.07	M+H[1+]	-0.0013	-3.0	yes
97.101_8.06	CE2061,	97.101	8.06	M-C3H4O2+H[1+]	-0.0002	-2.67	yes
123.1166_8.04	CE2061,	123.1166	8.04	M-HCOOH+H[1+]	-0.0003	-2.49	yes
837.5412_12.09	C02737, Phosphatidylserine	837.5412	12.09	M(C13)+H[1+]	-0.0058	2.58	yes

836.542_12.09	C02737, Phosphatidylserine	836.542	12.09	M+H[1+]	-0.0016	2.54	yes
469.2938_5.25	CE2207, 24-oxo-1alpha,23,25-trihydroxyvitamin D3	469.2938	5.25	M+Na[1+]	0.0013	2.68	yes
334.2819_8.46	CE2414, (3S,7R,11R)-phytanate	334.2819	8.46	M+Na[1+]	-0.0024	2.55	yes
303.2318_7.59	C02110, 11-cis-Retinal	303.2318	7.59	M+H2O+H[1+]	-0.0001	-3.67	yes
268.1038_0.44	C00330, Deoxyguanosine	268.1038	0.44	M+H[1+]	-0.0003	3.71	yes
398.3256_6.0	hdd2crn, trans-Hexadec-2-enoyl carnitine	398.3256	6.0	M+H[1+]	-0.0009	3.05	yes
366.141_6.59	C00611, N-Acetyllactosamine	366.141	6.59	M-H2O+H[1+]	0.0015	2.49	yes
304.2351_7.59	CE5013,	304.2351	7.59	M(C13)+H[1+]	-0.0002	-3.41	yes
427.361_6.46	odecrn, octadecenoyl carnitine	427.361	6.46	M(C13)+H[1+]	-0.0002	3.75	yes
426.3578_6.46	odecrn, octadecenoyl carnitine	426.3578	6.46	M+H[1+]	0.0	3.69	yes
451.3613_7.45	C02059, Phylloquinone	451.3613	7.45	M+H[1+]	0.0042	2.98	yes
153.0403_0.49	C00385, Xanthine	153.0403	0.49	M+H[1+]	-0.0004	-2.37	yes
303.2318_6.71	CE5575, 9-cis-retinal	303.2318	6.71	M+H2O+H[1+]	-0.0001	2.82	yes
343.224_6.72	C04805, 5(S)-HETE	343.224	6.72	M+Na[1+]	-0.0004	2.92	yes
320.266_8.78	prist, pristanic acid	320.266	8.78	M+Na[1+]	-0.0026	-4.26	yes
287.2358_8.81	CE1754, 9-cis-retinol	287.2358	8.81	M+H[1+]	-0.0012	-4.41	yes
304.2349_6.71	ocdcea, octadecenoate (n-C18:1)	304.2349	6.71	M+Na[1+]	-0.0024	2.83	yes
281.099_2.64	C00670, sn-glycero-3-Phosphocholine	281.099	2.64	M+Na[1+]	-0.0009	-2.99	yes
317.2117_4.66	CE5527,	317.2117	4.66	M+Na[1+]	0.0029	6.54	yes
153.1264_8.58	C00756, 1-Octanol	153.1264	8.58	M+Na[1+]	0.0013	-3.55	yes
285.2201_6.7	C14771, 14,15-EET	285.2201	6.7	M-H4O2+H[1+]	-0.0011	2.34	yes
239.2357_7.99	C00249, Hexadecanoic acid	239.2357	7.99	M-H2O+H[1+]	-0.0012	-2.82	yes
258.2507_8.47	C00249, Hexadecanoic acid	258.2507	8.47	M(C13)+H[1+]	-0.0002	-4.38	yes
283.2631_8.55	C01712, (9E)-Octadecenoic acid	283.2631	8.55	M+H[1+]	-0.0001	-3.72	yes
819.516_12.07	C02737, Phosphatidylserine	819.516	12.07	M-NH3+H[1+]	-0.0011	3.01	yes
150.0562_0.47	C00025, L-Glutamate	150.0562	0.47	M(S34)+H[1+]	-0.0001	-3.26	yes
182.1628_8.05	C16565,	182.1628	8.05	M+Na[1+]	0.0	-4.43	yes
335.2205_8.14	C04717, (9Z,11E)-(13S)-13-Hydroperoxyoctadeca-9,11-dienoic acid	335.2205	8.14	M+Na[1+]	0.0011	-2.89	yes
261.2208_8.56	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	261.2208	8.56	M-H2O+H[1+]	-0.0005	-5.75	yes
277.216_7.31	C16300, Stearidonic acid	277.216	7.31	M+H[1+]	-0.0002	-3.21	yes
182.1633_8.58	C16565,	182.1633	8.58	M+Na[1+]	0.0005	-3.52	yes
293.2448_7.35	C14771, 14,15-EET	293.2448	7.35	M-CO+H[1+]	-0.0026	-4.94	yes
356.2675_5.08	CE4786, nisinate	356.2675	5.08	M+H[1+]	-0.0035	4.34	yes
91.0582_0.45	C00213, Sarcosine	91.0582	0.45	M(C13)+H[1+]	-0.0002	-2.23	yes
326.2098_5.37	CE6504,	326.2098	5.37	M-H2O+H[1+]	0.0011	-2.24	yes
109.101_8.05	CE2577,	109.101	8.05	M-HCOOH+H[1+]	-0.0003	-3.01	yes
299.1968_4.63	C16300, Stearidonic acid	299.1968	4.63	M+Na[1+]	-0.0014	6.28	yes
371.0367_0.42	C00130, IMP	371.0367	0.42	M+Na[1+]	0.0003	-2.29	yes
245.2253_8.07	C01595, Linoleate	245.2253	8.07	M-H4O2+H[1+]	-0.001	-3.31	yes
386.0483_0.44	C00144, GMP	386.0483	0.44	M+Na[1+]	0.001	-2.65	yes
284.267_8.55	C00712, (9Z)-Octadecenoic acid	284.267	8.55	M(C13)+H[1+]	0.0004	-3.76	yes
241.2185_8.55	ptdca, pentadecanoate	241.2185	8.55	M[1+]	0.0017	-2.84	yes
242.2221_8.55	ptdca, pentadecanoate	242.2221	8.55	M+H[1+]	-0.0019	-2.81	yes
335.2217_4.72	C04717, (9Z,11E)-(13S)-13-Hydroperoxyoctadeca-9,11-dienoic acid	335.2217	4.72	M+Na[1+]	0.0023	5.52	yes
263.2366_8.93	C01595, Linoleate	263.2366	8.93	M-H2O+H[1+]	-0.0003	-5.13	yes
245.2247_8.93	C01595, Linoleate	245.2247	8.93	M-H4O2+H[1+]	-0.0016	-5.03	yes
315.0788_0.43	C04640, 2-(Formamido)-N1-(5'-phosphoribosyl)acetamidine	315.0788	0.43	M(C13)+H[1+]	0.0006	-2.49	yes

550.3867_7.54	C04598, 2-Acetyl-1-alkyl-sn-glycero-3-phosphocholine	550.3867	7.54	M+H[1+]	-0.0	2.17	yes
407.3322_7.45	C05437, Zymosterol	407.3322	7.45	M+Na[1+]	0.0037	-2.2	yes
287.101_2.1	C04148, alpha-N-Phenylacetyl-L-glutamine	287.101	2.1	M+Na[1+]	0.0007	2.23	yes
265.1195_2.1	C04148, alpha-N-Phenylacetyl-L-glutamine	265.1195	2.1	M+H[1+]	0.0012	2.47	yes
283.0321_0.45	C05640, Cinnavalininate	283.0321	0.45	M-H2O+H[1+]	-0.0028	-2.4	yes
343.032_0.41	C16634, 5-Fluorouridine monophosphate	343.032	0.41	M+H[1+]	-0.0017	-2.75	yes
232.1201_4.07	CE5982,	232.1201	4.07	M-H2O+H[1+]	-0.0005	-3.44	yes
377.1954_3.76	CE1342, 18-Hydroxycortisol	377.1954	3.76	M-H[-]	-0.0016	-2.51	yes
368.1606_4.46	C04555, 3beta-Hydroxyandrost-5-en-17-one 3-sulfate	368.1606	4.46	M(C13)-H[-]	-0.0012	3.67	yes
367.1579_4.46	C04555, 3beta-Hydroxyandrost-5-en-17-one 3-sulfate	367.1579	4.46	M-H[-]	-0.0005	3.63	yes
253.0837_4.12	C16584, p-Hydroxyfelbamate	253.0837	4.12	M-H[-]	0.0007	3.32	yes
252.0856_4.12	C16601, 2-Hydroxycarbamazepine	252.0856	4.12	M(C13)-H[-]	-0.0004	3.19	yes
251.0824_4.12	C16601, 2-Hydroxycarbamazepine	251.0824	4.12	M-H[-]	-0.0002	3.18	yes
208.0755_4.12	C16604, 2-Hydroxyiminostilbene	208.0755	4.12	M-H[-]	-0.0013	4.18	yes
101.0239_0.44	C02045,	101.0239	0.44	M-H2O-H[-]	-0.0005	4.21	yes
171.006_0.45	C01620,	171.006	0.45	M+Cl[-]	-0.0001	2.87	yes
699.4947_10.9	C00416, Phosphatidate	699.4947	10.9	M-H[-]	-0.0023	-3.14	yes
229.0107_0.44	C00199, D-Ribulose 5-phosphate	229.0107	0.44	M-H[-]	-0.0012	2.58	yes
319.2274_6.69	C14779, 9(S)-HETE	319.2274	6.69	M-H[-]	-0.0004	-2.5	yes
320.2307_6.69	C04805, 5(S)-HETE	320.2307	6.69	M(C13)-H[-]	-0.0005	-2.53	yes
89.0243_0.47	C01013, 3-Hydroxypropanoate	89.0243	0.47	M-H[-]	-0.0001	2.79	yes
360.0692_0.45	C06376, N-Acetyl-D-galactosamine 6-phosphate	360.0692	0.45	M+CH3COO[-]	-0.0004	4.07	yes
267.073_0.45	C00760, Cellulose	267.073	0.45	M-2H[2-]	0.0008	3.14	yes
317.2103_6.3	C04849, (5Z,9E,14Z)-(8xi,11R,12S)-11,12-Epoxy-8-hydroxyicosa-5,9,14-trienoic acid	317.2103	6.3	M-H2O-H[-]	-0.0019	-2.61	yes
196.0548_0.44	C00800, L-Gulonate	196.0548	0.44	M(C13)-H[-]	0.0004	2.51	yes
834.5231_12.05	C02737, Phosphatidylserine	834.5231	12.05	M-H[-]	-0.006	-2.65	yes
339.1995_10.29	CE6435,	339.1995	10.29	M-H2O-H[-]	0.003	-3.31	yes
700.4988_10.9	C00416, Phosphatidate	700.4988	10.9	M(C13)-H[-]	-0.0016	-2.55	yes
304.2364_7.98	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	304.2364	7.98	M(C13)-H[-]	0.0001	2.69	yes
303.2328_7.98	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	303.2328	7.98	M-H[-]	-0.0001	2.62	yes
195.0505_0.43	C16356, 1,7-Dimethyluric acid	195.0505	0.43	M-H[-]	-0.0018	3.3	yes
327.2326_7.86	C15647, 2-Acyl-1-(1-alkenyl)-sn-glycero-3-phosphate	327.2326	7.86	M-2H[2-]	0.0008	2.34	yes
301.217_7.57	C04805, 5(S)-HETE	301.217	7.57	M-H2O-H[-]	-0.0002	3.18	yes
160.0619_0.47	C00329, D-Glucosamine	160.0619	0.47	M-H2O-H[-]	0.0004	2.89	yes
353.2289_4.51	C00584, Prostaglandin E2	353.2289	4.51	M+H[1+]	-0.0034	-2.76	yes
211.0719_2.18	C00526, Deoxyuridine	211.0719	2.18	M-H2O+H[1+]	0.0006	-3.96	yes
198.0842_0.44	C00327, L-Citrulline	198.0842	0.44	M+Na[1+]	-0.0008	5.81	yes
114.056_0.42	C03912, (S)-1-Pyrroline-5-carboxylate	114.056	0.42	M+H[1+]	0.001	-2.48	yes
154.0593_0.43	C00300, Creatine	154.0593	0.43	M+Na[1+]	0.0005	-2.49	yes
90.0554_0.43	C00041, L-Alanine	90.0554	0.43	M+H[1+]	0.0004	-3.72	yes
511.2558_4.29	CE2303, 9-hydroxy-10-O-D-glucuronoside-12Z-octadecenoate	511.2558	4.29	M+Na[1+]	0.0044	2.48	yes
111.1175_4.31	CE6506,	111.1175	4.31	M-HCOOH+H[1+]	0.0006	2.66	yes
139.1118_4.31	CE6506,	139.1118	4.31	M-H2O+H[1+]	0.0001	2.52	yes
575.1162_0.44	C00760, Cellulose	575.1162	0.44	M+K[1+]	-0.0054	3.09	yes
559.1503_0.44	C00760, Cellulose	559.1503	0.44	M+Na[1+]	0.0022	2.83	yes
462.1772_4.03	C16643, Morphine-3-glucuronide	462.1772	4.03	M+H[1+]	0.0013	-3.74	yes
174.0546_1.42	C16596, 5-Phenyl-1,3-oxazinane-2,4-dione	174.0546	1.42	M-H2O+H[1+]	-0.0003	-4.5	yes

359.2581_5.95	CE6027, 24,25,26,27-tetranor-23-oxo-hydroxyvitamin D3	359.2581	5.95	M+H[1+]	0.0	-2.59	yes
427.3617_6.46	odecrn, octadecenoyl carnitine	427.3617	6.46	M(C13)+H[1+]	0.0005	3.29	yes
426.3584_6.46	odecrn, octadecenoyl carnitine	426.3584	6.46	M+H[1+]	0.0006	3.25	yes
269.2271_7.95	CE5014, anhydroretinol	269.2271	7.95	M+H[1+]	0.0007	-2.55	yes
270.2306_7.95	CE5014, anhydroretinol	270.2306	7.95	M(C13)+H[1+]	0.0008	-2.48	yes
422.3212_6.01	C02990, L-Palmitoylcarnitine	422.3212	6.01	M+Na[1+]	-0.003	2.54	yes
400.3425_6.36	C02990, L-Palmitoylcarnitine	400.3425	6.36	M+H[1+]	0.0003	5.4	yes
401.3452_6.36	C02990, L-Palmitoylcarnitine	401.3452	6.36	M(C13)+H[1+]	-0.0004	5.3	yes
450.3557_6.29	stcrn, stearoylcarnitine	450.3557	6.29	M+Na[1+]	0.0003	3.22	yes
447.3271_6.04	tmndnccrn, Timnodonyl carnitine	447.3271	6.04	M(C13)+H[1+]	-0.0028	2.71	yes
398.327_6.05	hdd2crn, trans-Hexadec-2-enoyl carnitine	398.327	6.05	M+H[1+]	0.0005	3.74	yes
399.3298_6.03	hdd2crn, trans-Hexadec-2-enoyl carnitine	399.3298	6.03	M(C13)+H[1+]	-0.0001	3.1	yes
425.3459_6.15	lneldccrn, Linoelaidyl carnitine	425.3459	6.15	M(C13)+H[1+]	0.0004	3.39	yes
424.3427_6.15	lneldccrn, Linoelaidyl carnitine	424.3427	6.15	M+H[1+]	0.0006	3.17	yes
451.3567_6.3	dlnlcgcrn, dihomo-gamma-linolenyl carnitine	451.3567	6.3	M(C13)+H[1+]	-0.0045	3.11	yes
458.1151_2.25	C00061, FMN	458.1151	2.25	M(C13)+H[1+]	-0.0002	-3.2	yes
324.062_0.46	C00055, CMP	324.062	0.46	M+H[1+]	0.0028	2.59	yes
169.0266_10.18	C05851,	169.0266	10.18	M+Na[1+]	0.0005	2.63	yes
280.2365_7.65	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	280.2365	7.65	M(C13)+H[1+]	0.0012	-3.22	yes
279.2304_7.66	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	279.2304	7.66	M+H[1+]	-0.0015	-3.06	yes
152.0317_2.56	C01879, 5-Oxoproline	152.0317	2.56	M+Na[1+]	-0.0002	2.63	yes
172.9588_12.15	C14453, 4-Bromophenol	172.9588	12.15	M+H[1+]	-0.0009	2.79	yes
303.2326_6.68	C04805, 5(S)-HETE	303.2326	6.68	M-H2O+H[1+]	0.0008	-2.65	yes
413.0469_1.89	C01194, 1-Phosphatidyl-D-myo-inositol	413.0469	1.89	M+Na[1+]	0.0013	-2.47	yes
158.0918_0.4	C00327, L-Citrulline	158.0918	0.4	M-H2O+H[1+]	-0.0006	-5.11	yes
146.0352_0.46	C00555, 4-Aminobutanal	146.0352	0.46	M+NaCl[1+]	0.0009	2.62	yes
382.0367_0.46	C16619, 6-Thioguanosine monophosphate	382.0367	0.46	M(S34)+H[1+]	-0.0016	-3.42	yes
260.0742_0.42	CE2847, fructoseglycine	260.0742	0.42	M+Na[1+]	0.0001	-2.59	yes
222.1622_7.98	CE5325, 6(S)-hydroxy-tetradeca-4E,8Z-dienoate	222.1622	7.98	M-H2O+H[1+]	0.0008	-2.56	yes
321.2411_7.14	C04805, 5(S)-HETE	321.2411	7.14	M+H[1+]	-0.0013	-2.36	yes
303.2325_7.58	C04805, 5(S)-HETE	303.2325	7.58	M-H2O+H[1+]	0.0007	3.27	yes
285.222_7.57	C04805, 5(S)-HETE	285.222	7.57	M-H4O2+H[1+]	0.0008	3.37	yes
244.0768_0.43	C01132, N-Acetyl-D-galactosamine	244.0768	0.43	M+Na[1+]	-0.0024	-3.02	yes
305.2484_7.98	C00473, Retinol	305.2484	7.98	M+H2O+H[1+]	0.0008	2.49	yes
287.2372_7.98	C00473, Retinol	287.2372	7.98	M+H[1+]	0.0002	2.45	yes
288.2407_7.98	C00473, Retinol	288.2407	7.98	M(C13)+H[1+]	0.0003	2.32	yes
363.2158_3.66	C01124, 18-Hydroxycorticosterone	363.2158	3.66	M+H[1+]	-0.0008	3.49	yes
273.2201_4.66	C00619, 3-Oxo-delta4-steroid	273.2201	4.66	M+H[1+]	-0.0012	3.54	yes
489.2457_4.65	5adtststeroneglc, 5alpha-Dihydrotestosterone glucuronide	489.2457	4.65	M+Na[1+]	-0.0002	3.27	yes
647.4999_8.87	C00165, Diacylglycerol	647.4999	8.87	M-H2O+H[1+]	-0.0035	-3.28	yes
306.2519_7.98	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	306.2519	7.98	M(C13)+H[1+]	0.001	2.47	yes
320.2668_8.78	C05480, 3alpha-Hydroxy-5beta-pregnane-20-one	320.2668	8.78	M(C13)+H[1+]	0.0002	2.76	yes
319.2637_8.78	C05480, 3alpha-Hydroxy-5beta-pregnane-20-one	319.2637	8.78	M+H[1+]	0.0005	2.7	yes
255.2111_4.69	C00523, Androsterone	255.2111	4.69	M-H4O2+H[1+]	0.0004	3.72	yes
311.1972_3.58	C01227, 3beta-Hydroxyandrost-5-en-17-one	311.1972	3.58	M+Na[1+]	-0.001	3.26	yes
304.2363_7.57	CE5013,	304.2363	7.57	M(C13)+H[1+]	0.001	3.26	yes
347.2222_3.68	C05474, 3alpha,11beta,21-Trihydroxy-20-oxo-5beta-pregnan-18-al	347.2222	3.68	M-H2O+H[1+]	0.0005	3.93	yes

361.2015_3.87	C01780, Aldosterone	361.2015	3.87	M+H[1+]	0.0005	4.13	yes
370.2955_5.52	C00836, Sphinganine	370.2955	5.52	M+HCOONa[1+]	0.0027	2.94	yes
296.0651_0.4	C00055, CMP	296.0651	0.4	M-CO+H[1+]	0.0009	3.44	yes
532.3807_7.65	C04598, 2-Acetyl-1-alkyl-sn-glycero-3-phosphocholine	532.3807	7.65	M-H2O+H[1+]	0.0046	2.55	yes
376.2592_5.34	CE5719, 9'-carboxy-gama-chromanol	376.2592	5.34	M+H[1+]	-0.0016	2.23	yes
423.3238_6.01	CE7144, 13'-hydroxy-alpha-tocotrienol	423.3238	6.01	M-H2O+H[1+]	-0.0019	2.47	yes
607.3526_9.01	CE4754, dynorphin B (6-9)	607.3526	9.01	M[1+]	-0.0028	-2.41	yes
283.2641_9.01	C01530, Octadecanoic acid	283.2641	9.01	M-H[-]	-0.0001	2.7	yes
128.0353_0.44	C01879, 5-Oxoproline	128.0353	0.44	M-H[-]	-0.0	2.63	yes
256.2362_8.43	C00249, Hexadecanoic acid	256.2362	8.43	M(C13)-H[-]	-0.0001	6.71	yes
255.2329_8.43	C00249, Hexadecanoic acid	255.2329	8.43	M-H[-]	-0.0	6.08	yes
279.0381_0.43	C00299, Uridine	279.0381	0.43	M+Cl[-]	-0.0003	2.74	yes
243.0622_0.43	C00299, Uridine	243.0622	0.43	M-H[-]	-0.0	2.63	yes
281.2486_8.52	C01712, (9E)-Octadecenoic acid	281.2486	8.52	M-H[-]	-0.0	3.33	yes
465.249_4.65	ahandrostanglc, Etiocholan-3alpha-ol-17-one 3-glucuronide	465.249	4.65	M-H[-]	-0.0004	2.98	yes
349.2356_8.52	C05476, Tetrahydrocorticosterone	349.2356	8.52	M-H[-]	-0.0028	3.09	yes
571.2882_7.52	C05791, D-Urobilinogen	571.2882	7.52	M-H2O-H[-]	-0.0043	2.64	yes
282.2519_8.52	C00712, (9Z)-Octadecenoic acid	282.2519	8.52	M(C13)-H[-]	-0.0001	3.68	yes
347.2202_8.04	C05472, Urocortisol	347.2202	8.04	M-H2O-H[-]	-0.0025	3.21	yes
280.2366_8.04	C01595, Linoleate	280.2366	8.04	M(C13)-H[-]	0.0003	2.55	yes
132.0301_0.43	C00402, D-Aspartate	132.0301	0.43	M-H[-]	-0.0001	2.9	yes
167.0171_3.35	C01185, Nicotinate D-ribonucleotide	167.0171	3.35	M-2H[2-]	0.0002	-2.52	yes
312.1715_7.36	CE7110, 5,6-epoxy,18R-HEPE	312.1715	7.36	M-H2O-H[-]	-0.0016	7.26	yes
263.1034_2.06	C04148, alpha-N-Phenylacetyl-L-glutamine	263.1034	2.06	M-H[-]	-0.0003	2.56	yes
268.076_0.43	C00294, Inosine	268.076	0.43	M(C13)-H[-]	-0.0009	2.82	yes
267.0734_0.44	C00294, Inosine	267.0734	0.44	M-H[-]	-0.0001	3.37	yes
146.046_0.42	C00025, L-Glutamate	146.046	0.42	M-H[-]	0.0001	2.42	yes
300.0469_0.44	CE3075, sorbitol 3-phosphate	300.0469	0.44	M+ACN-H[-]	-0.0021	3.0	yes
178.051_1.88	C01586, Hippurate	178.051	1.88	M-H[-]	0.0001	-2.79	yes
306.0766_0.44	C00051, Glutathione	306.0766	0.44	M-H[-]	0.0001	-2.65	yes
121.0293_3.15	C00180, Benzoate	121.0293	3.15	M-H[-]	-0.0002	2.41	yes
319.2278_6.68	C14771, 14,15-EET	319.2278	6.68	M-H[-]	-0.0	-2.71	yes
320.2311_6.68	C14771, 14,15-EET	320.2311	6.68	M(C13)-H[-]	-0.0001	-2.65	yes
301.2167_6.68	C14771, 14,15-EET	301.2167	6.68	M-H2O-H[-]	-0.0005	-2.62	yes
279.2329_8.04	C01595, Linoleate	279.2329	8.04	M-H[-]	-0.0	-4.44	yes
295.2277_6.42	C14826, 12(13)-EpOME	295.2277	6.42	M-H[-]	-0.0001	-3.36	yes
296.2311_6.42	C14826, 12(13)-EpOME	296.2311	6.42	M(C13)-H[-]	-0.0001	-3.37	yes
183.9881_0.1	C05698, Selenohomocysteine	183.9881	0.1	M+H[1+]	0.0009	-2.55	yes
327.2277_8.53	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	327.2277	8.53	M+Na[1+]	-0.0018	2.4	yes
324.2083_8.6	CE2540, timnodonate	324.2083	8.6	M+Na[1+]	0.0023	3.96	yes
613.1595_0.47	C00127, Glutathione disulfide	613.1595	0.47	M+H[1+]	0.0002	-5.19	yes
255.2113_4.65	C00523, Androsterone	255.2113	4.65	M-H4O2+H[1+]	0.0006	2.5	yes
273.2217_4.65	C00523, Androsterone	273.2217	4.65	M-H2O+H[1+]	0.0004	2.48	yes
282.2797_5.76	C02934, 3-Dehydrosphinganine	282.2797	5.76	M-H2O+H[1+]	0.0006	2.79	yes
300.2903_5.76	C02934, 3-Dehydrosphinganine	300.2903	5.76	M+H[1+]	0.0006	2.73	yes
301.2927_5.76	C02934, 3-Dehydrosphinganine	301.2927	5.76	M(C13)+H[1+]	-0.0004	2.6	yes
322.2715_5.75	C02934, 3-Dehydrosphinganine	322.2715	5.75	M+Na[1+]	-0.0002	3.11	yes

301.2168_6.32	C04686, (13E)-(15S)-15-Hydroxy-9-oxoprosta-11,13-dienoate	301.2168	6.32	M-H4O2+H[1+]	0.0006	-2.37	yes
393.2211_8.45	C05963,	393.2211	8.45	M+Na[1+]	-0.0037	5.23	yes
353.2305_4.45	C00584, Prostaglandin E2	353.2305	4.45	M+H[1+]	-0.0018	-2.89	yes
353.2306_4.8	C00584, Prostaglandin E2	353.2306	4.8	M+H[1+]	-0.0017	-3.86	yes
239.2362_8.44	C00249, Hexadecanoic acid	239.2362	8.44	M-H2O+H[1+]	-0.0007	3.52	yes
258.2507_8.44	C00249, Hexadecanoic acid	258.2507	8.44	M(C13)+H[1+]	-0.0002	3.19	yes
257.2478_8.44	C00249, Hexadecanoic acid	257.2478	8.44	M+H[1+]	0.0003	3.09	yes
489.2473_4.64	5adtststeroneglc, 5alpha-Dihydrotestosterone glucuronide	489.2473	4.64	M+Na[1+]	0.0014	3.09	yes
183.988_12.93	C05698, Selenohomocysteine	183.988	12.93	M+H[1+]	0.0008	-2.76	yes
302.3059_5.9	C00836, Sphinganine	302.3059	5.9	M+H[1+]	0.0005	2.34	yes
583.2556_4.96	C00500, Biliverdin	583.2556	4.96	M+H[1+]	0.0005	-4.78	yes
583.2561_5.21	C00500, Biliverdin	583.2561	5.21	M+H[1+]	0.001	-4.11	yes
173.0429_0.41	C00121, D-Ribose	173.0429	0.41	M+Na[1+]	0.0008	3.41	yes
431.2443_4.65	CE5730,	431.2443	4.65	M+Na[1+]	0.0038	2.39	yes
591.3154_3.08	C05791, D-Urobilinogen	591.3154	3.08	M+H[1+]	-0.0023	-2.82	yes
607.2571_8.73	C00486, Bilirubin	607.2571	8.73	M+Na[1+]	0.0043	3.29	yes
585.2745_8.73	C00486, Bilirubin	585.2745	8.73	M+H[1+]	0.0037	2.79	yes
363.2169_3.84	C01124, 18-Hydroxycorticosterone	363.2169	3.84	M+H[1+]	0.0003	2.31	yes
569.3112_2.96	C01079, Protoporphyrinogen IX	569.3112	2.96	M+H[1+]	-0.0011	-6.08	yes
562.403_10.59	C05200, 3-Hexaprenyl-4,5-dihydroxybenzoate	562.403	10.59	M[1+]	0.0008	2.57	yes
242.1023_2.53	C00864, Pantothenate	242.1023	2.53	M+Na[1+]	0.0023	2.58	yes
181.0627_2.52	C02909, (2-Naphthyl)methanol	181.0627	2.52	M+Na[1+]	0.0002	3.05	yes
168.0623_5.61	C02946, 4-Acetamidobutanoate	168.0623	5.61	M+Na[1+]	-0.0009	2.94	yes
180.0662_2.53	CE5536, adrenochrome	180.0662	2.53	M+H[1+]	0.0007	2.88	yes
174.0392_0.41	C00242, Guanine	174.0392	0.41	M+Na[1+]	0.0005	2.92	yes
359.2203_6.16	C04849, (5Z,9E,14Z)-(8xi,11R,12S)-11,12-Epoxy-8-hydroxyicosa-5,9,14-trienoic acid	359.2203	6.16	M+Na[1+]	0.0009	3.34	yes
377.1461_2.42	C00255, Riboflavin	377.1461	2.42	M+H[1+]	0.0005	3.62	yes
283.0198_0.46	CE3075, sorbitol 3-phosphate	283.0198	0.46	M+Na[1+]	0.0008	2.63	yes
136.0761_0.62	C03758, Dopamine	136.0761	0.62	M-H2O+H[1+]	0.0004	2.61	yes
167.0708_5.61	C05581, 3-Methoxy-4-hydroxyphenylacetaldehyde	167.0708	5.61	M+H[1+]	0.0005	3.16	yes
94.0658_0.61	CE2172,	94.0658	0.61	M-C3H4O2+H[1+]	0.0006	2.4	yes
118.0867_0.42	C00719, Betaine	118.0867	0.42	M+H[1+]	0.0004	-3.09	yes
139.9885_12.14	C00227, Acetyl phosphate	139.9885	12.14	M[1+]	0.001	-2.88	yes
140.9961_12.14	C00227, Acetyl phosphate	140.9961	12.14	M+H[1+]	0.0013	-2.63	yes
137.0464_0.44	C00262, Hypoxanthine	137.0464	0.44	M+H[1+]	0.0006	-2.84	yes
159.0273_0.43	C00262, Hypoxanthine	159.0273	0.43	M+Na[1+]	-0.0005	-2.59	yes
138.0489_0.44	C00262, Hypoxanthine	138.0489	0.44	M(C13)+H[1+]	-0.0003	-3.78	yes
120.0812_0.64	C00483, Tyramine	120.0812	0.64	M-H2O+H[1+]	0.0004	-2.8	yes
150.0541_0.43	C05578, 5,6-Dihydroxyindole	150.0541	0.43	M+H[1+]	-0.0009	-2.63	yes
167.09_0.64	C02076, Sedoheptulose	167.09	0.64	M-CO2+H[1+]	-0.0015	-2.65	yes
124.0614_0.42	C00242, Guanine	124.0614	0.42	M-CO+H[1+]	-0.0003	-4.52	yes
252.0885_4.11	C01136, S-Acetyldihydrolipoamide	252.0885	4.11	M(S34)+H[1+]	-0.0003	-2.66	yes
149.0603_0.64	C05581, 3-Methoxy-4-hydroxyphenylacetaldehyde	149.0603	0.64	M-H2O+H[1+]	0.0006	-3.06	yes
166.0867_0.64	CE2172,	166.0867	0.64	M+H[1+]	0.0004	-2.77	yes
116.0711_0.42	C00148, L-Proline	116.0711	0.42	M+H[1+]	0.0005	-2.92	yes
155.0475_0.41	C06608, Diethylphosphoric acid	155.0475	0.41	M+H[1+]	0.0007	-3.24	yes
114.0662_0.41	C00300, Creatine	114.0662	0.41	M-H2O+H[1+]	0.0	-3.16	yes

313.0318_0.43	C05382, D-Sedoheptulose 7-phosphate	313.0318	0.43	M+Na[1+]	0.0022	-3.28	yes
307.0445_0.43	C00294, Inosine	307.0445	0.43	M+K[1+]	0.0009	-2.66	yes
445.3686_9.77	CE5838,	445.3686	9.77	M-H2O+H[1+]	0.001	3.83	yes
442.3445_5.61	CE5843, 13'-carboxy-alpha-tocopherol	442.3445	5.61	M-H2O+H[1+]	0.0004	2.43	yes
473.345_6.08	c226crn, cervonyl carnitine	473.345	6.08	M(C13)+H[1+]	-0.0005	3.12	yes
472.3421_6.08	c226crn, cervonyl carnitine	472.3421	6.08	M+H[1+]	-0.0	2.79	yes
427.3615_6.43	odecrn, octadecenoyl carnitine	427.3615	6.43	M(C13)+H[1+]	0.0003	2.44	yes
426.3583_6.43	odecrn, octadecenoyl carnitine	426.3583	6.43	M+H[1+]	0.0005	2.5	yes
446.3258_5.84	lneldccrn, Linoelaidyl carnitine	446.3258	5.84	M+Na[1+]	0.0017	3.12	yes
415.3602_6.55	CE5655, 13'-hydroxy-gama-tocopherol	415.3602	6.55	M-H2O+H[1+]	0.0032	3.15	yes
398.327_6.21	hdd2crn, trans-Hexadec-2-enoyl carnitine	398.327	6.21	M+H[1+]	0.0005	2.43	yes
218.1381_0.46	pcrn, propionyl-carnitine	218.1381	0.46	M+H[1+]	-0.0006	3.27	yes
450.3583_6.3	stcrn, stearoylcarnitine	450.3583	6.3	M+Na[1+]	0.0029	2.45	yes
447.3299_6.07	tmndnccrn, Timnodonyl carnitine	447.3299	6.07	M(C13)+H[1+]	0.0	2.41	yes
424.3428_6.12	lneldccrn, Linoelaidyl carnitine	424.3428	6.12	M+H[1+]	0.0007	2.42	yes
425.346_6.12	lneldccrn, Linoelaidyl carnitine	425.346	6.12	M(C13)+H[1+]	0.0005	2.37	yes
451.3602_6.3	dlnlcgcrn, dihomo-gamma-linolenyl carnitine	451.3602	6.3	M(C13)+H[1+]	-0.001	2.92	yes
429.3773_6.8	stcrn, stearoylcarnitine	429.3773	6.8	M(C13)+H[1+]	0.0005	2.47	yes
428.374_6.8	stcrn, stearoylcarnitine	428.374	6.8	M+H[1+]	0.0006	2.39	yes
425.3461_6.33	lneldccrn, Linoelaidyl carnitine	425.3461	6.33	M(C13)+H[1+]	0.0006	2.38	yes
449.346_6.11	arachdcrn, C20:4 carnitine	449.346	6.11	M(C13)+H[1+]	0.0005	3.19	yes
448.3426_6.11	arachdcrn, C20:4 carnitine	448.3426	6.11	M+H[1+]	0.0005	2.81	yes
414.3584_6.55	hpdcacrn, heptadecanoyl carnitine	414.3584	6.55	M+H[1+]	0.0006	2.34	yes
456.4035_7.22	arachcrn, arachidyl carnitine	456.4035	7.22	M+H[1+]	-0.0012	2.8	yes
474.3566_6.21	clpndcrn, clupanodonyl carnitine	474.3566	6.21	M+H[1+]	-0.0012	4.44	yes
429.2994_8.04	CE2204, 25-hydroxyvitamin D3-26,23-lactone	429.2994	8.04	M+H[1+]	-0.0005	4.25	yes
281.248_8.05	C01595, Linoleate	281.248	8.05	M+H[1+]	0.0005	-3.68	yes
263.2374_8.05	C01595, Linoleate	263.2374	8.05	M-H2O+H[1+]	0.0005	-3.6	yes
245.2269_8.05	C01595, Linoleate	245.2269	8.05	M-H4O2+H[1+]	0.0006	-3.58	yes
401.2669_7.53	C13856, 2-Arachidonoylglycerol	401.2669	7.53	M+Na[1+]	0.0006	2.36	yes
320.2272_6.42	C00909, Leukotriene A4	320.2272	6.42	M(C13)+H[1+]	-0.003	-3.3	yes
319.2247_6.42	C00909, Leukotriene A4	319.2247	6.42	M+H[1+]	-0.0021	-3.14	yes
329.2481_6.77	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	329.2481	6.77	M+Na[1+]	0.0029	-2.39	yes
305.248_6.85	C01712, (9E)-Octadecenoic acid	305.248	6.85	M+Na[1+]	0.0028	-3.34	yes
309.0437_0.43	C03838, 5'-Phosphoribosylglycinamide	309.0437	0.43	M+Na[1+]	-0.0022	6.72	yes
307.2634_7.02	C01530, Octadecanoic acid	307.2634	7.02	M+Na[1+]	0.0026	-3.64	yes
85.1014_8.52	CE6506,	85.1014	8.52	M-C3H4O2+H[1+]	0.0002	-3.52	yes
139.1113_8.53	CE6506,	139.1113	8.53	M-H2O+H[1+]	-0.0004	-3.02	yes
121.1017_8.52	CE6506,	121.1017	8.52	M-H4O2+H[1+]	0.0006	-2.21	yes
325.2144_8.05	CE5013,	325.2144	8.05	M+Na[1+]	0.0005	-3.36	yes
283.2636_8.53	C01712, (9E)-Octadecenoic acid	283.2636	8.53	M+H[1+]	0.0004	-2.87	yes
291.0693_0.43	C00294, Inosine	291.0693	0.43	M+Na[1+]	-0.0008	4.79	yes
321.2428_6.98	C04805, 5(S)-HETE	321.2428	6.98	M+H[1+]	0.0004	-2.83	yes
447.238_12.2	CE5708, 15-oxo-Prostaglandin E2 glyceryl ester	447.238	12.2	M+Na[1+]	0.0026	2.97	yes
343.225_6.69	C14779, 9(S)-HETE	343.225	6.69	M+Na[1+]	0.0006	-2.44	yes
279.2321_7.64	C00249, Hexadecanoic acid	279.2321	7.64	M+Na[1+]	0.0026	-6.03	yes
261.2197_7.64	C14826, 12(13)-EpOME	261.2197	7.64	M-H4O2+H[1+]	-0.0015	-5.01	yes

303.2324_6.69	C01595, Linoleate	303.2324	6.69	M+Na[1+]	0.0029	-2.35	yes
325.2135_6.69	CE5013,	325.2135	6.69	M+Na[1+]	-0.0004	-2.94	yes
267.21_6.69	CE5013,	267.21	6.69	M-H4O2+H[1+]	-0.0007	-2.81	yes
285.2214_6.68	CE5013,	285.2214	6.68	M-H2O+H[1+]	0.0001	-2.41	yes
304.2359_6.68	CE5013,	304.2359	6.68	M(C13)+H[1+]	0.0006	-2.33	yes
153.1278_8.53	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	153.1278	8.53	M+2H[2+]	0.0004	-3.07	yes
375.2151_4.86	C00584, Prostaglandin E2	375.2151	4.86	M+Na[1+]	0.0008	-4.11	yes
567.2633_6.66	C00486, Bilirubin	567.2633	6.66	M-H2O+H[1+]	0.0031	2.71	yes
289.2164_3.85	C01227, 3beta-Hydroxyandrost-5-en-17-one	289.2164	3.85	M+H[1+]	0.0002	2.38	yes
306.2513_6.85	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	306.2513	6.85	M(C13)+H[1+]	0.0004	-3.76	yes
326.2201_8.06	arachd, arachidonic acid	326.2201	8.06	M+Na[1+]	-0.0016	-2.65	yes
277.2167_6.31	C14765, 13-OxoODE	277.2167	6.31	M-H2O+H[1+]	0.0005	-4.19	yes
330.2512_6.77	C06429, (4Z,7Z,10Z,13Z,16Z,19Z)-Docosahexaenoic acid	330.2512	6.77	M(C13)+H[1+]	0.0003	-2.74	yes
530.3584_7.01	C04230, 1-Acyl-sn-glycero-3-phosphocholine	530.3584	7.01	M+Na[1+]	0.0002	-2.65	yes
836.5425_12.14	C02737, Phosphatidylserine	836.5425	12.14	M+H[1+]	-0.0011	3.65	yes
858.5245_12.07	C02737, Phosphatidylserine	858.5245	12.07	M+Na[1+]	-0.0011	4.79	yes
835.5294_12.07	C02737, Phosphatidylserine	835.5294	12.07	M[1+]	-0.0069	4.39	yes
837.5464_12.14	C02737, Phosphatidylserine	837.5464	12.14	M(C13)+H[1+]	-0.0006	4.05	yes
83.0861_8.05	C02373, 4-Methylpentanal	83.0861	8.05	M-H2O+H[1+]	0.0006	-2.96	yes
155.1073_8.05	CE2577,	155.1073	8.05	M+H[1+]	0.0006	-3.24	yes
169.1227_8.05	CE2061,	169.1227	8.05	M+H[1+]	0.0004	-3.48	yes
97.1016_8.05	CE2061,	97.1016	8.05	M-C3H4O2+H[1+]	0.0004	-2.77	yes
133.1015_8.05	CE2061,	133.1015	8.05	M-H4O2+H[1+]	0.0004	-2.59	yes
247.2397_8.53	C00712, (9Z)-Octadecenoic acid	247.2397	8.53	M-H4O2+H[1+]	-0.0023	-3.12	yes
265.2531_8.53	C00712, (9Z)-Octadecenoic acid	265.2531	8.53	M-H2O+H[1+]	0.0005	-3.08	yes
280.2333_6.42	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	280.2333	6.42	M(C13)+H[1+]	-0.002	-3.22	yes
139.112_8.06	CE6506,	139.112	8.06	M-H2O+H[1+]	0.0003	-3.16	yes
83.0861_8.52	C02373, 4-Methylpentanal	83.0861	8.52	M-H2O+H[1+]	0.0006	-2.46	yes
365.1058_0.41	C06373, beta-D-Gal-(1->4)-D-Glc	365.1058	0.41	M+Na[1+]	0.0003	-3.19	yes
381.0792_0.4	C06373, beta-D-Gal-(1->4)-D-Glc	381.0792	0.4	M+K[1+]	0.0002	-2.37	yes
332.266_7.14	CE2510,	332.266	7.14	M+Na[1+]	-0.0026	-2.4	yes
280.2366_7.64	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	280.2366	7.64	M(C13)+H[1+]	0.0013	-6.42	yes
1138.4528_11.93	3ohxccoa, 3-Oxohexacosyl-CoA	1138.4528	11.93	M-H2O+H[1+]	0.0068	3.23	yes
1070.4642_11.94	CE2257, tetracosanoyl-CoA	1070.4642	11.94	M-CO2+H[1+]	0.0079	2.62	yes
468.3103_7.0	tmndnccrn, Timnodonyl carnitine	468.3103	7.0	M+Na[1+]	0.0018	2.26	yes
366.1401_6.57	C00611, N-Acetyllactosamine	366.1401	6.57	M-H2O+H[1+]	0.0006	-2.48	yes
282.0831_0.44	C00387, Guanosine	282.0831	0.44	M-H[-]	-0.0013	2.37	yes
129.055_1.96	C00233, 4-Methyl-2-oxopentanoate	129.055	1.96	M-H[-]	-0.0007	2.67	yes
128.0347_0.45	C01879, 5-Oxoproline	128.0347	0.45	M-H[-]	-0.0006	3.53	yes
339.9919_0.53	C03785, D-Tagatose 1,6-bisphosphate	339.9919	0.53	M(C13)-H[-]	-0.0002	3.0	yes
338.9882_0.53	C03785, D-Tagatose 1,6-bisphosphate	338.9882	0.53	M-H[-]	-0.0005	2.69	yes
466.2522_4.66	C11135, Androsterone glucuronide	466.2522	4.66	M(C13)-H[-]	-0.0006	2.85	yes
465.2489_4.66	C11135, Androsterone glucuronide	465.2489	4.66	M-H[-]	-0.0005	2.7	yes
226.9887_0.42	C00129, Isopentenyl diphosphate	226.9887	0.42	M-H2O-H[-]	0.0008	-3.25	yes
127.0503_0.4	C05100, 3-Ureidoisobutyrate	127.0503	0.4	M-H2O-H[-]	-0.0009	2.62	yes
378.2409_5.91	C06124, Sphingosine 1-phosphate	378.2409	5.91	M-H[-]	-0.0006	2.9	yes
86.0241_0.45	C00439, N-Formimino-L-glutamate	86.0241	0.45	M-2H[2-]	-0.0007	2.97	yes

215.0322_0.41	C00124, D-Galactose	215.0322	0.41	M+Cl[-]	-0.0001	2.77	yes
195.0502_0.42	C00124, D-Galactose	195.0502	0.42	M-H+O[-]	-0.0008	3.82	yes
74.0185_0.41	C00121, D-Ribose	74.0185	0.41	M-2H[2-]	-0.0006	2.46	yes
324.0929_0.43	C03410, N-Glycoloyl-neuraminate	324.0929	0.43	M-H[-]	-0.0007	2.71	yes
194.0198_0.44	C01194, 1-Phosphatidyl-D-myo-inositol	194.0198	0.44	M-2H[2-]	-0.0011	3.06	yes
784.1507_2.21	C00016, FAD	784.1507	2.21	M-H[-]	0.0009	2.4	yes
606.0739_0.49	C00203, UDP-N-acetyl-D-galactosamine	606.0739	0.49	M-H[-]	-0.0004	2.97	yes
607.0766_0.48	C00203, UDP-N-acetyl-D-galactosamine	607.0766	0.48	M(C13)-H[-]	-0.0011	2.62	yes
140.0113_0.42	C00346, Ethanolamine phosphate	140.0113	0.42	M-H[-]	-0.0005	2.45	yes
112.0399_0.46	C03912, (S)-1-Pyrroline-5-carboxylate	112.0399	0.46	M-H[-]	-0.0005	5.21	yes
271.2059_4.56	C00523, Androsterone	271.2059	4.56	M-H2O-H[-]	-0.0008	2.85	yes
154.0612_0.38	C00135, L-Histidine	154.0612	0.38	M-H[-]	-0.001	2.49	yes
101.0239_0.43	C00232, Succinate semialdehyde	101.0239	0.43	M-H[-]	-0.0005	2.92	yes
151.024_0.44	C01620,	151.024	0.44	M-H+O[-]	-0.0008	-3.34	yes
588.0752_0.51	C00325, GDP-L-fucose	588.0752	0.51	M-H[-]	0.0003	2.63	yes
255.2317_6.33	C00249, Hexadecanoic acid	255.2317	6.33	M-H[-]	-0.0012	2.63	yes
258.0404_1.33	C06377, D-Galactosamine 6-phosphate	258.0404	1.33	M-H[-]	0.002	2.32	yes
218.1027_0.63	C00864, Pantothenate	218.1027	0.63	M-H[-]	-0.0007	2.33	yes
346.0553_0.44	C00020, AMP	346.0553	0.44	M-H[-]	-0.0005	4.34	yes
351.2171_4.56	C05963,	351.2171	4.56	M-H2O-H[-]	-0.0005	-2.46	yes
352.2205_4.56	C00584, Prostaglandin E2	352.2205	4.56	M(C13)-H[-]	-0.0006	-2.49	yes
333.2066_4.56	C00584, Prostaglandin E2	333.2066	4.56	M-H2O-H[-]	-0.0005	-2.46	yes
363.2151_6.43	C05474, 3alpha,11beta,21-Trihydroxy-20-oxo-5beta-pregnan-18-al	363.2151	6.43	M-H[-]	-0.0026	-3.11	yes
393.2274_4.54	C05954, Prostaglandin B2	393.2274	4.54	M+CH3COO[-]	-0.0003	-2.57	yes
315.1961_4.56	C05954, Prostaglandin B2	315.1961	4.56	M-H2O-H[-]	-0.0004	-2.47	yes
334.21_4.56	C05954, Prostaglandin B2	334.21	4.56	M(C13)-H[-]	-0.0005	-2.45	yes
584.2592_8.73	C00486, Bilirubin	584.2592	8.73	M(C13)-H[-]	-0.0004	3.98	yes
583.2553_8.73	C00486, Bilirubin	583.2553	8.73	M-H[-]	-0.0009	3.8	yes
353.2325_4.92	C05959, 11-epi-Prostaglandin F2alpha	353.2325	4.92	M-H[-]	-0.0008	-2.63	yes
369.2277_4.38	C05959, 11-epi-Prostaglandin F2alpha	369.2277	4.38	M-H+O[-]	-0.0005	-3.23	yes
159.092_1.07	C00390, Ubiquinol	159.092	1.07	M-2H[2-]	-0.0001	-2.76	yes
138.0199_0.55	C00870, 4-Nitrophenol	138.0199	0.55	M-H[-]	0.0003	4.93	yes
142.9982_0.44	C01127, 4-Hydroxy-2-oxoglutarate	142.9982	0.44	M-H2O-H[-]	-0.0003	-2.55	yes
146.0454_0.42	C01110, 5-Amino-2-oxopentanoic acid	146.0454	0.42	M-H+O[-]	-0.0004	-2.36	yes
102.0555_0.42	C05145, 3-Aminoisobutyric acid	102.0555	0.42	M-H[-]	-0.0005	-2.2	yes
648.8542_11.89	C04884, N-Acetyl-D-galactosaminyl-(N-acetylneuraminyl)-D-galactosyl-D-glucosylceramide	648.8542	11.89	M-2H[2-]	-0.0035	-3.02	yes
88.0397_0.42	C00041, L-Alanine	88.0397	0.42	M-H[-]	-0.0007	-3.89	yes
135.0302_0.43	C01013, 3-Hydroxypropanoate	135.0302	0.43	M+HCOO[-]	0.0009	-3.0	yes
222.1618_7.97	CE5325, 6(S)-hydroxy-tetradeca-4E,8Z-dienoate	222.1618	7.97	M-H2O+H[1+]	0.0004	2.51	yes
317.212_4.56	C00584, Prostaglandin E2	317.212	4.56	M-H4O2+H[1+]	0.0009	2.83	yes
335.2225_4.56	C00584, Prostaglandin E2	335.2225	4.56	M-H2O+H[1+]	0.0008	2.83	yes
222.9976_0.38	C00279, D-Erythrose 4-phosphate	222.9976	0.38	M+Na[1+]	-0.0003	2.62	yes
375.215_4.88	C00584, Prostaglandin E2	375.215	4.88	M+Na[1+]	0.0007	5.82	yes
369.3543_9.89	C00187, Cholesterol	369.3543	9.89	M-H2O+H[1+]	0.0027	-2.47	yes
322.9936_0.61	C03785, D-Tagatose 1,6-bisphosphate	322.9936	0.61	M-H2O+H[1+]	0.0009	3.19	yes
378.96_0.53	C03785, D-Tagatose 1,6-bisphosphate	378.96	0.53	M+K[1+]	0.0012	2.89	yes
362.9868_0.53	C03785, D-Tagatose 1,6-bisphosphate	362.9868	0.53	M+Na[1+]	0.0015	2.66	yes

377.23_4.49	C05959, 11-epi-Prostaglandin F2alpha	377.23	4.49	M+Na[1+]	0.0001	2.64	yes
319.2266_4.49	C05959, 11-epi-Prostaglandin F2alpha	319.2266	4.49	M-H4O2+H[1+]	-0.0001	2.69	yes
265.2166_4.55	C04849, (5Z,9E,14Z)-(8xi,11R,12S)-11,12-Epoxy-8-hydroxyicosa-5,9,14-trienoic acid	265.2166	4.55	M-C3H4O2+H[1+]	0.0003	2.94	yes
116.0713_0.43	C00148, L-Proline	116.0713	0.43	M+H[1+]	0.0007	2.55	yes
298.0979_1.1	C00170, 5'-Methylthioadenosine	298.0979	1.1	M+H[1+]	0.001	2.39	yes
154.9965_0.11	C00036, Oxaloacetate	154.9965	0.11	M+Na[1+]	0.0013	2.49	yes
271.2064_4.56	C01227, 3beta-Hydroxyandrost-5-en-17-one	271.2064	4.56	M-H2O+H[1+]	0.0008	3.08	yes
289.2167_4.56	C01227, 3beta-Hydroxyandrost-5-en-17-one	289.2167	4.56	M+H[1+]	0.0005	2.76	yes
250.0914_0.43	C16255, [Dihydrolipoyllysine-residue acetyltransferase] S-acetyldihydrolipoyllysine	250.0914	0.43	M+H[1+]	-0.0016	2.33	yes
391.2853_9.04	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	391.2853	9.04	M-H2O+H[1+]	0.001	3.08	yes
336.2258_4.56	C05955, Prostaglandin C2	336.2258	4.56	M(C13)+H[1+]	0.0007	2.53	yes
299.2013_4.56	C05955, Prostaglandin C2	299.2013	4.56	M-H4O2+H[1+]	0.0008	2.84	yes
455.2969_6.64	CE5560, glycolithocholate	455.2969	6.64	M+Na[1+]	-0.0038	-2.31	yes
607.2535_8.73	C00486, Bilirubin	607.2535	8.73	M+Na[1+]	0.0007	2.84	yes
585.2712_8.73	C00486, Bilirubin	585.2712	8.73	M+H[1+]	0.0004	2.75	yes
586.2749_8.73	C00486, Bilirubin	586.2749	8.73	M(C13)+H[1+]	0.0007	2.65	yes
269.2264_7.53	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	269.2264	7.53	M-H4O2+H[1+]	0.0001	3.01	yes
287.2372_7.54	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	287.2372	7.54	M-H2O+H[1+]	0.0003	2.93	yes
300.2904_5.77	C12144, Phytosphingosine	300.2904	5.77	M-H2O+H[1+]	0.0007	4.55	yes
282.2798_5.77	C12144, Phytosphingosine	282.2798	5.77	M-H4O2+H[1+]	0.0007	4.88	yes
400.3427_6.34	C02990, L-Palmitoylcarnitine	400.3427	6.34	M+H[1+]	0.0005	2.73	yes
401.346_6.34	C02990, L-Palmitoylcarnitine	401.346	6.34	M(C13)+H[1+]	0.0004	2.73	yes
361.2745_7.29	C13856, 2-Arachidonoylglycerol	361.2745	7.29	M-H2O+H[1+]	0.0008	3.33	yes
399.145_0.4	C00019, S-Adenosyl-L-methionine	399.145	0.4	M+H[1+]	0.0005	2.7	yes
394.2951_5.5	ttdcrn, tetradecanoyl carnitine	394.2951	5.5	M+Na[1+]	0.0023	3.1	yes
348.0712_2.26	C00020, AMP	348.0712	2.26	M+H[1+]	0.0008	3.13	yes
426.3582_6.45	vacccrn, Vaccenyl carnitine	426.3582	6.45	M+H[1+]	0.0004	2.78	yes
427.3616_6.45	vacccrn, Vaccenyl carnitine	427.3616	6.45	M(C13)+H[1+]	0.0004	2.77	yes
401.2672_7.53	C13856, 2-Arachidonoylglycerol	401.2672	7.53	M+Na[1+]	0.0009	4.29	yes
380.2901_7.52	C13856, 2-Arachidonoylglycerol	380.2901	7.52	M(C13)+H[1+]	0.0024	3.84	yes
379.2847_7.53	C13856, 2-Arachidonoylglycerol	379.2847	7.53	M+H[1+]	0.0004	3.08	yes
370.2959_5.5	C00836, Sphinganine	370.2959	5.5	M+HCOONa[1+]	0.0031	3.27	yes
422.3273_5.9	lnlncacrn, alpha-linolenyl carnitine	422.3273	5.9	M+H[1+]	0.0008	2.52	yes
373.3144_5.83	ttdcrn, tetradecanoyl carnitine	373.3144	5.83	M(C13)+H[1+]	0.0002	2.63	yes
372.3119_5.83	ttdcrn, tetradecanoyl carnitine	372.3119	5.83	M+H[1+]	0.0011	2.62	yes
139.0507_0.44	C03680, 4-Imidazolone-5-propanoate	139.0507	0.44	M-H2O+H[1+]	0.0005	2.47	yes
414.3585_6.57	hpdcacrn, heptadecanoyl carnitine	414.3585	6.57	M+H[1+]	0.0007	2.57	yes
322.2714_5.77	C02934, 3-Dehydrosphinganine	322.2714	5.77	M+Na[1+]	-0.0003	2.54	yes
446.3263_6.11	tmndnccrn, Timnodonyl carnitine	446.3263	6.11	M+H[1+]	-0.0002	3.18	yes
302.306_5.91	C00836, Sphinganine	302.306	5.91	M+H[1+]	0.0006	3.05	yes
445.3682_9.77	CE5838,	445.3682	9.77	M-H2O+H[1+]	0.0006	2.76	yes
399.3301_5.99	hdd2crn, trans-Hexadec-2-enoyl carnitine	399.3301	5.99	M(C13)+H[1+]	0.0002	2.7	yes
398.327_5.99	hdd2crn, trans-Hexadec-2-enoyl carnitine	398.327	5.99	M+H[1+]	0.0005	2.64	yes
429.3726_9.7	CE5835,	429.3726	9.7	M-H2O+H[1+]	-0.0001	2.71	yes
318.3004_5.6	C12144, Phytosphingosine	318.3004	5.6	M+H[1+]	0.0001	3.33	yes
441.3402_5.63	CE7144, 13'-hydroxy-alpha-tocotrienol	441.3402	5.63	M+H[1+]	0.0039	2.47	yes
279.2324_6.43	ocdcya, octadecadienoate (n-C18:2)	279.2324	6.43	M[1+]	-0.0	-2.66	yes

376.2186_4.56	CE5828,	376.2186	4.56	M+Na[1+]	-0.0035	-2.53	yes
277.2169_6.11	C16300, Stearidonic acid	277.2169	6.11	M+H[1+]	0.0007	-4.45	yes
278.2202_6.11	C16300, Stearidonic acid	278.2202	6.11	M(C13)+H[1+]	0.0006	-2.51	yes
375.2149_4.56	C02198, Thromboxane A2	375.2149	4.56	M+Na[1+]	0.0006	-2.55	yes
307.2637_7.03	C01530, Octadecanoic acid	307.2637	7.03	M+Na[1+]	0.0029	-3.19	yes
243.2107_6.43	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	243.2107	6.43	M-H4O2+H[1+]	0.0	-2.97	yes
261.2217_6.43	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	261.2217	6.43	M-H2O+H[1+]	0.0004	-2.59	yes
280.2353_6.43	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	280.2353	6.43	M(C13)+H[1+]	0.0	-2.56	yes
308.2646_7.03	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	308.2646	7.03	M(C13)+H[1+]	-0.002	-2.8	yes
377.2304_4.91	C05959, 11-epi-Prostaglandin F2alpha	377.2304	4.91	M+Na[1+]	0.0005	-3.95	yes
297.1095_2.64	C00921, Dihydropteroate	297.1095	2.64	M-H2O+H[1+]	0.0001	-2.68	yes
393.2254_4.34	C05963,	393.2254	4.34	M+Na[1+]	0.0006	-3.79	yes
90.0557_0.42	C00041, L-Alanine	90.0557	0.42	M+H[1+]	0.0007	2.57	yes
192.0658_0.62	C16591, 3-Carbamoyl-2-phenylpropionic acid	192.0658	0.62	M-H2O+H[1+]	0.0003	2.38	yes
164.0719_0.62	C16591, 3-Carbamoyl-2-phenylpropionic acid	164.0719	0.62	M-HCOOH+H[1+]	0.0012	2.72	yes
509.3751_7.6	C04230, 1-Acyl-sn-glycero-3-phosphocholine	509.3751	7.6	M(C13)+H[1+]	-0.0045	2.33	yes
532.3733_7.62	C04598, 2-Acetyl-1-alkyl-sn-glycero-3-phosphocholine	532.3733	7.62	M-H2O+H[1+]	-0.0028	2.73	yes
243.0201_12.07	C07047, Ifosfamide	243.0201	12.07	M-H2O+H[1+]	-0.0014	4.29	yes
214.0514_1.39	C02712, N-Acetylmethionine	214.0514	1.39	M+Na[1+]	0.0005	2.54	yes
324.2901_7.19	C00836, Sphinganine	324.2901	7.19	M+Na[1+]	0.0027	-2.8	yes
835.5299_12.06	C02737, Phosphatidylserine	835.5299	12.06	M[1+]	-0.0064	-2.76	yes
370.0536_0.43	C06376, N-Acetyl-D-galactosamine 6-phosphate	370.0536	0.43	M+HCOONa[1+]	0.0026	-3.17	yes
409.2964_6.41	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	409.2964	6.41	M+H[1+]	0.0015	-2.38	yes
305.2482_7.97	CE1754, 9-cis-retinol	305.2482	7.97	M+H2O+H[1+]	0.0006	2.32	yes
317.2481_7.47	C05479, 5beta-Pregnane-3,20-dione	317.2481	7.47	M+H[1+]	0.0006	2.36	yes
285.2219_7.49	CE5013,	285.2219	7.49	M-H2O+H[1+]	0.0006	2.69	yes
367.2252_6.62	CE2961, 4-hydroxy-all-trans-retinyl acetate	367.2252	6.62	M+Na[1+]	0.0008	3.11	yes
309.2224_6.63	CE2961, 4-hydroxy-all-trans-retinyl acetate	309.2224	6.63	M-H4O2+H[1+]	0.0012	3.03	yes
327.2325_6.63	CE2961, 4-hydroxy-all-trans-retinyl acetate	327.2325	6.63	M-H2O+H[1+]	0.0007	2.95	yes
318.2506_7.47	C04042, 20alpha-Hydroxy-4-pregnen-3-one	318.2506	7.47	M(C13)+H[1+]	-0.0003	2.31	yes
431.3153_6.28	CE2203, 25-hydroxyvitamin D3-26,23-lactol	431.3153	6.28	M+H[1+]	-0.0003	4.7	yes
259.2051_7.97	C16300, Stearidonic acid	259.2051	7.97	M-H2O+H[1+]	-0.0005	2.94	yes
269.2271_7.96	CE5014, anhydroretinol	269.2271	7.96	M+H[1+]	0.0007	2.63	yes
270.2308_7.96	CE5014, anhydroretinol	270.2308	7.96	M(C13)+H[1+]	0.001	2.6	yes
306.2516_7.97	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	306.2516	7.97	M(C13)+H[1+]	0.0007	2.32	yes
509.3802_7.01	C04230, 1-Acyl-sn-glycero-3-phosphocholine	509.3802	7.01	M(C13)+H[1+]	0.0006	-2.27	yes
508.3766_7.01	C04230, 1-Acyl-sn-glycero-3-phosphocholine	508.3766	7.01	M+H[1+]	0.0004	-2.22	yes
322.2714_7.54	C00319, Sphingosine	322.2714	7.54	M+Na[1+]	-0.0003	-2.55	yes
300.29_7.54	C00319, Sphingosine	300.29	7.54	M+H[1+]	0.0003	-2.4	yes
311.236_7.86	C15492, all-trans-13,14-Dihydroretinol	311.236	7.86	M+Na[1+]	0.0014	2.99	yes
373.2156_7.86	C15492, all-trans-13,14-Dihydroretinol	373.2156	7.86	M+HCOOK[1+]	0.0017	3.39	yes
298.9941_0.46	CE3075, sorbitol 3-phosphate	298.9941	0.46	M+K[1+]	0.0016	-2.4	yes
334.2829_8.43	CE2414, (3S,7R,11R)-phytanate	334.2829	8.43	M+Na[1+]	-0.0014	2.49	yes
353.2328_3.94	C00584, Prostaglandin E2	353.2328	3.94	M+H[1+]	0.0005	4.0	yes
289.2171_3.86	C01227, 3beta-Hydroxyandrost-5-en-17-one	289.2171	3.86	M+H[1+]	0.0009	2.63	yes
321.2434_6.99	C04805, 5(S)-HETE	321.2434	6.99	M+H[1+]	0.001	3.45	yes
361.2016_3.86	C01780, Aldosterone	361.2016	3.86	M+H[1+]	0.0006	4.73	yes

508.3763_7.6	C04230, 1-Acyl-sn-glycero-3-phosphocholine	508.3763	7.6	M+H[1+]	0.0001	2.79	yes
292.2345_6.48	C00523, Androsterone	292.2345	6.48	M(C13)+H[1+]	-0.0008	2.21	yes
220.1187_0.8	C00864, Pantothenate	220.1187	0.8	M+H[1+]	0.0007	-2.96	yes
110.0206_8.71	C02218, 2-Aminoacrylate	110.0206	8.71	M+Na[1+]	-0.0007	5.21	yes
136.0437_6.41	C00155, L-Homocysteine	136.0437	6.41	M+H[1+]	0.001	4.21	yes
584.2589_4.96	C00500, Biliverdin	584.2589	4.96	M(C13)+H[1+]	0.0004	-3.58	yes
583.2561_4.96	C00500, Biliverdin	583.2561	4.96	M+H[1+]	0.001	-3.51	yes
350.2108_7.96	CE5138, 12-oxo-20-hydroxy-leukotriene B4	350.2108	7.96	M+H[1+]	0.002	2.29	yes
583.2566_5.22	C00500, Biliverdin	583.2566	5.22	M+H[1+]	0.0015	-2.77	yes
319.2643_7.71	C05480, 3alpha-Hydroxy-5beta-pregnane-20-one	319.2643	7.71	M+H[1+]	0.0011	-2.35	yes
393.2255_3.93	C05963,	393.2255	3.93	M+Na[1+]	0.0007	-2.47	yes
375.2149_5.37	C00584, Prostaglandin E2	375.2149	5.37	M+Na[1+]	0.0006	-3.58	yes
208.0002_0.39	C02532, D-O-Phosphoserine	208.0002	0.39	M+Na[1+]	0.002	-2.47	yes
404.2501_5.05	C01120, Sphinganine 1-phosphate	404.2501	5.05	M+Na[1+]	-0.0036	-2.27	yes
373.2352_6.96	C05476, Tetrahydrocorticosterone	373.2352	6.96	M+Na[1+]	0.0002	-2.3	yes

Supplementary Table 2. Comparative metabolomics data of jejunum tissue between “irradiated vs naïve” and “GT3 vs irradiated” treatment groups for 4.0 and 5.8 Gy exposure to PBI (LINAC) and TBI (Cobalt-60).

		PBI 4 Gy Irradiated vs. Naïve				PBI 4 Gy Irradiated vs. GT3				TBI 4 Gy Irradiated vs. Naïve				TBI 4 Gy Irradiated vs. GT3				PBI 5.8 Gy Irradiated vs. Naïve				PBI 5.8 Gy Irradiated vs. GT3				TBI 5.8 Gy Irradiated vs. Naïve				TBI 5.8 Gy Irradiated vs. GT3			
mz_RT	EmpiricalCompound	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)
785.1558_2.32	C00016, FAD	0.75625	0.99799	1.0724	0.1008	0.01491	0.11685	0.43933	-1.187	0.83294	0.90317	0.95403	-0.0679	0.44318	0.9997	0.78105	-0.3565	0.85558	0.99311	0.98672	-0.019	0.33965	0.53517	0.57001	-0.811	0.02646	0.99999	0.56501	-0.824	0.22422	0.83076	0.76606	-0.384
784.1517_2.32	C00016, FAD	0.94098	0.99799	1.0058	0.0084	0.018147	0.11685	0.49084	-1.027	0.48641	0.72075	0.83844	-0.2542	0.64158	0.9997	0.86518	-0.2089	0.86536	0.99311	0.98798	-0.017	0.3219	0.53517	0.5207	-0.941	0.011264	0.99999	0.51051	-0.97	0.42961	0.83076	0.85637	-0.224
346.0545_0.47	C00020, AMP	0.37751	0.99799	0.75264	-0.41	0.49657	0.55643	0.68072	-0.555	0.26602	0.59752	0.68528	-0.5452	0.46423	0.9997	0.80263	-0.3172	0.57899	0.99095	1.3256	0.4066	0.21269	0.53517	0.2297	-2.122	0.63137	0.99999	0.92234	-0.117	0.17899	0.83076	0.45539	-1.135
148.0604_0.47	C00025, L-Glutamate	0.69379	0.99991	0.90466	-0.1446	0.014065	0.16426	0.73826	-0.438	0.66904	0.7859	0.90438	-0.145	0.61851	0.99949	0.9139	-0.1299	0.67115	0.99931	0.88782	-0.172	0.36308	0.47929	0.62627	-0.675	0.52846	0.98126	0.86868	-0.203	0.50715	0.9067	0.9028	-0.148
150.0562_0.47	C00025, L-Glutamate	0.77277	0.99991	0.87352	-0.1951	0.15037	0.29391	0.70558	-0.503	0.29178	0.50562	0.69837	-0.5179	0.9888	0.99949	0.9478	-0.0774	0.3416	0.99931	0.68433	-0.547	0.38952	0.47929	0.73247	-0.449	0.35197	0.98126	0.72104	-0.472	0.43354	0.9067	0.87824	-0.187
566.0488_0.51	C00052, UDP-D-galactose	0.086334	0.99799	1.9051	0.9299	0.0041478	0.11218	0.20255	-2.304	0.2313	0.57785	1.4829	0.5685	0.56429	0.9997	0.77967	-0.3591	0.077944	0.99095	1.8658	0.8998	0.33119	0.53517	0.53683	-0.897	0.56901	0.99999	1.1474	0.1983	0.36605	0.83076	0.6776	-0.561
565.0473_0.51	C00052, UDP-D-galactose	0.090933	0.99799	2.0082	1.0059	0.011352	0.11361	0.17722	-2.496	0.16609	0.52246	1.6044	0.682	0.44875	0.9997	0.73853	-0.4373	0.069038	0.99095	2.2969	1.1997	0.31513	0.53517	0.48254	-1.051	0.5571	0.99999	1.1174	0.1601	0.38502	0.83076	0.7015	-0.511
74.0198_0.41	C00121, D-Ribose	0.91605	0.99799	0.92368	-0.1145	0.16553	0.25759	0.55669	-0.845	0.19615	0.54404	0.56128	-0.8332	0.82484	0.9997	0.99153	-0.0123	0.47819	0.99095	0.66536	-0.588	0.40372	0.53517	0.76954	-0.378	0.96962	0.99999	0.96886	-0.046	0.36908	0.83076	0.65142	-0.618
371.0367_0.42	C00130, IMP	0.6025	0.99991	1.066	0.0923	0.1539	0.2977	0.80353	-0.316	0.93121	0.95412	1.004	0.0058	0.44471	0.99949	0.91714	-0.1248	0.57484	0.99931	1.0998	0.1373	0.33279	0.47929	0.52418	-0.932	0.24694	0.98126	0.8538	-0.228	0.88075	0.9725	1.0045	0.0064
386.0483_0.44	C00144, GMP	0.5608	0.99991	1.1627	0.2175	0.24349	0.37945	0.73093	-0.452	0.67714	0.7924	1.1124	0.1537	0.52941	0.99949	0.84319	-0.2461	0.10454	0.99931	1.2888	0.366	0.32108	0.47929	0.50014	-1	0.71818	0.98126	0.94732	-0.078	0.16099	0.9067	0.85618	-0.224
133.0129_0.45	C00149, (S)-Malate	0.35116	0.99799	0.83034	-0.2682	0.17186	0.26191	0.67106	-0.576	0.18657	0.53878	0.75958	-0.3967	0.35818	0.9997	0.79283	-0.3349	0.20145	0.99095	0.75892	-0.398	0.35778	0.53517	0.61741	-0.696	0.13719	0.99999	0.72399	-0.466	0.33293	0.83076	0.7762	-0.366
134.0175_0.44	C00149, (S)-Malate	0.38393	0.99799	0.84031	-0.251	0.19117	0.27656	0.67403	-0.569	0.2485	0.58806	0.78234	-0.3541	0.41322	0.9997	0.79296	-0.3347	0.28469	0.99095	0.78703	-0.346	0.34278	0.53517	0.57224	-0.805	0.14831	0.99999	0.72351	-0.467	0.59107	0.83685	0.84177	-0.249
118.0862_0.44	C00183, L-Valine	0.39011	0.99991	0.8377	-0.2555	0.039128	0.16677	0.64323	-0.637	0.45967	0.63324	0.85492	-0.2262	0.3628	0.99949	0.8084	-0.3069	0.07198	0.99931	0.61025	-0.713	0.42356	0.47929	0.81791	-0.29	0.051269	0.98126	0.59662	-0.745	0.91621	0.98159	0.94756	-0.078
195.049_0.57	C00191, D-Glucuronate	0.47543	0.99991	1.1409	0.1902	0.006938	0.16426	0.26668	-1.907	0.94149	0.95911	0.75102	-0.4131	0.78182	0.99949	0.98027	-0.0288	0.30295	0.99931	1.4664	0.5523	0.27074	0.47929	0.35187	-1.507	0.81401	0.98126	1.1846	0.2444	0.79872	0.9402	0.6528	-0.615
652.079_0.51	C00203, UDP-N-acetyl-D-galactosamine	0.17159	0.99799	1.4569	0.5429	0.0060656	0.11218	0.31289	-1.676	0.97947	0.98662	0.9953	-0.0068	0.6706	0.9997	0.96097	-0.0574	0.082501	0.99095	1.3035	0.3824	0.41369	0.53517	0.80002	-0.322	0.11663	0.99999	0.72305	-0.468	0.99254	0.99736	1.0127	0.0182
606.0744_0.49	C00203, UDP-N-acetyl-D-galactosamine	0.32236	0.99799	1.7269	0.7882	0.0079235	0.11218	0.10572	-3.242	0.81051	0.89488	1.6652	0.7357	0.53382	0.9997	0.42532	-1.2334	0.13232	0.99095	2.011	1.0079	0.29618	0.53517	0.41428	-1.271	0.79767	0.99999	1.4463	0.5324	0.31763	0.83076	0.46701	-1.099
607.0792_0.49	C00203, UDP-N-acetyl-D-galactosamine	0.38707	0.99799	1.5688	0.6497	0.011764	0.11495	0.16903	-2.565	0.90854	0.94509	1.577	0.6571	0.62958	0.9997	0.46876	-1.0931	0.13758	0.99095	1.7667	0.8211	0.30689	0.53517	0.45421	-1.139	0.3196	0.99999	1.5255	0.6093	0.15822	0.83076	0.4964	-1.01
630.0721_0.5	C00203, UDP-N-acetyl-D-galactosamine	0.71406	0.99991	1.1007	0.1385	0.014924	0.16426	0.48536	-1.043	0.55834	0.71261	1.1839	0.2435	0.26344	0.99949	0.71969	-0.4746	0.019223	0.91863	1.6089	0.6861	0.32016	0.47929	0.49548	-1.013	0.46582	0.98126	0.88266	-0.18	0.72273	0.91638	0.90978	-0.136
91.0582_0.45	C00213, Sarcosine	0.67698	0.99991	0.85307	-0.2293	0.26842	0.40376	0.77853	-0.361	0.87187	0.91916	0.90661	-0.1414	0.86924	0.99949	0.96685	-0.0486	0.95676	0.99931	0.91439	-0.129	0.32885	0.47929	0.53382	-0.906	0.54447	0.98126	0.79778	-0.326	0.31545	0.9067	0.90249	-0.148
225.0892_2.47	C00214, Thymidine	0.57566	0.99991	0.78031	-0.3579	0.020012	0.16426	0.53028	-0.915	0.14676	0.43242	0.57567	-0.7967	0.6421	0.99949	0.84311	-0.2462	0.52152	0.99931	0.87003	-0.201	0.36287	0.47929	0.43731	-1.193	0.16049	0.98126	0.58429	-0.775	0.22684	0.9067	0.65347	-0.614
303.232_7.97	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.43042	0.99799	0.65524	-0.6099	0.15001	0.24475	0.41736	-1.261	0.048401	0.42112	0.3082	-1.6981	0.15877	0.9997	1.7075	0.7719	0.36799	0.99095	0.56328	-0.828	0.40611	0.53517	0.6466	-0.629	0.9515	0.99999	1.1062	0.1456	0.23346	0.83076	0.34773	-1.524
304.2355_7.97	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.43715	0.99799	0.66564	-0.5872	0.15014	0.24475	0.42946	-1.219	0.048977	0.42112	0.3198	-1.6447	0.15893	0.9997	1.6675	0.7377	0.37446	0.99095	0.57411	-0.801	0.40201	0.53517	0.64221	-0.639	0.95472	0.99999	1.1063	0.1458	0.23518	0.83076	0.35883	-1.479
83.0131_0.44	C00232, Succinate semialdehyde	0.56177	0.99799	1.1173	0.16	0.019848	0.11685	0.56416	-0.826	0.6489	0.7981	0.91579	-0.1269	0.80324	0.9997	0.93261	-0.1007	0.87824	0.99436	0.9491	-0.075	0.41954	0.53517	0.80613	-0.311	0.58291	0.99999	1.203	0.2666	0.1896	0.83076	0.62003	-0.69
279.2311_7.66	C00249, Hexadecanoic acid	0.003449	0.4184	0.25589	-1.9664	0.56255	0.65176	0.86901	-0.203	0.001315	0.14373	0.20156	-2.3107	0.45583	0.99949	1.3522	0.4354	0.05444	0.99931	0.3976	-1.331	0.27086	0.47929	0.31812	-1.652	0.005359	0.6509	0.25463	-1.974	0.43246	0.9067	1.2396	0.3099
257.247_8.47	C00249, Hexadecanoic acid	0.03466	0.61504	0.52132	-0.9398	0.19607	0.33536	1.1914	0.2526	0.05517	0.32339	0.53986	-0.8893	0.42846	0.99949	1.3543	0.4376	0.48542	0.99931	0.82596	-0.276	0.29888	0.47929	0.38187	-1.389	0.32124	0.98126	0.76997	-0.377	0.96353	0.98984	0.83105	-0.267
258.2507_8.47	C00249, Hexadecanoic acid	0.055576	0.72648	0.52504	-0.9295	0.25291	0.3876	1.1705	0.2271	0.066708	0.33649	0.52894	-0.9188	0.47792	0.99949	1.3583	0.4418	0.45851	0.99931	0.79806	-0.325	0.31172	0.47929	0.3992	-1.325	0.35891	0.98126	0.7766	-0.365	0.93825	0.98629	0.8181	-0.29
255.2317_8.44	C00249, Hexadecanoic acid	0.085229	0.99799	0.23535	-2.0871	0.71034	0.75248	1.0521	0.0733	0.079733	0.43501	0.23065	-2.1162	0.45566	0.9997	1.8569	0.8929	0.67825	0.99095	0.77865	-0.361	0.24437	0.53517	0.18398	-2.442	0.54778	0.99999	0.91178	-0.133	0.68334	0.86467	0.34462	-1.537
256.2341_8.44	C00249, Hexadecanoic acid	0.092619	0.99799	0.22757	-2.1356	0.65895	0.70557	1.0683	0.0954	0.083123	0.43593	0.22017	-2.1833	0.43803	0.9997	1.9373	0.954	0.68098	0.99095	0.7701	-0.377	0.2448	0.53517	0.17893	-2.483	0.54106	0.99999	0.88486	-0.176	0.7084	0.87171	0.34681	-1.528
239.2357_7.99	C00249, Hexadecanoic acid	0.14387	0.86169	0.07685	-3.7018	0.40469	0.51762	0.61841	-0.693	0.081003	0.36124	0.049276	-4.343	0.39071	0.99949	4.1096	2.039	0.53939	0.99931	0.54865	-0.866	0.27244	0.47929	0.057804	-4.113	0.69989	0.98126	0.68015	-0.556	0.45074	0.9067	0.16205	-2.626
137.0458_0.46	C00262, Hypoxanthine	0.011145	0.50391	1.5302	0.6137	0.0025844	0.15336	0.53711	-0.897	0.040569	0.30994	1.4015	0.487	0.25074	0.99949	1.1615	0.216	0.045682	0.99931	1.4772	0.5628	0.39895	0.47929	0.73655	-0.441	0.70662	0.98126	1.1592	0.2131	0.95505	0.98903	1.0573	0.0804
138.0493_0.45	C00262, Hypoxanthine	0.80563	0.99991	1.0182	0.026	0.00061902	0.14276	0.60085	-0.735	0.48722	0.65703	0.8946	-0.1607	0.40852	0.99949	1.1156	0.1578	0.68646	0.99931	0.92287	-0.116	0.38196	0.47929	0.69095	-0.533	0.71318	0.98126	1.0726	0.1012	0.63802	0.90677	0.90411	-0.145
283.0686_0.47	C00294, Inosine	0.48341	0.99799	0.65084	-0.6196	0.96534	0.97318	0.98203	-0.026	0.51066	0.73105	0.65201	-0.617	0.38459	0.9997	0.75465	-0.4061	0.1632	0.99095	0.40509	-1.304	0.37838	0.53517	0.67455	-0.568	0.059581	0.99999	0.34758	-1.525	0.6446	0.84979	0.85523	-0.226
121.0271_2.3	C00299, Uridine	0.78355	0.99799	1.1121	0.1533	0.010686	0.11227	0.31814	-1.652	0.18458	0.53786	1.3472	0.43	0.01638	0.9997	0.42213	-1.2442	0.41112	0.99095	1.2567	0.3297	0.38209	0.53517	0.70983	-0.494	0.75319	0.99999	0.98346	-0.024	0.18431	0.83076	0.54248	-0.882
588.0781_0.5	C00325, GDP-L-fucose	0.38107	0.99799	1.2321	0.3011	0.0048516	0.11218	0.27531	-1.861	0.42168	0.69311	0.59684	-0.7446	0.29673	0.9997	1.3863	0.4713	0.37595	0.99095	1.2452	0.3163	0.38162	0.53517	0.67316	-0.571	0.87297	0.99999	0.89317	-0.163	0.54504	0.83197	0.85455	-0.227
268.1038_0.44	C00330, Deoxyguanosine	0.015244	0.51452	1.8182	0.8625	0.30389	0.43703	0.81952	-0.287	0.029968	0.29612	1.8167	0.8613	0.45698	0.99949	0.84583	-0.2416	0.007563	0.72622	2.6992	1.4326	0.27926	0.47929	0.3798	-1.397	0.086947	0.98126	1.4716	0.5574	0.73192	0.91842	1.1393	0.1881
322.0574_0.44	C00364, dTMP	0.13173	0.86169	1.432	0.5181	0.030189	0.16668	0.56127	-0.833	0.56627	0.71646	1.2405	0.3109	0.90738	0.99949	1.0158	0.0227	0.12036	0.99931	1.592	0.6709	0.34317	0.47929	0.53992	-0.889	0.12503	0.98126	0.63663	-0.651	0.37712	0.9067	1.2671	0.3415
305.0553_0.44	C00364, dTMP	0.42183	0.99991	0.82998	-0.2688	0.049788	0.17602	0.7583	-0.399	0.34151	0.53869	0.80499	-0.313	0.33275	0.99949	0.87238	-0.197	0.38096	0.99931	0.7966	-0.328	0.3445	0.47929	0.57466	-0.799	0.87793	0.99347	1.1687	0.2249	0.57262	0.90677	0.71614	-0.482
341.0711_0.44	C00364, dTMP	0.69999	0.99991	1.2408	0.3112	0.039279	0.16677	0.35985	-1.475	0.032903	0.30545	0.56727	-0.8179	0.1765	0.99949	1.2806	0.3568	0.3806	0.99931	1.1661	0.2217	0.30491	0.47929	0.45635	-1.132	0.55244	0.98126	1.4405	0.5266	0.45702	0.9067	0.62193	-0.685
149.0112_0.45	C00366, Urate	0.33835	0.99799	0.65664	-0.6068	0.071398	0.17356	0.53962	-0.89	0.050897	0.42112	0.42503	-1.2344	0.96175	0.9997	0.95157	-0.0716	0.25669	0.99095	0.56545	-0.823	0.35289	0.53517	0.61083	-0.711	0.75868	0.99999	1.7614	0.8168	0.76398	0.89868	3.4167	1.7726
167.0197_0.44	C00366, Urate	0.88384	0.99799	0.92281	-0.1159	0.89948	0.92012	0.96198	-0.056	0.45046	0.70942	0.70906	-0.496	0.12173	0.9997	0.72956	-0.4549	0.52168	0.99095	0.71459	-0.485	0.33119	0.53517	0.56207	-0.831	0.10663	0.99999	0.51544	-0.956	0.38359	0.83076	1.1806	0.2395
264.1034_2.07	C00378, Thiamin	0.19522	0.99799	1.8307	0.8724	0.051846	0.14981	0.29762	-1.749	0.88366	0.92983	0.89001	-0.1681	0.56142	0.9997	0.65652	-0.6071	0.43274	0.99095	1.1356	0.1835	0.40245	0.53517	0.80307	-0.316	0.20833	0.99999	2.643	1.4022	0.20504	0.83076	0.29614	-1.756
153.0403_0.49	C00385, Xanthine	0.57242	0.99991	0.92437	-0.1135	0.46526	0.56913	0.86549	-0.208	0.15182	0.43298	1.1717	0.2286	0.20697	0.99949	0.82336	-0.2804	0.35982	0.99931	0.86147	-0.215	0.35199	0.47929	0.57098	-0.808	0.045293	0.98126	0.70059	-0.513	0.78321	0.93673	1.0067	0.0096
159.0912_1.06	C00398, Tryptamine	0.88068	0.99799	0.75654	-0.4025	0.25783	0.33436	0.47596	-1.071	0.29993	0.62761	0.40633	-1.2993	0.8674	0.9997	0.95881	-0.0607	0.49917	0.99095	0.44586	-1.165	0.40093	0.53517	0.77573	-0.366	0.88093	0.99999	0.73322	-0.448	0.3085	0.83076	0.56497	-0.824
224.0664_3.49	C00475, Cytidine	0.018233	0.66552	4.5801	2.1954	0.073654	0.17536	0.24069	-2.055	0.121	0.46807	0.76919	-0.3786	0.62372	0.9997	2.2069	1.142	0.00156	0.84236	2.7703	1.47	0.24817	0.53517	0.36975	-1.435	0.12578	0.99999	5.0588	2.3388	0.40225	0.83076	0.32412	-1.625
226.0825_2.46	C00475, Cytidine	0.70535	0.99991	0.81168	-0.301	0.017946	0.16426	0.59443	-0.75	0.1857	0.46235	0.58604	-0.7709	0.72979	0.99949	0.93167	-0.1021	0.5635	0.99931	0.88526	-0.176	0.36629	0.47929	0.44483	-1.169	0.19773	0.98126	0.59174	-0.757	0.33148	0.9067	0.6751	-0.567
263.2367_8.08	C00517, Hexadecanal	0.10864	0.86169	0.19614	-2.3501	0.42409	0.5334	0.72427	-0.465	0.046352	0.31681	0.13552	-2.8835	0.21319	0.99949	2.1502	1.1044	0.51125	0.99931	0.59278	-0.754	0.2721	0.47929	0.17934	-2.479	0.39499	0.98126	0.656	-0.608	0.62175	0.90677	0.29573	-1.758
204.0845_1.05	C00525, D-Tryptophan	0.84553	0.99799	0.71857	-0.4768	0.24637	0.32374	0.51579	-0.955	0.2173	0.56302	0.37776	-1.4044	0.96364	0.9997	0.8656	-0.2082	0.45506	0.99095	0.43374	-1.205	0.40368	0.53517	0.80002	-0.322	0.48011	0.99999	0.52269	-0.936	0.66859	0.86071	0.82803	-0.272
203.0813_1.05	C00525, D-Tryptophan	0.86539	0.99799	0.74105	-0.4324	0.23077	0.30968	0.52387	-0.933	0.24897	0.58806	0.41301	-1.2758	0.99892	0.99972	0.87442	-0.1936	0.47012	0.99095	0.45933	-1.122	0.40337	0.53517	0.7984	-0.325	0.50548	0.99999	0.5494	-0.864	0.6308	0.84356	0.80786	-0.308
366.141_6.59	C00611, N-Acetyllactosamine	0.47651	0.99991	0.92818	-0.1075	0.22327	0.36218	1.161	0.2154	0.51959	0.68473	1.0495	0.0697	0.91856	0.99949	1.0168	0.024	0.041319	0.99931	1.2235	0.2911	0.33307	0.47929	0.54737	-0.869	0.31598	0.98126	0.90375	-0.146	0.19737	0.9067	1.1806	0.2395
281.099_2.64	C00670, sn-glycero-3-Phosphocholine	0.6225	0.99991	0.78557	-0.3482	0.057516	0.18384	0.27095	-1.884	0.28321	0.49986	0.56148	-0.8327	0.71083	0.99949	0.75972	-0.3965	0.50443	0.99931	0.65736	-0.605	0.31171	0.47929	0.39651	-1.335	0.79154	0.98126	0.89479	-0.16	0.024358	0.9067	0.25166	-1.99
407.2792_5.05	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	0.039523	0.86081	86.7	6.438	0.025839	0.12092	0.002876	-8.442	0.66829	0.80995	4.9737	2.3143	0.55325	0.9997	0.98172	-0.0266	0.13614	0.99095	65.366	6.0305	0.72307	0.726	0.2452	-2.028	0.34978	0.99999	100.73	6.6544	0.83926	0.92827	0.12317	-3.021
408.2827_5.05	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	0.039884	0.86081	90.522	6.5002	0.034709	0.13067	0.003716	-8.072	0.85005	0.91326	5.4772	2.4534	0.66044	0.9997	0.92365	-0.1146	0.13834	0.99095	70.234	6.1341	0.73307	0.73514	0.24499	-2.029	0.29152	0.99999	105.57	6.7221	0.76038	0.89656	0.12882	-2.957
409.2954_6.41	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	0.81014	0.99991	1.023	0.0328	0.037674	0.16677	0.51715	-0.951	0.31445	0.52047	1.2756	0.3512	0.55025	0.99949	0.88158	-0.1818	0.29165	0.99931	0.63991	-0.644	0.55101	0.55984	1.3426	0.4251	0.53357	0.98126	1.2515	0.3236	0.9595	0.98903	0.96988	-0.044
284.267_8.55	C00712, (9Z)-Octadecenoic acid	0.11147	0.86169	0.53417	-0.9046	0.59105	0.67671	0.90123	-0.15	0.12909	0.41686	0.54282	-0.8815	0.54909	0.99949	1.2335	0.3028	0.65032	0.99931	1.6344	0.7087	0.27049	0.47929	0.24413	-2.034	0.63862	0.98126	1.118	0.1609	0.64065	0.90677	0.47505	-1.074
140.0105_0.45	C00740, D-Serine	0.067944	0.95051	1.3328	0.4145	0.0023934	0.11218	0.49531	-1.014	0.30488	0.63111	1.1991	0.262	0.21652	0.9997	0.786	-0.3474	0.14494	0.99095	1.3073	0.3866	0.41508	0.53517	0.79295	-0.335	0.68595	0.99999	1.062	0.0868	0.59592	0.83685	0.92319	-0.115
183.961_0.41	C00740, D-Serine	0.2667	0.99799	1.2698	0.3446	0.026815	0.12123	0.64842	-0.625	0.69349	0.82317	0.86208	-0.2141	0.61703	0.9997	1.0889	0.1229	0.3056	0.99095	1.2604	0.3339	0.32842	0.53517	0.53521	-0.902	0.80021	0.99999	1.0059	0.0084	0.3439	0.83076	0.86428	-0.21
86.025_0.46	C00740, D-Serine	0.46946	0.99799	1.1665	0.2222	0.013629	0.11655	0.46175	-1.115	0.56711	0.7654	0.90933	-0.1371	0.18221	0.9997	0.71389	-0.4862	0.96429	0.99784	0.98966	-0.015	0.40498	0.53517	0.73925	-0.436	0.27178	0.99999	0.81515	-0.295	0.52663	0.83076	1.1249	0.1698
145.0614_0.41	C00740, D-Serine	0.98639	0.99867	0.92445	-0.1133	0.24639	0.32374	0.63362	-0.658	0.20234	0.54825	0.53748	-0.8957	0.7612	0.9997	1.0123	0.0177	0.66549	0.99095	0.71497	-0.484	0.41711	0.53517	0.8081	-0.307	0.73215	0.99999	0.81437	-0.296	0.54723	0.83197	0.76851	-0.38
153.1264_8.58	C00756, 1-Octanol	0.11678	0.86169	0.45604	-1.1328	0.61364	0.69403	0.90251	-0.148	0.13332	0.42104	0.4705	-1.0877	0.50918	0.99949	1.2616	0.3352	0.8925	0.99931	0.91281	-0.132	0.29774	0.47929	0.37704	-1.407	0.52556	0.98126	0.92691	-0.11	0.68514	0.90677	0.49397	-1.018
267.0721_0.46	C00760, Cellulose	0.023959	0.73363	1.9121	0.9352	0.00045015	0.11218	0.27988	-1.837	0.63403	0.79225	1.1809	0.2399	0.27642	0.9997	1.3066	0.3858	0.053166	0.99095	1.9939	0.9956	0.38765	0.53517	0.67387	-0.569	0.6723	0.99999	1.0807	0.112	0.81778	0.92135	1.05	0.0704
195.0496_0.43	C00800, L-Gulonate	0.01094	0.54771	0.43005	-1.2174	0.39482	0.45986	0.76736	-0.382	0.038629	0.42112	0.52735	-0.9232	0.43388	0.9997	0.76103	-0.394	0.007721	0.99095	0.41096	-1.283	0.3176	0.53517	0.53479	-0.903	0.11049	0.99999	0.60334	-0.729	0.33522	0.83076	0.55781	-0.842
324.2856_7.2	C00836, Sphinganine	0.27084	0.97806	0.62079	-0.6878	0.096758	0.22764	0.4943	-1.017	0.04191	0.31038	0.38889	-1.3626	0.82564	0.99949	0.88371	-0.1784	0.64537	0.99931	0.88225	-0.181	0.35119	0.47929	0.46145	-1.116	0.55924	0.98126	0.94067	-0.088	0.39044	0.9067	0.42179	-1.245
218.1021_0.67	C00864, Pantothenate	0.38724	0.99799	0.54525	-0.875	0.2294	0.30883	0.52355	-0.934	0.13212	0.4787	0.35898	-1.478	0.97348	0.9997	1.0041	0.0059	0.38001	0.99095	0.4732	-1.08	0.32896	0.53517	0.52689	-0.924	0.16592	0.99999	0.42877	-1.222	0.64212	0.84869	0.62383	-0.681
318.2128_6.3	C00909, Leukotriene A4	0.34237	0.99799	0.45429	-1.1383	0.83004	0.862	1.032	0.0454	0.042651	0.42112	0.22174	-2.1731	0.129	0.9997	2.2325	1.1587	0.63599	0.99095	0.68237	-0.551	0.2863	0.53517	0.2963	-1.755	0.05716	0.99999	0.24301	-2.041	0.34267	0.83076	1.5269	0.6106
112.0393_0.47	C01110, 5-Amino-2-oxopentanoic acid	0.063751	0.95051	1.6923	0.759	0.02901	0.125	0.53409	-0.905	0.32303	0.64192	1.4512	0.5372	0.88444	0.9997	0.94336	-0.0841	0.11174	0.99095	1.7266	0.7879	0.35032	0.53517	0.57525	-0.798	0.73435	0.99999	1.2511	0.3233	0.6425	0.84869	0.74528	-0.424
131.055_0.42	C01110, 5-Amino-2-oxopentanoic acid	0.75842	0.99799	0.86667	-0.2064	0.21144	0.29302	0.51773	-0.95	0.14607	0.49756	0.50774	-0.9778	0.78684	0.9997	0.87599	-0.191	0.38296	0.99095	0.61681	-0.697	0.38688	0.53517	0.70463	-0.505	0.97423	0.99999	1.1394	0.1882	0.24632	0.83076	0.42507	-1.234
151.0247_0.45	C01110, 5-Amino-2-oxopentanoic acid	0.90734	0.99799	0.96955	-0.0446	0.039686	0.13493	0.61892	-0.692	0.67562	0.81303	0.83152	-0.2662	0.44411	0.9997	0.85097	-0.2328	0.54871	0.99095	0.75913	-0.398	0.38109	0.53517	0.68755	-0.54	0.27362	0.99999	0.67884	-0.559	0.4261	0.83076	0.84719	-0.239
308.079_0.44	C01169, S-Succinyldihydrolipoamide	0.9599	0.99799	0.91892	-0.122	0.07573	0.17695	0.59893	-0.74	0.4823	0.7181	0.72613	-0.4617	0.85007	0.9997	1.0438	0.0619	0.74909	0.99095	1.0734	0.1021	0.34185	0.53517	0.52814	-0.921	0.76337	0.99999	0.95049	-0.073	0.94259	0.97602	0.87197	-0.198
307.2629_8.28	C01530, Octadecanoic acid	0.38869	0.99991	0.71106	-0.492	0.36369	0.48858	0.65166	-0.618	0.025723	0.29096	0.37001	-1.4344	0.072531	0.99949	1.8372	0.8775	0.20707	0.99931	0.5581	-0.841	0.40894	0.47929	0.7226	-0.469	0.28084	0.98126	0.66215	-0.595	0.68411	0.90677	0.74277	-0.429
402.3433_6.34	C01561, Calcidiol	0.078221	0.83776	1.6934	0.7599	0.011539	0.16426	0.52994	-0.916	0.41505	0.60253	1.3163	0.3965	0.18063	0.99949	1.3891	0.4741	0.09763	0.99931	1.7725	0.8258	0.3453	0.47929	0.57706	-0.793	0.7774	0.98126	1.0847	0.1173	0.72435	0.91656	1.0791	0.1098
245.2253_8.07	C01595, Linoleate	0.11766	0.86169	0.16879	-2.5667	0.4326	0.54052	0.72308	-0.468	0.0539	0.32222	0.11602	-3.1075	0.21246	0.99949	2.5798	1.3673	0.5641	0.99931	0.63006	-0.666	0.26738	0.47929	0.14762	-2.76	0.59094	0.98126	0.77059	-0.376	0.48406	0.9067	0.24032	-2.057
279.2319_8.06	C01595, Linoleate	0.17236	0.99799	0.3946	-1.3415	0.23754	0.31596	0.42119	-1.248	0.023614	0.42112	0.18255	-2.4536	0.31409	0.9997	1.5902	0.6692	0.44294	0.99095	0.66601	-0.586	0.30054	0.53517	0.25851	-1.952	0.52178	0.99999	1.0417	0.0589	0.45275	0.83076	0.21976	-2.186
280.2349_8.06	C01595, Linoleate	0.17543	0.99799	0.40722	-1.2961	0.23105	0.30982	0.42754	-1.226	0.023206	0.42112	0.19073	-2.3904	0.31296	0.9997	1.5709	0.6516	0.44383	0.99095	0.67266	-0.572	0.29951	0.53517	0.26349	-1.924	0.52198	0.99999	1.0487	0.0686	0.46208	0.83076	0.22822	-2.132
245.2247_8.93	C01595, Linoleate	0.27879	0.98794	0.26709	-1.9046	0.11221	0.24589	0.24105	-2.053	0.30818	0.51677	0.26845	-1.8973	0.89199	0.99949	1.2206	0.2876	0.3117	0.99931	0.51003	-0.971	0.3145	0.47929	0.10161	-3.299	0.68737	0.98126	0.77739	-0.363	0.069721	0.9067	0.091183	-3.455
263.2366_8.93	C01595, Linoleate	0.27939	0.98794	0.26907	-1.894	0.14645	0.28922	0.2357	-2.085	0.332	0.53162	0.27355	-1.8701	0.97339	0.99949	1.1866	0.2468	0.28431	0.99931	0.50438	-0.987	0.35692	0.47929	0.10386	-3.267	0.69733	0.98126	0.77941	-0.36	0.067875	0.9067	0.088496	-3.498
283.2631_8.55	C01712, (9E)-Octadecenoic acid	0.11322	0.86169	0.53656	-0.8982	0.51905	0.6158	0.88412	-0.178	0.12443	0.41343	0.53991	-0.8892	0.53356	0.99949	1.2405	0.311	0.65592	0.99931	1.644	0.7172	0.27074	0.47929	0.24168	-2.049	0.64698	0.98126	1.1419	0.1914	0.64389	0.90677	0.4637	-1.109
282.2561_8.07	C01712, (9E)-Octadecenoic acid	0.12441	0.86169	0.72773	-0.4585	0.36477	0.48907	0.78516	-0.349	0.001429	0.14373	0.43936	-1.1865	0.44268	0.99949	1.1562	0.2094	0.29429	0.99931	0.79657	-0.328	0.30229	0.47929	0.4532	-1.142	0.64934	0.98126	1.1363	0.1844	0.45237	0.9067	0.49592	-1.012
281.2476_8.53	C01712, (9E)-Octadecenoic acid	0.20337	0.99799	0.28019	-1.8355	0.32389	0.39359	0.63036	-0.666	0.13675	0.48282	0.23373	-2.0971	0.52853	0.9997	1.6652	0.7357	0.93667	0.99784	0.96412	-0.053	0.28651	0.53517	0.24084	-2.054	0.861	0.99999	1.5649	0.646	0.47158	0.83076	0.16619	-2.589
430.2955_4.57	C01921, Glycocholate	0.44265	0.99991	2.1041	1.0732	0.032301	0.16668	0.064232	-3.961	0.001476	0.14373	0.026364	-5.2453	0.13036	0.99949	19.957	4.3188	0.42053	0.99931	1.2264	0.2944	0.19917	0.47929	0.22915	-2.126	0.26141	0.98126	1.1322	0.1792	0.77586	0.93456	0.52969	-0.917
504.271_4.57	C01921, Glycocholate	0.46936	0.99991	1.5414	0.6243	0.026664	0.16426	0.10766	-3.215	0.002059	0.16224	0.048929	-4.3532	0.16734	0.99949	10.786	3.4311	0.29246	0.99931	1.4759	0.5616	0.22711	0.47929	0.2866	-1.803	0.48824	0.98126	1.3319	0.4135	0.52741	0.9067	0.31436	-1.67
464.3008_4.57	C01921, Glycocholate	0.48635	0.99799	2.1364	1.0952	0.029548	0.12649	0.047155	-4.407	0.001823	0.38945	0.023061	-5.4384	0.12318	0.9997	17.284	4.1114	0.46291	0.99095	1.1117	0.1528	0.19085	0.53517	0.24933	-2.004	0.24072	0.99999	1.1077	0.1475	0.87723	0.94701	0.56037	-0.836
488.2981_4.57	C01921, Glycocholate	0.54616	0.99991	1.4429	0.529	0.033196	0.16668	0.11626	-3.105	0.000766	0.13087	0.038883	-4.6847	0.16613	0.99949	13.232	3.726	0.32986	0.99931	1.3797	0.4643	0.26714	0.47929	0.36862	-1.44	0.23114	0.98126	0.8926	-0.164	0.69068	0.90731	0.55656	-0.845
446.29_4.88	C01921, Glycocholate	0.67806	0.99799	0.40241	-1.3133	0.092178	0.19323	0.13385	-2.901	0.031835	0.42112	0.009643	-6.6963	0.12193	0.9997	25.66	4.6815	0.2687	0.99095	0.75092	-0.413	0.17557	0.53517	0.19176	-2.383	0.56107	0.99999	0.30904	-1.694	0.60439	0.83731	0.68034	-0.556
448.3059_4.59	C01921, Glycocholate	0.69019	0.99991	1.016	0.0229	0.044881	0.17054	0.078801	-3.666	0.002469	0.17881	0.012747	-6.2937	0.11792	0.99949	25.647	4.6807	0.40123	0.99931	0.88826	-0.171	0.1594	0.47929	0.18903	-2.403	0.28572	0.98126	0.61371	-0.704	0.6599	0.90677	0.51318	-0.962
451.3613_7.45	C02059, Phylloquinone	0.42585	0.99991	1.353	0.4362	0.96095	0.97322	0.98708	-0.019	0.12156	0.41007	2.6496	1.4058	0.55123	0.99949	1.2818	0.3582	0.057052	0.99931	3.3847	1.759	0.40538	0.47929	0.69949	-0.516	0.017662	0.98126	4.8136	2.2671	0.43972	0.9067	0.4905	-1.028
303.2318_7.59	C02110, 11-cis-Retinal	0.82999	0.99991	1.0509	0.0716	0.59169	0.67718	0.85032	-0.234	0.55697	0.71208	0.87014	-0.2007	0.89199	0.99949	1.1083	0.1484	0.007972	0.72622	0.34685	-1.528	0.50159	0.51593	1.2045	0.2685	0.23593	0.98126	0.68423	-0.547	0.85034	0.96299	0.94322	-0.084
391.2844_5.87	C02528, Chenodeoxycholate	0.047311	0.89638	142.78	7.1577	0.080839	0.18265	0.004899	-7.673	0.44704	0.70717	21.708	4.4401	0.91361	0.9997	0.2303	-2.1184	0.027218	0.99095	51.956	5.6992	0.55885	0.57939	0.28367	-1.818	0.075289	0.99999	146.01	7.1899	0.45848	0.83076	0.041938	-4.576
392.2879_5.87	C02528, Chenodeoxycholate	0.054704	0.91256	139.89	7.1282	0.09	0.19027	0.005019	-7.638	0.43204	0.70021	22.533	4.4939	0.92077	0.9997	0.21199	-2.2379	0.037302	0.99095	54.007	5.7551	0.58827	0.60185	0.27943	-1.839	0.075087	0.99999	147.21	7.2017	0.41567	0.83076	0.040896	-4.612
321.2815_9.04	C02528, Chenodeoxycholate	0.54567	0.99991	0.2695	-1.8916	0.04047	0.16677	0.23273	-2.103	0.39012	0.58228	0.22216	-2.1703	0.67615	0.99949	1.3624	0.4461	0.3718	0.99931	0.29442	-1.764	0.27675	0.47929	0.15515	-2.688	0.75059	0.98126	0.35141	-1.509	0.009079	0.9067	0.16886	-2.566
347.2914_9.18	C02528, Chenodeoxycholate	0.73807	0.99991	0.39035	-1.3572	0.037736	0.16677	0.11791	-3.084	0.67542	0.7907	0.3245	-1.6237	0.65673	0.99949	1.4314	0.5174	0.37695	0.99931	0.30248	-1.725	0.40565	0.47929	0.26728	-1.904	0.74624	0.98126	0.68642	-0.543	0.007292	0.9067	0.098629	-3.342
223.1691_6.45	C02679, Dodecanoic acid	0.071236	0.82093	0.33138	-1.5934	0.12054	0.25649	1.5713	0.652	0.032503	0.30465	0.26375	-1.9228	0.61804	0.99949	1.0895	0.1237	0.7843	0.99931	0.86354	-0.212	0.29916	0.47929	0.34199	-1.548	0.060399	0.98126	0.33756	-1.567	0.49631	0.9067	0.994	-0.009
214.0491_1.35	C02712, N-Acetylmethionine	0.88908	0.99991	1.0571	0.08	0.016209	0.16426	0.40972	-1.287	0.37973	0.57408	0.79419	-0.3324	0.67807	0.99949	0.76563	-0.3853	0.81498	0.99931	0.99438	-0.008	0.31706	0.47929	0.49963	-1.001	0.75851	0.98126	0.90647	-0.142	0.17255	0.9067	0.7249	-0.464
858.5241_12.03	C02737, Phosphatidylserine	0.041072	0.6537	1.5591	0.6407	0.88075	0.91692	0.98911	-0.016	0.11794	0.40607	1.2845	0.3612	0.51852	0.99949	1.1114	0.1524	0.68692	0.99931	1.1104	0.1511	0.40173	0.47929	0.72736	-0.459	0.30852	0.98126	1.1759	0.2338	0.26015	0.9067	1.2399	0.3103
837.5412_12.09	C02737, Phosphatidylserine	0.10787	0.86169	1.5236	0.6075	0.96146	0.97322	0.96677	-0.049	0.14049	0.42971	1.359	0.4426	0.041635	0.99949	1.3563	0.4397	0.88393	0.99931	1.0516	0.0725	0.38978	0.47929	0.66681	-0.585	0.42575	0.98126	1.219	0.2857	0.30294	0.9067	1.248	0.3196
836.542_12.09	C02737, Phosphatidylserine	0.18521	0.89258	1.4302	0.5162	0.6201	0.69684	1.0483	0.0681	0.2603	0.48947	1.2425	0.3132	0.04414	0.99949	1.4124	0.4982	0.94583	0.99931	0.99651	-0.005	0.3998	0.47929	0.72027	-0.473	0.53182	0.98126	1.1697	0.2262	0.20523	0.9067	1.3139	0.3938
819.516_12.07	C02737, Phosphatidylserine	0.5225	0.99991	1.0904	0.1248	0.45949	0.56373	1.1104	0.1511	0.33275	0.53162	1.3234	0.4043	0.58979	0.99949	1.0897	0.1239	0.87048	0.99931	0.89331	-0.163	0.49383	0.50993	1.1499	0.2015	0.38798	0.98126	1.4186	0.5045	0.74967	0.92518	0.80643	-0.31
400.3413_6.34	C02990, L-Palmitoylcarnitine	0.026311	0.59142	1.55	0.6323	0.022934	0.16426	0.58261	-0.779	0.53006	0.69227	1.1956	0.2577	0.18676	0.99949	1.3705	0.4547	0.029837	0.99931	1.6488	0.7215	0.3385	0.47929	0.55325	-0.854	0.19356	0.98126	1.2874	0.3645	0.62757	0.90677	0.91276	-0.132
401.344_6.34	C02990, L-Palmitoylcarnitine	0.056935	0.73113	1.4938	0.579	0.031356	0.16668	0.59337	-0.753	0.63357	0.76466	1.1538	0.2064	0.18002	0.99949	1.3981	0.4835	0.053268	0.99931	1.6092	0.6863	0.34074	0.47929	0.558	-0.842	0.23084	0.98126	1.2856	0.3624	0.60244	0.90677	0.89744	-0.156
308.2665_8.28	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	0.37743	0.99991	0.70113	-0.5123	0.38414	0.5044	0.64243	-0.638	0.022445	0.28773	0.34855	-1.5206	0.068808	0.99949	1.9367	0.9536	0.20043	0.99931	0.54511	-0.875	0.4107	0.47929	0.72714	-0.46	0.27105	0.98126	0.65238	-0.616	0.70868	0.91327	0.73133	-0.451
305.2463_8.27	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	0.39532	0.99799	0.618	-0.6943	0.21626	0.29704	0.42038	-1.25	0.038942	0.42112	0.26013	-1.9427	0.13482	0.9997	1.9133	0.9361	0.43638	0.99095	0.60851	-0.717	0.3851	0.53517	0.53202	-0.91	0.73785	0.99999	0.88818	-0.171	0.30899	0.83076	0.40598	-1.301
306.2511_8.29	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	0.48837	0.99799	0.60663	-0.7211	0.29872	0.37087	0.42048	-1.25	0.043629	0.42112	0.19946	-2.3258	0.094433	0.9997	2.4767	1.3084	0.4461	0.99095	0.57672	-0.794	0.4044	0.53517	0.50124	-0.996	0.61455	0.99999	0.69974	-0.515	0.43829	0.83076	0.46815	-1.095
289.2519_8.3	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	0.53234	0.99991	0.78276	-0.3534	0.37793	0.49817	0.62489	-0.678	0.039045	0.30994	0.38882	-1.3628	0.07247	0.99949	1.998	0.9986	0.24758	0.99931	0.57852	-0.79	0.41181	0.47929	0.71514	-0.484	0.64385	0.98126	0.97529	-0.036	0.73284	0.91842	0.61796	-0.694
299.0717_0.56	C03492, D-4'-Phosphopantothenate	0.65749	0.99799	0.80614	-0.3109	0.088659	0.18893	0.57727	-0.793	0.30441	0.63111	0.65164	-0.6179	0.51049	0.9997	0.81294	-0.2988	0.40332	0.99095	0.65422	-0.612	0.36144	0.53517	0.64057	-0.643	0.83797	0.99999	1.6347	0.709	0.24113	0.83076	0.29411	-1.766
336.0443_0.45	C03492, D-4'-Phosphopantothenate	0.95159	0.99799	0.98752	-0.0181	0.35573	0.42326	0.7343	-0.446	0.29907	0.62688	0.7385	-0.4373	0.22301	0.9997	0.75924	-0.3974	0.16833	0.99095	0.63733	-0.65	0.3576	0.53517	0.62024	-0.689	0.59942	0.99999	1.6848	0.7526	0.28637	0.83076	0.39984	-1.323
298.0687_0.48	C03492, D-4'-Phosphopantothenate	0.99777	0.99881	0.92574	-0.1113	0.074985	0.17673	0.55997	-0.837	0.50505	0.73015	0.71885	-0.4762	0.4569	0.9997	0.82051	-0.2854	0.32106	0.99095	0.60703	-0.72	0.40626	0.53517	0.73416	-0.446	0.17447	0.99999	0.55483	-0.85	0.91389	0.95991	0.96357	-0.054
309.0443_0.43	C03838, 5'-Phosphoribosylglycinamide	0.075532	0.83776	1.6647	0.7353	0.0076935	0.16426	0.36476	-1.455	0.39963	0.58832	1.3464	0.4292	0.40407	0.99949	1.1716	0.2284	0.041456	0.99931	1.7813	0.833	0.36797	0.47929	0.63571	-0.654	0.029412	0.98126	2.9716	1.5713	0.28741	0.9067	0.51246	-0.964
263.1021_2.07	C04148, alpha-N-Phenylacetyl-L-glutamine	0.18878	0.99799	1.7733	0.8265	0.064778	0.16508	0.32249	-1.633	0.9831	0.98947	0.90063	-0.151	0.58337	0.9997	0.67871	-0.5591	0.37622	0.99095	1.1793	0.2379	0.40161	0.53517	0.78665	-0.346	0.21846	0.99999	2.5151	1.3306	0.20491	0.83076	0.29681	-1.752
265.1195_2.1	C04148, alpha-N-Phenylacetyl-L-glutamine	0.2158	0.93875	1.6002	0.6782	0.055256	0.18221	0.37501	-1.415	0.9756	0.98342	0.93272	-0.1005	0.60535	0.99949	0.71372	-0.4866	0.44051	0.99931	1.1498	0.2014	0.39889	0.47929	0.78052	-0.358	0.21299	0.98126	2.7122	1.4395	0.25579	0.9067	0.31662	-1.659
287.101_2.1	C04148, alpha-N-Phenylacetyl-L-glutamine	0.32706	0.99991	1.4038	0.4894	0.056187	0.18291	0.33552	-1.576	0.85981	0.91308	0.85537	-0.2254	0.72635	0.99949	0.69316	-0.5288	0.49391	0.99931	1.0778	0.1081	0.39273	0.47929	0.75702	-0.402	0.27013	0.98126	2.1674	1.116	0.22323	0.9067	0.34352	-1.542
508.3748_7.01	C04230, 1-Acyl-sn-glycero-3-phosphocholine	0.80276	0.99991	0.89075	-0.1669	0.19885	0.33819	0.6204	-0.689	0.047382	0.31681	0.45824	-1.1258	0.1586	0.99949	1.56	0.6415	0.98731	0.99931	0.9183	-0.123	0.34825	0.47929	0.59617	-0.746	0.43952	0.98126	0.77896	-0.36	0.19304	0.9067	0.49372	-1.018
325.025_0.45	C04242, 5-Fluorodeoxyuridine monophosphate	0.15019	0.99799	1.7005	0.766	0.046729	0.14404	0.41339	-1.274	0.60325	0.77861	1.1617	0.2163	0.26967	0.9997	0.68932	-0.5368	0.92823	0.99784	0.91813	-0.123	0.55604	0.57696	1.3198	0.4003	0.78881	0.99999	0.85147	-0.232	0.61322	0.83744	1.3573	0.4407
368.161_4.47	C04555, 3beta-Hydroxyandrost-5-en-17-one 3-sulfate	0.04652	0.89506	3.2406	1.6963	0.030057	0.12747	0.15171	-2.721	0.92977	0.95795	0.34244	-1.5461	0.3188	0.9997	2.3217	1.2152	0.20541	0.99095	1.1177	0.1605	0.31137	0.53517	0.48759	-1.036	0.28698	0.99999	2.5984	1.3776	0.79596	0.91377	0.36258	-1.464
367.1577_4.46	C04555, 3beta-Hydroxyandrost-5-en-17-one 3-sulfate	0.098741	0.99799	2.7683	1.469	0.034285	0.13067	0.16337	-2.614	0.79922	0.88993	0.45918	-1.1229	0.23727	0.9997	1.7829	0.8342	0.37199	0.99095	1.0182	0.026	0.30421	0.53517	0.49199	-1.023	0.56172	0.99999	2.0567	1.0403	0.83133	0.92509	0.4009	-1.319

320.266_8.78	prist, pristanic acid	0.66664	0.99991	0.59469	-0.7498	0.063832	0.19322	0.1245	-3.006	0.61767	0.75367	0.50411	-0.9882	0.66824	0.99949	1.1501	0.2017	0.25756	0.99931	0.33398	-1.582	0.38805	0.47929	0.33123	-1.594	0.94124	0.99511	0.65363	-0.613	0.005294	0.9067	0.15878	-2.655
242.2221_8.55	ptdca, pentadecanoate	0.10834	0.86169	0.36064	-1.4714	0.77879	0.8377	0.93854	-0.092	0.12776	0.41644	0.37715	-1.4068	0.67257	0.99949	1.174	0.2314	0.65915	0.99931	0.66241	-0.594	0.32854	0.47929	0.46424	-1.107	0.60573	0.98126	0.92262	-0.116	0.55053	0.9067	0.40135	-1.317
241.2185_8.55	ptdca, pentadecanoate	0.16261	0.86169	0.35361	-1.4998	0.47291	0.57415	0.87568	-0.192	0.15049	0.43298	0.35159	-1.5081	0.46722	0.99949	1.3017	0.3804	0.78108	0.99931	0.69081	-0.534	0.29585	0.47929	0.37509	-1.415	0.5026	0.98126	0.71489	-0.484	0.64632	0.90677	0.49093	-1.026
429.3765_6.81	stcrn, stearoylcarnitine	0.032407	0.61236	2.0219	1.0157	0.25455	0.38869	0.79258	-0.335	0.070966	0.34071	1.8628	0.8974	0.14573	0.99949	1.3876	0.4726	0.10957	0.99931	1.8236	0.8668	0.3948	0.47929	0.7096	-0.495	0.46421	0.98126	1.3822	0.4669	0.61897	0.90677	1.0902	0.1246
428.3733_6.82	stcrn, stearoylcarnitine	0.032561	0.61236	1.9595	0.9705	0.26556	0.40151	0.80106	-0.32	0.071974	0.34233	1.8186	0.8628	0.14127	0.99949	1.3845	0.4693	0.10059	0.99931	1.8045	0.8516	0.38484	0.47929	0.67922	-0.558	0.40545	0.98126	1.3766	0.4611	0.6898	0.90731	1.0639	0.0893
526.3875_10.19	tetteticrn, Tetracosatetraenoyl carnitine	0.88462	0.99991	0.79286	-0.3349	0.012795	0.16426	0.12767	-2.97	0.22979	0.48047	0.44837	-1.1572	0.6752	0.99949	0.81838	-0.2892	0.5185	0.99931	0.50959	-0.973	0.38285	0.47929	0.58194	-0.781	0.41876	0.98126	0.63823	-0.648	0.87919	0.97187	0.64751	-0.627
463.2304_4.35	tststeroneglc, testosterone glucuronide	0.08665	0.99799	12.807	3.6788	0.10953	0.20831	0.062092	-4.009	0.89653	0.93894	1.0741	0.1031	0.89861	0.9997	1.0349	0.0495	0.1969	0.99095	1.917	0.9388	0.45554	0.53517	0.80251	-0.317	0.041798	0.99999	3.6262	1.8585	0.31609	0.83076	0.56983	-0.811
300.2894_5.76	ttdcrn, tetradecanoyl carnitine	0.026918	0.59142	2.2584	1.1753	0.59622	0.6805	1.0797	0.1106	0.082378	0.36124	1.7054	0.7701	0.52031	0.99949	0.85875	-0.2197	0.20475	0.99931	1.432	0.518	0.38148	0.47929	0.69184	-0.532	0.36771	0.98126	1.2699	0.3447	0.86763	0.96939	0.99292	-0.01
372.3094_5.83	ttdcrn, tetradecanoyl carnitine	0.13882	0.86169	1.6229	0.6986	0.039395	0.16677	0.41104	-1.283	0.75225	0.84565	1.006	0.0087	0.59611	0.99949	1.1489	0.2002	0.14108	0.99931	1.78	0.8319	0.33036	0.47929	0.49473	-1.015	0.16748	0.98126	1.967	0.976	0.21209	0.9067	0.50425	-0.988

Supplementary Table 3. Comparative metabolomics data of kidney tissue between "irradiated vs naïve" and "GT3 vs irradiated" treatment groups for 4.0 and 5.8 Gy exposure to PBI (LINAC) and TBI (Cobalt-60).

		PBI 4 Gy Irradiated vs. Naïve				PBI 4 Gy Irradiated vs. GT3				TBI 4 Gy Irradiated vs. Naïve				TBI 4 Gy Irradiated vs. GT3				PBI 5.8 Gy Irradiated vs. Naïve				PBI 5.8 Gy Irradiated vs. GT3				TBI 5.8 Gy Irradiated vs. Naïve				TBI 5.8 Gy Irradiated vs. GT3			
mz_RT	EmpiricalCompound	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)
489.2457_4.65	5adtststeroneglc, 5alpha-Dihydrotestosterone glucuronide	0.83348	0.99628	0.90749	-0.14005	0.86807	0.99964	1.0865	0.1196	0.93134	0.99993	0.9791	-0.0305	0.16376	0.94371	1.4852	0.5707	0.12432	0.8561	1.5245	0.6084	0.42886	0.99989	0.86212	-0.214	0.42964	0.64517	2.8904	1.5313	0.46104	0.76709	0.35709	-1.486
148.0604_0.47	C00025, L-Glutamate	0.19642	0.99628	1.1933	0.25496	0.93653	0.99964	1.0305	0.0434	0.13621	0.99993	1.2183	0.2849	0.032364	0.94371	0.82089	-0.285	0.073243	0.78057	1.3929	0.4781	0.90351	0.99989	0.99044	-0.0139	0.013201	0.20583	1.5278	0.6115	0.3699	0.74999	0.92094	-0.119
90.0554_0.43	C00041, L-Alanine	0.009898	0.80423	0.49858	-1.0041	0.3947	0.99964	1.1946	0.2565	0.1173	0.99993	0.66918	-0.5795	0.56283	0.94811	1.592	0.6709	0.072464	0.78057	0.66801	-0.5821	0.01267	0.99989	0.75326	-0.4088	0.28895	0.56939	1.9763	0.9828	0.3917	0.7501	0.59673	-0.745
296.0651_0.4	C00055, CMP	0.54342	0.99628	1.0929	0.12813	0.60692	0.99964	0.84943	-0.2354	0.99814	0.99993	0.80818	-0.3073	0.48849	0.94371	0.81401	-0.297	0.7581	0.98539	0.72942	-0.4552	0.5288	0.99989	1.2277	0.2959	0.8317	0.90508	0.875	-0.193	0.34593	0.74999	1.8347	0.8756
324.062_0.46	C00055, CMP	0.83703	0.99628	1.0698	0.097331	0.45395	0.99964	0.83694	-0.2568	0.69952	0.99993	0.94886	-0.0757	0.40705	0.94371	1.1321	0.179	0.38759	0.954	1.1015	0.1395	0.50821	0.99989	1.0665	0.0929	0.041451	0.27898	1.3142	0.3942	0.16118	0.74999	0.82229	-0.282
458.1151_2.25	C00061, FMN	0.42649	0.99628	0.83083	-0.26738	0.54429	0.99964	0.87694	-0.1895	0.62138	0.99993	0.91011	-0.1359	0.91247	0.99404	1.0028	0.004	0.10792	0.84488	1.4499	0.536	0.024062	0.99989	0.67961	-0.5572	0.16598	0.4769	1.4469	0.5329	0.24721	0.74999	0.68786	-0.54
647.4999_8.87	C00165, Diacylglycerol	0.27434	0.99628	1.215	0.28096	0.27156	0.99964	0.83459	-0.2609	0.52573	0.99993	0.84419	-0.2444	0.56615	0.94811	1.2193	0.286	0.27346	0.954	0.71399	-0.486	0.33224	0.99989	0.78469	-0.3498	0.96992	0.98337	1.1291	0.1751	0.99135	0.99709	0.90378	-0.146
229.0107_0.44	C00199, D-Ribulose 5-phosphate	0.26469	0.85589	1.2737	0.34899	0.4459	0.99807	1.1071	0.1468	0.43576	0.9993	1.3812	0.466	0.72601	0.97747	1.0109	0.0156	0.10066	0.77937	1.5465	0.629	0.48093	0.99753	0.92331	-0.1151	0.041589	0.2149	1.6544	0.7263	0.81984	0.94423	0.96914	-0.045
304.2364_7.98	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.33454	0.85589	1.5132	0.59756	0.55392	0.99807	0.76502	-0.3864	0.50224	0.9993	1.2178	0.2843	0.38817	0.97319	0.77933	-0.36	0.63421	0.98049	1.0943	0.13	0.70599	0.99753	1.1175	0.1602	0.23371	0.4684	1.2515	0.3237	0.075221	0.82425	0.81867	-0.289
303.2328_7.98	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.34969	0.85589	1.5151	0.59941	0.54519	0.99807	0.75368	-0.408	0.51583	0.9993	1.2119	0.2773	0.38487	0.97319	0.77649	-0.365	0.66643	0.99162	1.0824	0.1142	0.68995	0.99753	1.1242	0.1689	0.26454	0.49296	1.2332	0.3024	0.064419	0.82425	0.80767	-0.308
306.2519_7.98	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.41201	0.99628	1.4131	0.49888	0.61799	0.99964	0.7964	-0.3284	0.68821	0.99993	1.0767	0.1066	0.41074	0.94371	0.85273	-0.23	0.51573	0.96206	1.094	0.1296	0.54127	0.99989	1.126	0.1712	0.1557	0.46283	1.2072	0.2716	0.052969	0.74999	0.83869	-0.254
154.0593_0.43	C00300, Creatine	0.046934	0.99628	0.62022	-0.68916	0.72283	0.99964	0.92246	-0.1164	0.037836	0.99993	0.65521	-0.61	0.25702	0.94371	1.5327	0.6161	0.09339	0.81299	0.67487	-0.5673	0.77094	0.99989	0.95062	-0.0731	0.4022	0.62377	1.4048	0.4904	0.21648	0.74999	0.61816	-0.694
198.0842_0.44	C00327, L-Citrulline	0.001144	0.17057	3.0931	1.629	0.082987	0.99964	0.68976	-0.5358	0.21217	0.99993	7.3505	2.8778	0.79333	0.97865	1.2515	0.3237	0.008498	0.43606	2.2557	1.1735	0.67602	0.99989	1.1771	0.2353	0.000741	0.0926	14.146	3.8223	0.19146	0.74999	1.5331	0.6165
158.0918_0.4	C00327, L-Citrulline	0.096035	0.99628	0.49128	-1.0254	0.13454	0.99964	0.35539	-1.4925	0.023111	0.96203	0.35596	-1.4902	0.6368	0.96467	1.3776	0.4622	0.003503	0.29477	0.24583	-2.0243	0.68975	0.99989	1.5675	0.6485	0.002206	0.11522	0.3846	-1.379	0.91786	0.97095	1.3364	0.4184
160.0619_0.47	C00329, D-Glucosamine	0.54127	0.90912	0.80763	-0.30824	0.53132	0.99807	0.82338	-0.2804	0.67433	0.9993	0.84885	-0.2364	0.80332	0.98004	1.0366	0.0518	0.36703	0.94156	0.70981	-0.4945	0.49465	0.99753	1.1522	0.2044	0.4027	0.59207	1.4032	0.4887	0.44349	0.82583	0.72535	-0.463
700.4988_10.9	C00416, Phosphatidate	0.61539	0.91598	0.79888	-0.32395	0.84721	0.99807	1.1204	0.164	0.8678	0.9993	0.97513	-0.0363	0.70476	0.97747	0.95095	-0.073	0.79353	0.99743	0.84886	-0.2364	0.22535	0.99753	0.68196	-0.5522	0.095059	0.32711	0.47803	-1.065	0.25888	0.82425	1.3512	0.4342
699.4947_10.9	C00416, Phosphatidate	0.75328	0.9337	0.80477	-0.31335	0.82396	0.99807	1.0979	0.1347	0.74661	0.9993	1.009	0.013	0.71358	0.97747	0.95197	-0.071	0.9741	0.99743	0.87624	-0.1906	0.025669	0.99753	0.66902	-0.5799	0.15915	0.399	0.49301	-1.02	0.3817	0.82425	1.2981	0.3764
287.2372_7.98	C00473, Retinol	0.40556	0.99628	1.4096	0.49529	0.60385	0.99964	0.79437	-0.3321	0.64274	0.99993	1.0869	0.1203	0.36914	0.94371	0.84002	-0.252	0.53308	0.96498	1.0921	0.1272	0.5304	0.99989	1.1284	0.1743	0.16477	0.47438	1.2118	0.2772	0.057858	0.74999	0.84305	-0.246
288.2407_7.98	C00473, Retinol	0.40791	0.99628	1.4555	0.54148	0.61752	0.99964	0.78334	-0.3523	0.65998	0.99993	1.0832	0.1153	0.38091	0.94371	0.84066	-0.25	0.54844	0.96556	1.0983	0.1353	0.56133	0.99989	1.1387	0.1874	0.20835	0.50656	1.199	0.2618	0.058857	0.74999	0.8356	-0.259
305.2484_7.98	C00473, Retinol	0.4081	0.99628	1.4554	0.5414	0.60524	0.99964	0.77613	-0.3656	0.70016	0.99993	1.0777	0.108	0.4033	0.94371	0.84451	-0.244	0.54484	0.96526	1.0893	0.1234	0.52665	0.99989	1.1368	0.185	0.17115	0.4783	1.2095	0.2744	0.064211	0.74999	0.83434	-0.261
255.2111_4.69	C00523, Androsterone	0.48012	0.99628	1.0443	0.062491	0.19716	0.99964	0.58197	-0.781	0.41711	0.99993	1.2395	0.3097	0.7676	0.97865	0.87607	-0.191	0.2712	0.954	1.6009	0.6788	0.50363	0.99989	0.78815	-0.3435	0.19102	0.49578	3.4747	1.7969	0.42244	0.75355	0.38377	-1.382
211.0719_2.18	C00526, Deoxyuridine	0.007465	0.68236	0.33644	-1.5716	0.79198	0.99964	1.1848	0.2447	0.22055	0.99993	0.64317	-0.6367	0.82543	0.97917	0.76246	-0.391	0.035716	0.70562	0.4279	-1.2246	0.40913	0.99989	0.86239	-0.2136	0.63937	0.7871	0.99002	-0.014	0.27371	0.74999	0.36281	-1.463
146.0352_0.46	C00555, 4-Aminobutanal	0.19972	0.99628	1.1707	0.22742	0.83458	0.99964	1.03	0.0426	0.094975	0.99993	1.3006	0.3792	0.05221	0.94371	0.77691	-0.364	0.063536	0.77152	1.3927	0.4779	0.78893	0.99989	0.97714	-0.0334	0.039809	0.27898	1.3746	0.459	0.3218	0.74999	0.92257	-0.116
353.2289_4.51	C00584, Prostaglandin E2	0.032967	0.99628	0.28689	-1.8014	0.62307	0.99964	0.79661	-0.3281	0.007667	0.72345	0.20174	-2.3094	0.40314	0.94371	1.7066	0.7712	0.019933	0.61943	0.25887	-1.9497	0.84071	0.99989	1.5056	0.5904	0.012659	0.20447	0.22053	-2.181	0.46805	0.77021	0.64735	-0.627
273.2201_4.66	C00619, 3-Oxo-delta4-steroid	0.7962	0.99628	0.9396	-0.089887	0.34597	0.99964	0.72123	-0.4715	0.69056	0.99993	1.0826	0.1145	0.95496	0.99932	0.96618	-0.05	0.31576	0.954	1.4404	0.5265	0.55063	0.99989	0.83615	-0.2582	0.23921	0.53088	3.1232	1.643	0.38184	0.74999	0.37477	-1.416
575.1162_0.44	C00760, Cellulose	0.090462	0.99628	2.1439	1.1003	0.57171	0.99964	0.76171	-0.3927	0.021293	0.94369	2.2813	1.1899	0.41921	0.94371	0.78055	-0.357	0.003617	0.29477	2.4147	1.2719	0.1142	0.99989	1.4652	0.5511	0.006292	0.17029	3.6688	1.8753	0.36726	0.74999	0.70316	-0.508
559.1503_0.44	C00760, Cellulose	0.14741	0.99628	2.0446	1.0318	0.71896	0.99964	0.82186	-0.283	0.02985	0.99993	2.2704	1.1829	0.56307	0.94811	0.85378	-0.228	0.024224	0.6748	2.3054	1.205	0.066438	0.99989	1.6816	0.7499	0.016779	0.21338	3.5144	1.8133	0.39485	0.75072	0.69046	-0.534
267.073_0.45	C00760, Cellulose	0.18196	0.85589	1.4971	0.58219	0.76117	0.99807	0.90532	-0.1435	0.036223	0.9993	1.6531	0.7252	0.73587	0.97958	1.0304	0.0432	0.044185	0.67638	1.6639	0.7345	0.21734	0.99753	1.2174	0.2838	0.020127	0.14883	2.4466	1.2908	0.39007	0.82425	0.75615	-0.403
196.0548_0.44	C00800, L-Gulonate	0.72932	0.92738	1.1102	0.15078	0.8808	0.99807	1.0886	0.1225	0.28824	0.9993	1.7538	0.8105	0.76412	0.97958	1.0609	0.0853	0.90996	0.99743	1.1347	0.1823	0.51232	0.99753	0.73673	-0.4408	0.045806	0.22374	2.6204	1.3898	0.33271	0.82425	1.3291	0.4104
370.2955_5.52	C00836, Sphinganine	0.66813	0.99628	0.9578	-0.062208	0.8077	0.99964	0.72719	-0.4596	0.26935	0.99993	0.63274	-0.6603	0.33441	0.94371	2.7054	1.4358	0.33474	0.954	0.63165	-0.6628	0.78663	0.99989	1.1658	0.2213	0.41616	0.63498	0.70258	-0.509	0.60546	0.81935	0.7524	-0.41
89.0243_0.47	C01013, 3-Hydroxypropanoate	0.85483	0.96043	1.0502	0.070655	0.86271	0.99807	0.95329	-0.069	0.39255	0.9993	1.1942	0.256	0.78746	0.97958	0.96986	-0.044	0.49833	0.94815	1.0858	0.1187	0.36031	0.99753	0.93623	-0.0951	0.031551	0.18829	1.5033	0.5881	0.11102	0.82425	0.70846	-0.497
363.2158_3.66	C01124, 18-Hydroxycorticosterone	0.63037	0.99628	1.046	0.064903	0.49947	0.99964	1.4918	0.577	0.1593	0.99993	1.7282	0.7892	0.77165	0.97865	0.90067	-0.151	0.74225	0.98157	0.93531	-0.0965	0.611	0.99989	0.92854	-0.107	0.16988	0.4783	2.0487	1.0347	0.3308	0.74999	0.61197	-0.708
244.0768_0.43	C01132, N-Acetyl-D-galactosamine	0.25079	0.99628	0.83924	-0.25284	0.15605	0.99964	1.3319	0.4135	0.23413	0.99993	0.86769	-0.2047	0.48747	0.94371	0.91428	-0.129	0.44088	0.954	0.8798	-0.1848	0.15045	0.99989	1.2993	0.3777	0.76534	0.86877	0.98205	-0.026	0.42895	0.75404	0.80579	-0.312
413.0469_1.89	C01194, 1-Phosphatidyl-D-myo-inositol	0.20283	0.99628	0.55393	-0.85222	0.86181	0.99964	0.5831	-0.7782	0.81691	0.99993	3.6175	1.855	0.1348	0.94371	0.053845	-4.215	0.18002	0.92995	0.40711	-1.2965	0.65063	0.99989	2.0285	1.0204	0.048767	0.29507	0.30381	-1.719	0.91352	0.96829	1.03	0.0426
311.1972_3.58	C01227, 3beta-Hydroxyandrost-5-en-17-one	0.13037	0.99628	0.65116	-0.61891	0.42316	0.99964	1.2112	0.2765	0.13339	0.99993	10.101	3.3364	0.15731	0.94371	0.10888	-3.199	0.75336	0.98335	0.88296	-0.1796	0.52377	0.99989	0.92138	-0.1181	0.68624	0.81729	1.3232	0.4041	0.42184	0.75355	1.4703	0.5561
171.006_0.45	C01620,	0.17702	0.85589	1.5132	0.59756	0.5923	0.99807	1.1337	0.181	0.036256	0.9993	1.8756	0.9074	0.089341	0.97319	0.60537	-0.724	0.034987	0.65914	2.0574	1.0408	0.070043	0.99753	0.68784	-0.5399	0.022973	0.15777	2.1678	1.1162	0.42427	0.82462	0.80799	-0.308
361.2015_3.87	C01780, Aldosterone	0.61495	0.99628	1.1248	0.16971	0.63605	0.99964	1.2752	0.3507	0.38773	0.99993	1.2266	0.2947	0.79731	0.97865	1.0996	0.137	0.46812	0.954	1.1574	0.2109	0.083735	0.99989	0.76776	-0.3813	0.30126	0.57326	1.4277	0.5137	0.2631	0.74999	0.6873	-0.541
152.0317_2.56	C01879, 5-Oxoproline	0.76096	0.99628	1.1477	0.19869	0.60711	0.99964	0.81325	-0.2982	0.32553	0.99993	1.4461	0.5322	0.25026	0.94371	1.3787	0.4633	0.82763	0.99458	0.91137	-0.1339	0.24091	0.99989	1.2645	0.3386	0.039238	0.27737	1.8643	0.8986	0.40512	0.75316	0.82466	-0.278
101.0239_0.44	C02045,	0.45688	0.87872	1.1604	0.21461	0.591	0.99807	1.1041	0.1429	0.29265	0.9993	1.2584	0.3316	0.36882	0.97319	0.80177	-0.319	0.008374	0.46405	1.3149	0.395	0.97125	0.99753	1.0083	0.0119	0.034288	0.19266	1.6656	0.7361	0.31651	0.82425	0.77734	-0.363
834.5231_12.05	C02737, Phosphatidylserine	0.74677	0.93046	0.97729	-0.033136	0.43009	0.99807	0.75364	-0.4081	0.83688	0.9993	0.97095	-0.0425	0.38648	0.97319	0.82795	-0.272	0.89648	0.99743	1.085	0.1178	0.24138	0.99753	0.55993	-0.8367	0.037774	0.20337	0.66082	-0.598	0.13272	0.82425	1.366	0.45
422.3212_6.01	C02990, L-Palmitoylcarnitine	0.29128	0.99628	0.25612	-1.9651	0.6374	0.99964	0.97113	-0.0423	0.55452	0.99993	0.31747	-1.6553	0.044083	0.94371	1.8012	0.849	0.37676	0.954	0.2246	-2.1546	0.86512	0.99989	0.97642	-0.0344	0.74464	0.85589	0.45404	-1.139	0.37062	0.74999	0.52066	-0.942
400.3425_6.36	C02990, L-Palmitoylcarnitine	0.43882	0.99628	0.42788	-1.2247	0.73722	0.99964	1.0886	0.1224	0.46144	0.99993	0.41266	-1.277	0.001668	0.76652	2.5826	1.3688	0.4005	0.954	0.35411	-1.4977	0.10133	0.99989	1.4654	0.5513	0.84507	0.91011	0.6302	-0.666	0.39158	0.7501	0.64654	-0.629
401.3452_6.36	C02990, L-Palmitoylcarnitine	0.44623	0.99628	0.40402	-1.3075	0.68973	0.99964	1.1097	0.1502	0.46368	0.99993	0.38341	-1.383	0.001834	0.76652	2.7033	1.4347	0.43389	0.954	0.34171	-1.5492	0.14748	0.99989	1.4325	0.5186	0.85086	0.91264	0.60137	-0.734	0.37122	0.74999	0.6282	-0.671
298.0687_0.48	C03492, D-4'-Phosphopantothenate	0.83981	0.95662	1.0101	0.01446	0.71025	0.99807	1.2616	0.3353	0.59674	0.9993	1.1057	0.145	0.25058	0.97319	0.74198	-0.431	0.73079	0.99319	1.1657	0.2212	0.64196	0.99753	0.81979	-0.2867	0.043979	0.22086	1.8481	0.8861	0.078263	0.82425	0.60792	-0.718
114.056_0.42	C03912, (S)-1-Pyrroline-5-carboxylate	0.047722	0.99628	0.41155	-1.2809	0.72182	0.99964	1.1944	0.2563	0.64023	0.99993	0.84199	-0.2481	0.26516	0.94371	0.5494	-0.864	0.28647	0.954	0.57991	-0.7861	0.23325	0.99989	0.70319	-0.508	0.29775	0.57257	0.62686	-0.674	0.66564	0.85119	0.88035	-0.184
368.1606_4.46	C04555, 3beta-Hydroxyandrost-5-en-17-one 3-sulfate	0.010409	0.54405	3.2956	1.7206	0.13668	0.99807	0.73582	-0.4426	0.094085	0.9993	2.5363	1.3428	0.74782	0.97958	1.5882	0.6674	0.080184	0.76246	2.0403	1.0288	0.98445	0.99778	1.0278	0.0395	0.33179	0.54968	3.156	1.6581	0.82036	0.94423	0.92715	-0.109
367.1579_4.46	C04555, 3beta-Hydroxyandrost-5-en-17-one 3-sulfate	0.010958	0.54405	3.3796	1.7569	0.13102	0.99807	0.74388	-0.4269	0.15752	0.9993	2.564	1.3584	0.7375	0.97958	1.5325	0.6159	0.087478	0.76607	2.0896	1.0632	0.86368	0.99753	0.98077	-0.028	0.40855	0.59794	3.1102	1.637	0.7683	0.93119	0.93724	-0.094
532.3807_7.65	C04598, 2-Acetyl-1-alkyl-sn-glycero-3-phosphocholine	0.2234	0.99628	1.9093	0.93301	0.28781	0.99964	0.56197	-0.8314	0.49853	0.99993	1.1524	0.2047	0.66301	0.96467	0.91797	-0.123	0.2289	0.94889	1.39	0.4751	0.33674	0.99989	0.79405	-0.3327	0.48769	0.68647	1.2529	0.3253	0.51126	0.78011	0.80681	-0.31
320.2307_6.69	C04805, 5(S)-HETE	0.14304	0.85589	0.15822	-2.66	0.58547	0.99807	2.2002	1.1376	0.66578	0.9993	0.36783	-1.4429	0.62007	0.97491	1.9959	0.997	0.36972	0.94156	0.28957	-1.788	0.49718	0.99753	1.6891	0.7563	0.044474	0.22127	0.064386	-3.957	0.41737	0.82425	2.0557	1.0396
303.2326_6.68	C04805, 5(S)-HETE	0.14921	0.99628	0.17414	-2.5217	0.5582	0.99964	1.8262	0.8688	0.62886	0.99993	0.36918	-1.4376	0.63022	0.96467	1.8763	0.9079	0.4009	0.954	0.31424	-1.6701	0.55634	0.99989	1.4914	0.5767	0.03817	0.2755	0.062762	-3.994	0.36423	0.74999	2.3633	1.2408
321.2411_7.14	C04805, 5(S)-HETE	0.17088	0.99628	0.69975	-0.51509	0.22587	0.99964	1.2779	0.3538	0.25086	0.99993	0.76267	-0.3909	0.69184	0.97057	1.1067	0.1462	0.23833	0.95138	0.73877	-0.4368	0.57576	0.99989	1.1258	0.1709	0.45189	0.66171	0.83223	-0.265	0.44341	0.76076	0.79964	-0.323
301.217_7.57	C04805, 5(S)-HETE	0.25298	0.85589	2.2487	1.1691	0.7314	0.99807	0.73038	-0.4533	0.14032	0.9993	1.8384	0.8785	0.17098	0.97319	0.62779	-0.672	0.34719	0.94156	1.4148	0.5006	0.81603	0.99753	0.9649	-0.0515	0.2348	0.46873	1.5431	0.6258	0.45825	0.83299	0.81259	-0.299
303.2325_7.58	C04805, 5(S)-HETE	0.25422	0.99628	1.9991	0.99937	0.74106	0.99964	0.77349	-0.3705	0.10672	0.99993	1.5972	0.6755	0.12237	0.94371	0.69081	-0.534	0.21459	0.94889	1.434	0.52	0.75726	0.99989	0.95771	-0.0623	0.18649	0.49142	1.4913	0.5766	0.53739	0.78886	0.85861	-0.22
285.222_7.57	C04805, 5(S)-HETE	0.345	0.99628	1.8868	0.91593	0.76632	0.99964	0.76442	-0.3876	0.08749	0.99993	1.4912	0.5765	0.16064	0.94371	0.70304	-0.508	0.13328	0.88202	1.3723	0.4566	0.63843	0.99989	0.92177	-0.1175	0.24396	0.53403	1.3534	0.4366	0.61899	0.82583	0.8717	-0.198
317.2103_6.3	C04849, (5Z,9E,14Z)-(8xi,11R,12S)-11,12-Epoxy-8-hydroxyicosa-5,9,14-trienoic acid	0.23575	0.85589	0.42692	-1.228	0.75198	0.99807	1.1948	0.2568	0.96199	0.9993	0.85891	-0.2194	0.88639	0.98524	1.3592	0.4427	0.45487	0.94156	0.61262	-0.7069	0.83879	0.99753	0.95307	-0.0693	0.039966	0.21197	0.16501	-2.599	0.29607	0.82425	1.6533	0.7254
347.2222_3.68	C05474, 3alpha,11beta,21-Trihydroxy-20-oxo-5beta-pregnan-18-al	0.93007	0.99628	1.0574	0.08057	0.98481	0.99964	1.045	0.0635	0.82499	0.99993	1.0773	0.1074	0.53204	0.94371	1.161	0.2154	0.90747	0.99638	0.90692	-0.141	0.16089	0.99989	0.87198	-0.1976	0.51256	0.70507	0.81334	-0.298	0.63893	0.83843	0.83349	-0.263
320.2668_8.78	C05480, 3alpha-Hydroxy-5beta-pregnane-20-one	0.52296	0.99628	2.0446	1.0318	0.84293	0.99964	1.2167	0.283	0.22944	0.99993	1.7517	0.8088	0.3789	0.94371	0.71167	-0.491	0.21199	0.94889	2.1015	1.0714	0.92066	0.99989	1.0021	0.003	0.040662	0.27898	3.2592	1.7045	0.20324	0.74999	0.63721	-0.65
319.2637_8.78	C05480, 3alpha-Hydroxy-5beta-pregnane-20-one	0.55428	0.99628	1.9113	0.93453	0.90652	0.99964	1.1603	0.2145	0.26547	0.99993	1.6211	0.697	0.40108	0.94371	0.73514	-0.444	0.23757	0.95138	1.9264	0.9459	0.9381	0.99989	1.0157	0.0224	0.041441	0.27898	3.0445	1.6062	0.18009	0.74999	0.6292	-0.668
169.0266_10.18	C05851,	0.80177	0.99628	1.1234	0.16792	0.82971	0.99964	1.321	0.4017	0.91157	0.99993	1.0256	0.0365	0.92601	0.99517	1.1611	0.2155	0.05359	0.76092	1.6934	0.7599	0.34557	0.99989	0.77341	-0.3707	0.039037	0.27737	3.5723	1.8368	0.25372	0.74999	0.55139	-0.859
360.0692_0.45	C06376, N-Acetyl-D-galactosamine 6-phosphate	0.36281	0.85589	0.78232	-0.35417	0.64759	0.99807	1.0538	0.0756	0.57863	0.9993	0.86543	-0.2085	0.56617	0.97491	1.2182	0.2848	0.32771	0.94156	1.2859	0.3628	0.060933	0.99753	0.6879	-0.5397	0.006579	0.11139	1.9863	0.9901	0.018311	0.82425	0.75559	-0.404
280.2365_7.65	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	0.37431	0.99628	0.67505	-0.56693	0.84127	0.99964	0.82444	-0.2785	0.15343	0.99993	0.53412	-0.9048	0.96106	0.99932	1.0611	0.0855	0.10868	0.84488	0.4411	-1.1808	0.13879	0.99989	1.5005	0.5855	0.018152	0.21536	0.32576	-1.618	0.50978	0.78011	1.284	0.3607
279.2304_7.66	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	0.42328	0.99628	0.70976	-0.49459	0.83108	0.99964	0.83375	-0.2623	0.19965	0.99993	0.58054	-0.7845	0.81313	0.97917	1.0293	0.0416	0.13579	0.88708	0.47772	-1.0658	0.16867	0.99989	1.4334	0.5194	0.022239	0.22921	0.35926	-1.477	0.51636	0.78062	1.2458	0.3171
172.9588_12.15	C14453, 4-Bromophenol	0.86471	0.99628	1.0176	0.025176	0.95228	0.99964	0.99717	-0.0041	0.98417	0.99993	1.0038	0.0055	0.19801	0.94371	1.0886	0.1224	0.1664	0.92628	1.1372	0.1855	0.72402	0.99989	1.0309	0.0439	0.031406	0.26172	1.1619	0.2164	0.40676	0.75316	0.93588	-0.096
319.2274_6.69	C14779, 9(S)-HETE	0.16145	0.85589	0.17677	-2.5001	0.55995	0.99807	2.1117	1.0784	0.77598	0.9993	0.4055	-1.3022	0.61964	0.97491	1.893	0.9207	0.41557	0.94156	0.32046	-1.6418	0.50178	0.99753	1.5411	0.624	0.046296	0.22477	0.062728	-3.995	0.36504	0.82425	2.5233	1.3353
327.2326_7.86	C15647, 2-Acyl-1-(1-alkenyl)-sn-glycero-3-phosphate	0.44021	0.87438	1.1825	0.24182	0.53132	0.99807	0.88858	-0.1704	0.64037	0.9993	1.0652	0.0911	0.21371	0.97319	0.70037	-0.514	0.9895	0.99743	0.88316	-0.1793	0.66977	0.99753	0.8692	-0.2022	0.31534	0.53732	1.2992	0.3776	0.29316	0.82425	0.84807	-0.238
195.0505_0.43	C16356, 1,7-Dimethyluric acid	0.85317	0.96043	1.1064	0.14591	0.99746	0.99808	1.0596	0.0835	0.54313	0.9993	1.2541	0.3267	0.098265	0.97319	0.50123	-0.996	0.97912	0.99743	1.1643	0.2195	0.26808	0.99753	0.52719	-0.9236	0.34487	0.55643	1.57	0.6508	0.26265	0.82425	0.59317	-0.753
253.0837_4.12	C16584, p-Hydroxyfelbamate	0.90495	0.97508	0.88788	-0.17157	0.016034	0.99807	1.3455	0.4281	0.44075	0.9993	1.1719	0.2289	0.14636	0.97319	1.3777	0.4623	0.42093	0.94156	1.2854	0.3622	0.52187	0.99753	1.0925	0.1277	0.15529	0.39438	1.4822	0.5678	0.52377	0.84266	0.89291	-0.163
174.0546_1.42	C16596, 5-Phenyl-1,3-oxazinane-2,4-dione	0.057978	0.99628	0.60803	-0.71778	0.92942	0.99964	1.0168	0.0241	0.004113	0.57734	0.43871	-1.1887	0.00925	0.94371	3.5343	1.8214	0.067427	0.77152	0.55443	-0.8509	0.23064	0.99989	1.5844	0.664	0.019033	0.21853	0.59131	-0.758	0.79265	0.90978	1.1996	0.2626
252.0856_4.12	C16601, 2-Hydroxycarbamazepine	0.85045	0.96043	0.92464	-0.11304	0.018786	0.99807	1.3212	0.4018	0.39583	0.9993	1.2002	0.2633	0.13482	0.97319	1.3434	0.4259	0.37753	0.94156	1.3317	0.4132	0.54239	0.99753	1.0821	0.1138	0.1125	0.34419	1.5681	0.649	0.38215	0.82425	0.85559	-0.225
251.0824_4.12	C16601, 2-Hydroxycarbamazepine	0.8752	0.96713	0.91902	-0.12183	0.019138	0.99807	1.3174	0.3977	0.40779	0.9993	1.1939	0.2557	0.13124	0.97319	1.3515	0.4346	0.39718	0.94156	1.3183	0.3986	0.53073	0.99753	1.0879	0.1216	0.11075	0.34419	1.5705	0.6512	0.3645	0.82425	0.84678	-0.24
208.0755_4.12	C16604, 2-Hydroxyiminostilbene	0.91542	0.97823	0.88765	-0.17194	0.005797	0.99807	1.3777	0.4623	0.39688	0.9993	1.1942	0.256	0.13283	0.97319	1.3603	0.4439	0.39542	0.94156	1.3104	0.39	0.53784	0.99753	1.0887	0.1226	0.12895	0.36742	1.5388	0.6218	0.51134	0.83898	0.89139	-0.166
382.0367_0.46	C16619, 6-Thioguanosine monophosphate	0.1162	0.99628	0.83197	-0.26539	0.65318	0.99964	1.0914	0.1262	0.45621	0.99993	0.90425	-0.1452	0.42912	0.94371	1.2286	0.297	0.78256	0.98914	0.97057	-0.0431	0.65798	0.99989	1.0825	0.1144	0.061151	0.31771	1.1899	0.2508	0.014104	0.74999	0.74667	-0.421
462.1772_4.03	C16643, Morphine-3-glucuronide	0.011003	0.84693	0.23027	-2.1186	0.28332	0.99964	9.1571	3.1949	0.009624	0.84777	0.23097	-2.1142	0.047472	0.94371	5.8305	2.5436	0.21804	0.94889	0.4703	-1.0883	0.71583	0.99989	1.4097	0.4954	0.083853	0.36772	0.40743	-1.295	0.7124	0.877	0.93112	-0.103
377.1954_3.76	CE1342, 18-Hydroxycortisol	0.045728	0.81909	0.18401	-2.4421	0.79501	0.99807	1.2634	0.3373	0.28592	0.9993	0.41207	-1.2791	0.35278	0.97319	0.4942	-1.017	0.10375	0.77937	0.20417	-2.2922	0.87852	0.99753	0.91493	-0.1283	0.43739	0.62645	0.53187	-0.911	0.86095	0.95745	0.76927	-0.378
511.2558_4.29	CE2303, 9-hydroxy-10-O-D-glucuronoside-12Z-octadecenoate	0.73655	0.99628	0.80345	-0.31572	0.047587	0.99964	1.2951	0.3731	0.72941	0.99993	1.0349	0.0495	0.42114	0.94371	1.2414	0.3119	0.85988	0.99638	1.1774	0.2356	0.45078	0.99989	1.1443	0.1945	0.44585	0.65853	1.1449	0.1953	0.222	0.74999	0.77775	-0.363
260.0742_0.42	CE2847, fructoseglycine	0.37893	0.99628	0.89462	-0.16066	0.37009	0.99964	1.1813	0.2404	0.59629	0.99993	0.93526	-0.0966	0.91018	0.99265	1.0032	0.0046	0.80783	0.99304	1.0311	0.0442	0.50494	0.99989	1.083	0.115	0.055422	0.30937	1.4134	0.4992	0.041137	0.74999	0.62525	-0.677
607.3526_9.01	CE4754, dynorphin B (6-9)	0.5999	0.99628	0.90117	-0.15014	0.59736	0.99964	0.84861	-0.2368	0.68226	0.99993	0.93194	-0.1017	0.48904	0.94371	0.82292	-0.281	0.8138	0.99304	1.0576	0.0808	0.55469	0.99989	0.85626	-0.2239	0.18248	0.48789	0.73366	-0.447	0.95655	0.98726	1.0138	0.0197
304.2363_7.57	CE5013,	0.26642	0.99628	2.0595	1.0423	0.73451	0.99964	0.75263	-0.41	0.11238	0.99993	1.6112	0.6881	0.12435	0.94371	0.67587	-0.565	0.22419	0.94889	1.4473	0.5333	0.71264	0.99989	0.9413	-0.0873	0.22046	0.51525	1.4691	0.5549	0.5343	0.78886	0.84716	-0.239
270.2306_7.95	CE5014, anhydroretinol	0.16406	0.99628	1.3866	0.47151	0.30132	0.99964	0.76848	-0.3799	0.37564	0.99993	1.1801	0.2389	0.048001	0.94371	0.68436	-0.547	0.11733	0.85114	1.3792	0.4638	0.34159	0.99989	0.87526	-0.1922	0.17345	0.47893	1.2432	0.314	0.24444	0.74999	0.90065	-0.151
269.2271_7.95	CE5014, anhydroretinol	0.1722	0.99628	1.3726	0.45694	0.29965	0.99964	0.77198	-0.3734	0.39828	0.99993	1.1573	0.2108	0.043742	0.94371	0.70578	-0.503	0.12333	0.8561	1.3593	0.4429	0.34959	0.99989	0.88638	-0.174	0.15362	0.46247	1.2561	0.3289	0.35317	0.74999	0.92543	-0.112
222.1622_7.98	CE5325, 6(S)-hydroxy-tetradeca-4E,8Z-dienoate	0.48642	0.99628	1.3951	0.48034	0.61326	0.99964	0.77668	-0.3646	0.85552	0.99993	1.043	0.0608	0.35631	0.94371	0.81402	-0.297	0.74727	0.98164	1.0475	0.0669	0.50472	0.99989	1.1384	0.187	0.39531	0.61701	1.1054	0.1446	0.042658	0.74999	0.85691	-0.223
376.2592_5.34	CE5719, 9'-carboxy-gama-chromanol	0.98373	0.99637	0.99781	-0.0031587	0.32544	0.99964	1.2232	0.2907	0.62476	0.99993	0.94941	-0.0749	0.45327	0.94371	1.1274	0.173	0.21588	0.94889	1.2979	0.3762	0.25381	0.99989	0.79675	-0.3278	0.59684	0.75481	0.93961	-0.09	0.45354	0.76373	1.1031	0.1416
359.2581_5.95	CE6027, 24,25,26,27-tetranor-23-oxo-hydroxyvitamin D3	0.70714	0.99628	1.0912	0.12589	0.70058	0.99964	0.91601	-0.1266	0.41356	0.99993	1.2269	0.295	0.04142	0.94371	0.47025	-1.089	0.34765	0.954	1.3482	0.4311	0.80797	0.99989	0.92445	-0.1133	0.066111	0.32684	1.6175	0.6937	0.2267	0.74999	0.83456	-0.261
339.1995_10.29	CE6435,	0.65196	0.91959	1.1124	0.15368	0.73016	0.99807	0.92079	-0.1191	0.63386	0.9993	1.2577	0.3308	0.68146	0.97491	1.3718	0.4561	0.073041	0.74135	1.2223	0.2896	0.95987	0.99753	1.0536	0.0753	0.001815	0.078811	1.6149	0.6915	0.016135	0.82425	0.68675	-0.542
139.1118_4.31	CE6506,	0.56678	0.99628	0.73359	-0.44696	0.045157	0.99964	1.3267	0.4078	0.82951	0.99993	0.96478	-0.0517	0.43832	0.94371	1.2214	0.2885	0.99003	0.99707	1.0585	0.0821	0.31926	0.99989	1.2698	0.3446	0.54457	0.72438	1.0778	0.1081	0.31957	0.74999	0.81715	-0.291
111.1175_4.31	CE6506,	0.59987	0.99628	0.72406	-0.46582	0.037351	0.99964	1.3807	0.4654	0.7674	0.99993	0.97518	-0.0363	0.46321	0.94371	1.229	0.2974	0.91528	0.99638	1.0896	0.1238	0.35142	0.99989	1.2357	0.3053	0.51005	0.70439	1.0866	0.1198	0.32589	0.74999	0.82333	-0.28
423.3238_6.01	CE7144, 13'-hydroxy-alpha-tocotrienol	0.28917	0.99628	0.26706	-1.9048	0.70625	0.99964	0.95457	-0.0671	0.51226	0.99993	0.33092	-1.5955	0.085184	0.94371	1.5339	0.6172	0.32634	0.954	0.22641	-2.143	0.78124	0.99989	1.0709	0.0988	0.61925	0.77274	0.40572	-1.301	0.49294	0.77696	0.6616	-0.596
451.3567_6.3	dlnlcgcrn, dihomo-gamma-linolenyl carnitine	0.43837	0.99628	0.65204	-0.61697	0.71634	0.99964	1.0368	0.0521	0.63398	0.99993	0.70727	-0.4997	0.020733	0.94371	1.8442	0.883	0.6214	0.96556	0.68397	-0.548	0.97677	0.99989	0.98022	-0.0288	0.6311	0.78081	1.1589	0.2127	0.72646	0.88126	0.80842	-0.307
399.3298_6.03	hdd2crn, trans-Hexadec-2-enoyl carnitine	0.41148	0.99628	0.26407	-1.921	0.7594	0.99964	1.034	0.0482	0.30473	0.99993	0.19435	-2.3633	0.021174	0.94371	3.5551	1.8299	0.36729	0.954	0.19245	-2.3774	0.24526	0.99989	1.3583	0.4418	0.73243	0.8488	0.37717	-1.407	0.35375	0.74999	0.60092	-0.735
398.327_6.05	hdd2crn, trans-Hexadec-2-enoyl carnitine	0.50524	0.99628	0.30384	-1.7186	0.68152	0.99964	1.0599	0.0839	0.63671	0.99993	0.29291	-1.7715	0.009658	0.94371	2.8993	1.5357	0.46273	0.954	0.21425	-2.2227	0.20577	0.99989	1.4802	0.5658	0.85551	0.9162	0.44761	-1.16	0.48537	0.77491	0.58256	-0.78
425.3459_6.15	lneldccrn, Linoelaidyl carnitine	0.41299	0.99628	0.47702	-1.0679	0.66218	0.99964	1.0517	0.0728	0.46249	0.99993	0.45668	-1.1307	0.014677	0.94371	2.352	1.2339	0.52238	0.96399	0.44892	-1.1555	0.089784	0.99989	1.4015	0.487	0.89546	0.93711	0.86315	-0.212	0.2839	0.74999	0.53259	-0.909
424.3427_6.15	lneldccrn, Linoelaidyl carnitine	0.41955	0.99628	0.4953	-1.0136	0.66926	0.99964	1.0532	0.0747	0.48688	0.99993	0.48467	-1.0449	0.019357	0.94371	2.1962	1.135	0.51556	0.96206	0.46369	-1.1088	0.072048	0.99989	1.4044	0.49	0.91887	0.94938	0.85872	-0.22	0.306	0.74999	0.5595	-0.838
426.3584_6.46	odecrn, octadecenoyl carnitine	0.55386	0.99628	0.58404	-0.77586	0.58643	0.99964	1.1602	0.2144	0.73965	0.99993	0.62027	-0.689	0.017423	0.94371	2.1007	1.0708	0.79789	0.99304	0.61958	-0.6906	0.069124	0.99989	1.3979	0.4832	0.79506	0.8866	0.98925	-0.016	0.43424	0.75664	0.62724	-0.673
427.3617_6.46	odecrn, octadecenoyl carnitine	0.55764	0.99628	0.55981	-0.83698	0.58733	0.99964	1.1841	0.2438	0.73919	0.99993	0.59012	-0.7609	0.016718	0.94371	2.1813	1.1252	0.80152	0.99304	0.59176	-0.7569	0.082669	0.99989	1.4234	0.5093	0.79333	0.88592	0.97601	-0.035	0.42091	0.75355	0.6027	-0.73
450.3557_6.29	stcrn, stearoylcarnitine	0.48278	0.99628	0.62348	-0.68158	0.75193	0.99964	1.0062	0.0089	0.79433	0.99993	0.72046	-0.473	0.018089	0.94371	1.8175	0.862	0.64844	0.96671	0.64134	-0.6408	0.93133	0.99989	0.9957	-0.0062	0.73469	0.85006	1.0752	0.1046	0.79721	0.91251	0.81151	-0.301
447.3271_6.04	tmndnccrn, Timnodonyl carnitine	0.59079	0.99628	0.67081	-0.57602	0.52365	0.99964	1.0954	0.1314	0.84782	0.99993	0.85866	-0.2199	0.035221	0.94371	1.5099	0.5945	0.78267	0.98914	0.68886	-0.5377	0.41168	0.99989	1.2186	0.2852	0.50144	0.69769	1.3021	0.3809	0.35667	0.74999	0.61646	-0.698

Supplementary Table 4. Comparative metabolomics data of lung tissue between "irradiated vs naïve" and "GT3 vs irradiated" treatment groups for 4.0 and 5.8 Gy exposure to PBI (LINAC) and TBI (Cobalt-60).

		PBI 4 Gy Irradiated vs. Naïve				PBI 4 Gy Irradiated vs. GT3				TBI 4 Gy Irradiated vs. Naïve				TBI 4 Gy Irradiated vs. GT3				PBI 5.8 Gy Irradiated vs. Naïve				PBI 5.8 Gy Irradiated vs. GT3				TBI 5.8 Gy Irradiated vs. Naïve				TBI 5.8 Gy Irradiated vs. GT3			
mz_RT	EmpiricalCompound	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)
1138.4528_11.93	3ohxccoa, 3-Oxohexacosyl-CoA	0.036973	0.63665	1.3031	0.38195	0.29928	0.81752	0.92399	-0.1141	0.1705	0.63219	1.1665	0.2222	0.25543	0.76376	1.0717	0.0998	0.36343	0.6602	1.1546	0.2074	0.6858	0.87426	1.0461	0.0651	0.2011	0.72205	1.1458	0.1964	0.008879	0.99459	1.2004	0.2635
489.2473_4.64	5adtststeroneglc, 5alpha-Dihydrotestosterone glucuronide	0.014981	0.55658	3.8511	1.9453	0.35443	0.8216	0.58362	-0.7769	0.008394	0.57762	3.5567	1.8306	0.82884	0.92837	1.4334	0.5195	0.002432	0.61158	7.6142	2.9287	0.24511	0.6522	0.4886	-1.033	0.014438	0.65597	14.4	3.848	0.51921	0.99459	0.29128	-1.78
465.249_4.65	ahandrostanglc, Etiocholan-3alpha-ol-17-one 3-glucuronide	0.030634	0.46597	3.7681	1.9139	0.36999	0.90573	0.58271	-0.7792	0.021138	0.32936	3.4751	1.7971	0.93798	0.97021	1.3635	0.4473	0.008436	0.40888	7.7065	2.9461	0.28058	0.72481	0.50411	-0.988	0.027096	0.68442	12.109	3.598	0.57365	0.97554	0.35931	-1.477
456.4035_7.22	arachcrn, arachidyl carnitine	0.41657	0.77216	1.3207	0.4013	0.91677	0.98437	1.0895	0.1236	0.26262	0.658	4.6932	2.2306	0.8104	0.92766	0.38326	-1.384	0.26039	0.63093	1.4692	0.555	0.47532	0.76195	1.3498	0.4328	0.02304	0.65597	2.5545	1.353	0.77363	0.99459	0.95217	-0.071
326.2201_8.06	arachd, arachidonic acid	0.20366	0.69542	1.2345	0.30398	0.92088	0.98682	0.98166	-0.0267	0.017453	0.62084	1.3724	0.4567	0.39345	0.80644	1.0743	0.1034	0.13403	0.61158	1.321	0.4017	0.19015	0.63008	0.77989	-0.359	0.53821	0.88973	1.0934	0.1288	0.57198	0.99459	1.1037	0.1423
449.346_6.11	arachdcrn, C20:4 carnitine	0.19422	0.69542	1.7238	0.78562	0.79973	0.94932	1.2385	0.3086	0.083172	0.62084	2.3448	1.2295	0.23628	0.75876	1.7125	0.7761	0.05955	0.61158	4.2436	2.0853	0.30557	0.68844	0.62135	-0.687	0.012867	0.65597	7.9492	2.9908	0.21012	0.99459	0.49237	-1.022
448.3426_6.11	arachdcrn, C20:4 carnitine	0.21012	0.69542	1.7196	0.78209	0.77466	0.94349	1.2475	0.3191	0.10599	0.62084	2.3712	1.2456	0.24297	0.76013	1.6705	0.7403	0.078577	0.61158	4.3747	2.1292	0.25767	0.66164	0.61449	-0.703	0.02298	0.65597	7.4966	2.9062	0.2116	0.99459	0.5097	-0.972
146.046_0.42	C00025, L-Glutamate	0.16473	0.57493	1.3572	0.44064	0.65469	0.96194	1.0494	0.0696	0.25049	0.48959	1.2244	0.2921	0.15552	0.85896	1.1586	0.2124	0.047348	0.40888	1.651	0.7234	0.18941	0.71367	0.80927	-0.305	0.21628	0.70307	1.2439	0.3149	0.32437	0.97554	1.1872	0.2475
306.0766_0.44	C00051, Glutathione	0.073198	0.52458	0.1443	-2.7928	0.28084	0.90573	2.0655	1.0465	0.84581	0.90601	0.75513	-0.405	0.29493	0.85896	1.6708	0.7406	0.26305	0.5299	0.93224	-0.101	0.047008	0.71367	0.51848	-0.948	0.56787	0.97448	0.41486	-1.269	0.63199	0.97554	1.32	0.4006
173.0429_0.41	C00121, D-Ribose	0.065537	0.66599	0.5569	-0.8445	0.014283	0.81752	1.7435	0.802	0.81686	0.91809	1.0017	0.0025	0.3225	0.78345	1.1516	0.2037	0.4382	0.70823	1.1842	0.244	0.26374	0.66219	0.80845	-0.307	0.9726	0.99995	0.95587	-0.065	0.70763	0.99459	0.91414	-0.13
613.1595_0.47	C00127, Glutathione disulfide	0.000828	0.31434	0.056577	-4.1436	0.16072	0.81752	3.8239	1.9351	0.062489	0.62084	0.28277	-1.822	0.094818	0.67902	3.8749	1.9541	0.88158	0.94224	0.73208	-0.45	0.43674	0.74531	0.75536	-0.405	0.29439	0.78975	0.5844	-0.775	0.64454	0.99459	0.39932	-1.324
116.0711_0.42	C00148, L-Proline	0.5664	0.8393	1.0869	0.12023	0.94887	0.99343	0.95929	-0.06	0.52832	0.74962	1.0856	0.1185	0.80501	0.92766	1.0447	0.0631	0.32344	0.64302	1.4653	0.5512	0.033116	0.6184	0.65929	-0.601	0.90469	0.99877	0.84966	-0.235	0.24845	0.99459	1.3551	0.4384
121.0293_3.15	C00180, Benzoate	0.30576	0.62185	1.3872	0.47221	0.31948	0.90573	1.3328	0.4145	0.19031	0.47823	1.4008	0.4862	0.38042	0.85896	1.3044	0.3833	0.05952	0.40888	1.9612	0.9717	0.96623	0.98923	0.98008	-0.029	0.042732	0.68442	2.7727	1.4713	0.27627	0.97554	0.58381	-0.776
327.2277_8.53	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.043321	0.63665	1.5764	0.65666	0.71687	0.92871	1.0516	0.0725	0.015151	0.62084	2.062	1.0441	0.46935	0.80931	0.8093	-0.305	0.060935	0.61158	1.6566	0.7283	0.4585	0.75723	0.85132	-0.232	0.5453	0.89518	1.1095	0.15	0.17077	0.99459	1.4292	0.5153
306.2513_6.85	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.15612	0.6945	0.20279	-2.302	0.26832	0.81752	2.7265	1.447	0.28076	0.65851	0.26517	-1.915	0.2131	0.74846	1.4833	0.5688	0.43092	0.70477	0.30109	-1.732	0.71605	0.88904	1.5244	0.6082	0.53234	0.88973	0.54325	-0.88	0.84046	0.99491	0.60701	-0.72
153.1278_8.53	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.47011	0.79651	1.137	0.18528	0.40823	0.82217	1.1279	0.1737	0.097618	0.62084	2.1165	1.0817	0.51675	0.82172	0.64581	-0.631	0.34972	0.65767	1.2493	0.3212	0.81907	0.93095	0.92495	-0.113	0.71662	0.95198	1.0293	0.0417	0.15214	0.99459	1.2604	0.3339
140.9961_12.14	C00227, Acetyl phosphate	0.10783	0.6945	0.89446	-0.16091	0.49285	0.83853	1.0344	0.0487	0.35107	0.67009	0.94006	-0.089	0.40273	0.80644	1.0512	0.0721	0.32044	0.64146	1.0736	0.1024	0.046711	0.6184	0.86557	-0.208	0.7022	0.94771	1.0301	0.0427	0.87395	0.99502	0.98449	-0.023
139.9885_12.14	C00227, Acetyl phosphate	0.12855	0.6945	0.89854	-0.15434	0.78512	0.94664	1.0147	0.0211	0.46184	0.72417	0.95675	-0.064	0.67746	0.87902	1.0237	0.0338	0.20022	0.61476	1.0971	0.1336	0.034629	0.6184	0.82806	-0.272	0.85209	0.99047	1.0174	0.0249	0.93578	0.99664	0.98833	-0.017
124.0614_0.42	C00242, Guanine	0.59059	0.85213	1.0859	0.1189	0.2194	0.81752	1.1938	0.2555	0.43918	0.7154	1.1966	0.2589	0.13411	0.68823	1.2849	0.3616	0.172	0.61158	1.5473	0.6297	0.006309	0.6184	0.76199	-0.392	0.17671	0.6978	1.5331	0.6165	0.79645	0.99459	0.93045	-0.104
174.0392_0.41	C00242, Guanine	0.62753	0.87348	1.0661	0.092398	0.26791	0.81752	1.1629	0.2178	0.53867	0.75521	1.0847	0.1173	0.0266	0.63307	1.23	0.2986	0.35912	0.65986	1.2198	0.2867	0.092763	0.6184	0.86144	-0.215	0.42342	0.86047	1.1655	0.2209	0.91885	0.99664	0.97572	-0.035
256.2362_8.43	C00249, Hexadecanoic acid	0.000153	0.045958	1.6426	0.71595	0.79836	0.97304	0.98108	-0.0276	0.002858	0.32936	1.4781	0.5638	0.54059	0.89499	0.94478	-0.082	0.60845	0.74753	0.93443	-0.098	0.93079	0.98923	1.0277	0.0395	0.87086	0.99561	0.9916	-0.012	0.49812	0.97554	1.1329	0.1801
255.2329_8.43	C00249, Hexadecanoic acid	0.000323	0.04868	1.5118	0.59624	0.72167	0.96194	0.97444	-0.0374	0.021182	0.32936	1.4429	0.529	0.82214	0.93543	0.96515	-0.051	0.26719	0.5299	0.84608	-0.241	0.75346	0.89615	1.0542	0.0762	0.90883	0.99561	0.99958	-6E-04	0.75239	0.97554	1.0704	0.0982
239.2362_8.44	C00249, Hexadecanoic acid	0.007898	0.50491	1.4023	0.48782	0.66534	0.91253	1.0361	0.0512	0.079036	0.62084	2.5886	1.3722	0.51597	0.82158	0.56645	-0.82	0.32365	0.64302	0.85766	-0.222	0.64764	0.85884	1.1146	0.1566	0.71295	0.94952	1.0336	0.0477	0.31788	0.99459	1.1987	0.2615
258.2507_8.44	C00249, Hexadecanoic acid	0.012797	0.53241	1.4453	0.53135	0.90102	0.98276	0.99003	-0.0145	0.07428	0.62084	2.7236	1.4455	0.47405	0.81046	0.53539	-0.901	0.26356	0.63193	0.82684	-0.274	0.70995	0.88651	1.0741	0.1032	0.81209	0.98358	0.97125	-0.042	0.26693	0.99459	1.2767	0.3524
257.2478_8.44	C00249, Hexadecanoic acid	0.014914	0.55658	1.3618	0.44546	0.75437	0.93682	1.0268	0.0381	0.078464	0.62084	2.5117	1.3286	0.51828	0.82172	0.58154	-0.782	0.24099	0.62664	0.82564	-0.276	0.67513	0.87002	1.0911	0.1258	0.87349	0.99433	1.0137	0.0197	0.32275	0.99459	1.2052	0.2693
279.2321_7.64	C00249, Hexadecanoic acid	0.11105	0.6945	0.68794	-0.53964	0.14308	0.81752	1.6057	0.6832	0.36635	0.67848	1.1786	0.237	0.85957	0.94537	1.0773	0.1074	0.57017	0.76843	0.87121	-0.199	0.35844	0.70998	0.75382	-0.408	0.023719	0.65597	0.52564	-0.928	0.17199	0.99459	1.4464	0.5325
377.1461_2.42	C00255, Riboflavin	0.59792	0.85589	0.55421	-0.8515	0.20495	0.81752	1.417	0.5029	0.67192	0.84117	0.55454	-0.851	0.011063	0.63307	2.0159	1.0114	0.7239	0.85737	0.88304	-0.179	0.088008	0.6184	0.71811	-0.478	0.87123	0.99433	0.83282	-0.264	0.64244	0.99459	1.1344	0.1819
159.0273_0.43	C00262, Hypoxanthine	0.4512	0.7884	0.8923	-0.1644	0.21478	0.81752	1.139	0.1878	0.81027	0.91589	0.9554	-0.066	0.056148	0.63845	1.2258	0.2937	0.35993	0.65986	1.1239	0.1685	0.048825	0.6184	0.88046	-0.184	0.37715	0.85167	1.1565	0.2098	0.58897	0.99459	0.90773	-0.14
137.0464_0.44	C00262, Hypoxanthine	0.46048	0.79384	1.1434	0.19335	0.31254	0.81752	1.0845	0.117	0.52658	0.74962	1.1096	0.1501	0.049398	0.63845	1.2532	0.3256	0.22177	0.62157	1.4364	0.5225	0.036238	0.6184	0.81213	-0.3	0.42063	0.86047	1.1715	0.2283	0.39843	0.99459	1.1419	0.1915
138.0489_0.44	C00262, Hypoxanthine	0.55211	0.83451	1.0959	0.13211	0.4373	0.83068	1.0785	0.1091	0.59347	0.78665	1.0738	0.1027	0.065988	0.64532	1.261	0.3346	0.25562	0.62714	1.4463	0.5324	0.012918	0.6184	0.75773	-0.4	0.44547	0.86047	1.1745	0.2321	0.50693	0.99459	1.1071	0.1468
291.0693_0.43	C00294, Inosine	0.35159	0.73826	0.78797	-0.34379	0.22927	0.81752	0.83896	-0.2533	0.28466	0.65851	0.77074	-0.376	0.97335	0.98843	0.93093	-0.103	0.17493	0.61158	1.3571	0.4405	0.071138	0.6184	0.72423	-0.465	0.46477	0.86437	1.2148	0.2807	0.6397	0.99459	1.0734	0.1022
307.0445_0.43	C00294, Inosine	0.47516	0.80037	1.116	0.1583	0.48953	0.83827	0.92984	-0.105	0.9218	0.97128	0.98574	-0.021	0.68145	0.88088	1.1306	0.1771	0.024651	0.61158	2.1548	1.1076	0.044996	0.6184	0.67177	-0.574	0.09946	0.65597	1.5905	0.6694	0.1948	0.99459	1.2122	0.2776
268.076_0.43	C00294, Inosine	0.6678	0.8171	1.0097	0.013889	0.1635	0.90573	0.80358	-0.3155	0.3477	0.59032	0.76317	-0.39	0.83694	0.93578	1.0011	0.0016	0.028178	0.40888	1.687	0.7544	0.091013	0.71367	0.67881	-0.559	0.31117	0.81662	1.2949	0.3729	0.57862	0.97554	1.0909	0.1256
267.0734_0.44	C00294, Inosine	0.95979	0.97318	0.94459	-0.08224	0.23538	0.90573	0.87532	-0.1921	0.44819	0.66657	0.82728	-0.274	0.91167	0.96624	0.93989	-0.089	0.012124	0.40888	1.6129	0.6897	0.022607	0.71367	0.68271	-0.551	0.17385	0.68442	1.3002	0.3787	0.39547	0.97554	1.12	0.1635
279.0381_0.43	C00299, Uridine	0.068733	0.5046	1.413	0.49879	0.03932	0.90573	1.9107	0.9341	0.95822	0.97439	1.0146	0.0209	0.23159	0.85896	1.5352	0.6185	0.046422	0.40888	2.053	1.0378	0.40934	0.7298	0.7893	-0.341	0.1276	0.68442	1.2341	0.3035	0.8751	0.97554	1.0978	0.1347
243.0622_0.43	C00299, Uridine	0.18047	0.57493	1.3529	0.43602	0.03973	0.90573	1.9302	0.9487	0.86208	0.91605	0.97497	-0.037	0.15987	0.85896	1.6146	0.6912	0.032618	0.40888	2.1137	1.0798	0.32391	0.72481	0.76165	-0.393	0.24005	0.74491	1.218	0.2845	0.82621	0.97554	1.0823	0.1141
114.0662_0.41	C00300, Creatine	0.58528	0.84925	1.0186	0.026648	0.30468	0.81752	1.2378	0.3077	0.22864	0.63886	1.4903	0.5756	0.96078	0.98495	0.98926	-0.016	0.23092	0.62301	1.6204	0.6963	0.024997	0.6184	0.73755	-0.439	0.33693	0.82905	1.2552	0.3279	0.7771	0.99459	1.0693	0.0967
132.0301_0.43	C00402, D-Aspartate	0.25563	0.57728	1.2335	0.30271	0.58039	0.92433	1.1817	0.2409	0.64984	0.80165	0.95222	-0.071	0.028551	0.85896	1.2936	0.3714	0.042697	0.40888	1.8438	0.8827	0.13618	0.71367	0.76089	-0.394	0.83657	0.99561	0.88205	-0.181	0.057917	0.97554	1.5005	0.5854
120.0812_0.64	C00483, Tyramine	0.74954	0.90448	0.71143	-0.49121	0.82672	0.95751	0.85954	-0.2184	0.50573	0.74001	0.55927	-0.838	0.22442	0.75395	1.3717	0.456	0.56626	0.76748	1.1441	0.1942	0.038034	0.6184	0.47471	-1.075	0.61899	0.91673	0.61784	-0.695	0.46965	0.99459	1.214	0.2798
607.2571_8.73	C00486, Bilirubin	0.040292	0.63665	2.8522	1.5121	0.29906	0.81752	0.61251	-0.7072	0.011105	0.594	3.391	1.7617	0.40747	0.80782	0.85303	-0.229	0.026352	0.61158	3.9713	1.9896	0.40165	0.72904	0.66505	-0.588	0.14164	0.68578	2.3583	1.2377	0.45976	0.99459	1.1537	0.2063
585.2745_8.73	C00486, Bilirubin	0.05122	0.63928	2.7322	1.4501	0.26774	0.81752	0.57642	-0.7948	0.02356	0.62084	2.7967	1.4837	0.46643	0.80931	0.90176	-0.149	0.037159	0.61158	3.6104	1.8522	0.36382	0.70998	0.63368	-0.658	0.2125	0.72507	2.1472	1.1024	0.541	0.99459	1.0357	0.0506
567.2633_6.66	C00486, Bilirubin	0.33649	0.72724	1.1848	0.24462	0.91253	0.98398	1.0103	0.0147	0.3093	0.65851	1.2368	0.3066	0.31878	0.78345	1.1246	0.1694	0.13516	0.61158	1.4661	0.552	0.23614	0.64744	0.79118	-0.338	0.37257	0.85123	1.2856	0.3625	0.65738	0.99459	1.0371	0.0525
583.2561_5.21	C00500, Biliverdin	0.048188	0.63665	2.2876	1.1939	0.006302	0.81752	0.28186	-1.8269	0.15112	0.62084	1.5566	0.6384	0.34289	0.78861	0.51248	-0.964	0.19395	0.61467	1.4455	0.5316	0.46091	0.75767	1.182	0.2412	0.42251	0.86047	1.4877	0.5731	0.2931	0.99459	2.1689	1.117
583.2556_4.96	C00500, Biliverdin	0.24483	0.69775	1.364	0.44787	0.00305	0.81733	0.29637	-1.7545	0.62153	0.80537	0.90256	-0.148	0.22824	0.75876	0.5742	-0.8	0.62867	0.80403	0.91051	-0.135	0.71954	0.89059	1.2095	0.2744	0.64179	0.92496	1.0054	0.0078	0.56996	0.99459	1.6114	0.6883
255.2113_4.65	C00523, Androsterone	0.036981	0.63665	3.6679	1.875	0.34414	0.82008	0.61105	-0.7106	0.031457	0.62084	3.4971	1.8061	0.78578	0.92251	1.5275	0.6111	0.015135	0.61158	7.8135	2.966	0.21145	0.64161	0.47294	-1.08	0.017202	0.65597	12.552	3.6498	0.56871	0.99459	0.36988	-1.435
273.2217_4.65	C00523, Androsterone	0.038267	0.63665	3.5318	1.8204	0.37458	0.82217	0.62895	-0.669	0.029697	0.62084	3.3734	1.7542	0.76499	0.91806	1.5649	0.6461	0.01429	0.61158	7.5684	2.92	0.21422	0.64161	0.47183	-1.084	0.017029	0.65597	12.49	3.6427	0.55862	0.99459	0.35789	-1.482
353.2306_4.8	C00584, Prostaglandin E2	0.00481	0.46941	0.20787	-2.2663	0.34137	0.82008	1.2707	0.3456	0.032222	0.62084	0.35258	-1.504	0.45318	0.80811	1.2757	0.3512	0.17214	0.61158	0.48485	-1.044	0.45025	0.75373	0.74231	-0.43	0.060232	0.65597	0.38665	-1.371	0.75805	0.99459	0.76685	-0.383
353.2305_4.45	C00584, Prostaglandin E2	0.020094	0.5663	0.065143	-3.9403	0.055502	0.81752	3.3175	1.7301	0.097827	0.62084	0.186	-2.427	0.36222	0.79362	1.0872	0.1206	0.17438	0.61158	0.15863	-2.656	0.85862	0.94686	1.6848	0.7526	0.1912	0.70766	0.28475	-1.812	0.77404	0.99459	0.4616	-1.115
375.2151_4.86	C00584, Prostaglandin E2	0.17157	0.6945	0.5659	-0.82137	0.56875	0.86502	1.3048	0.3839	0.50321	0.73945	0.81161	-0.301	0.38454	0.80053	1.462	0.5479	0.29036	0.63316	1.9945	0.996	0.069017	0.6184	0.20117	-2.314	0.15922	0.69669	0.55608	-0.847	0.44577	0.99459	1.1831	0.2425
366.1401_6.57	C00611, N-Acetyllactosamine	0.91018	0.96154	1.0093	0.013395	0.21943	0.81752	0.8968	-0.1572	0.58414	0.77915	0.94799	-0.077	0.32308	0.78345	1.0896	0.1238	0.40674	0.69856	1.1155	0.1577	0.42563	0.74026	0.88437	-0.177	0.41672	0.86047	1.1242	0.1689	0.84937	0.99491	0.95848	-0.061
282.2519_8.52	C00712, (9Z)-Octadecenoic acid	0.30154	0.61744	1.2634	0.33728	0.55874	0.92433	1.1016	0.1396	0.011973	0.32936	1.7242	0.7859	0.20884	0.85896	0.80183	-0.319	0.17528	0.40888	1.4182	0.504	0.53124	0.80121	0.85601	-0.224	0.85231	0.99561	1.02	0.0285	0.75479	0.97554	1.0921	0.1271
265.2531_8.53	C00712, (9Z)-Octadecenoic acid	0.43984	0.78121	1.1329	0.18004	0.3561	0.82217	1.1428	0.1926	0.079884	0.62084	1.927	0.9464	0.53281	0.82976	0.71292	-0.488	0.2699	0.63193	1.2682	0.3428	0.80123	0.92227	0.93114	-0.103	0.56669	0.90567	1.074	0.103	0.25379	0.99459	1.2054	0.2695
247.2397_8.53	C00712, (9Z)-Octadecenoic acid	0.48782	0.80352	1.1243	0.16908	0.40256	0.82217	1.13	0.1763	0.098342	0.62084	1.9374	0.9541	0.57702	0.85159	0.71101	-0.492	0.34322	0.65333	1.2393	0.3096	0.85848	0.94686	0.9374	-0.093	0.59626	0.91423	1.0657	0.0917	0.23391	0.99459	1.2222	0.2895
118.0867_0.42	C00719, Betaine	0.67001	0.8791	0.75933	-0.3972	0.52531	0.8499	0.93449	-0.0977	0.82059	0.91849	0.82557	-0.277	0.71975	0.89629	1.0923	0.1273	0.71213	0.84918	1.048	0.0676	0.027148	0.6184	0.54909	-0.865	0.44026	0.86047	0.6765	-0.564	0.49128	0.97554	1.2244	0.2921
302.3059_5.9	C00836, Sphinganine	0.047634	0.63665	1.753	0.80983	0.29264	0.81752	0.82766	-0.2729	0.1049	0.62084	1.8167	0.8613	0.94566	0.97967	0.99188	-0.012	0.91169	0.95439	0.98786	-0.018	0.088406	0.6184	1.6172	0.6935	0.047557	0.65597	1.8417	0.8811	0.97008	0.99664	0.97638	-0.034
242.1023_2.53	C00864, Pantothenate	0.27929	0.70183	1.5726	0.65314	0.97454	0.99844	0.92851	-0.107	0.1278	0.62084	1.7606	0.816	0.041877	0.63307	1.8637	0.8982	0.091237	0.61158	2.1331	1.0929	0.34785	0.70998	0.7145	-0.485	0.056917	0.65597	1.8332	0.8744	0.034362	0.99459	1.6704	0.7402
319.2247_6.42	C00909, Leukotriene A4	0.081586	0.67661	0.085279	-3.5517	0.1359	0.81752	3.226	1.6897	0.27717	0.65851	0.17105	-2.548	0.5288	0.82666	1.1099	0.1505	0.21777	0.62157	0.11854	-3.077	0.58991	0.82324	2.4202	1.2751	0.48259	0.87655	0.3006	-1.734	0.58682	0.99459	0.5851	-0.773
320.2272_6.42	C00909, Leukotriene A4	0.08495	0.67661	0.07962	-3.6507	0.1404	0.81752	3.2908	1.7184	0.28924	0.65851	0.16987	-2.558	0.61824	0.86077	1.0645	0.0901	0.25499	0.62714	0.12567	-2.992	0.68903	0.8754	2.1854	1.1279	0.43504	0.86047	0.26383	-1.922	0.61295	0.99459	0.60725	-0.72
569.3112_2.96	C01079, Protoporphyrinogen IX	0.010017	0.51849	0.41911	-1.2546	0.93573	0.99133	1.0209	0.0299	0.000295	0.26436	0.36428	-1.457	0.36888	0.79362	2.1798	1.1242	0.31777	0.63987	0.83376	-0.262	0.22499	0.64161	0.45314	-1.142	0.012854	0.65597	0.54269	-0.882	0.76305	0.99459	1.0381	0.0539
363.2169_3.84	C01124, 18-Hydroxycorticosterone	0.64741	0.87494	0.969	-0.045426	0.30925	0.81752	1.9223	0.9429	0.049307	0.62084	2.2003	1.1377	0.15588	0.70436	1.5495	0.6318	0.24778	0.62664	1.6382	0.7121	0.55219	0.80675	0.72446	-0.465	0.21885	0.73165	4.1858	2.0655	0.63876	0.99459	0.316	-1.662
252.0885_4.11	C01136, S-Acetyldihydrolipoamide	0.14328	0.6945	1.7684	0.82241	0.3156	0.81752	1.0807	0.112	0.1869	0.63877	1.5694	0.6503	0.082604	0.66413	1.2537	0.3262	0.17349	0.61158	1.9702	0.9784	0.044769	0.6184	0.83636	-0.258	0.094652	0.65597	2.1771	1.1224	0.59015	0.99459	0.94468	-0.082
167.0171_3.35	C01185, Nicotinate D-ribonucleotide	0.85547	0.91434	1.0061	0.0087403	0.95262	0.98574	1.0034	0.0049	0.10328	0.47625	1.0644	0.09	0.045771	0.85896	0.93723	-0.094	0.75778	0.83551	0.98387	-0.023	0.74343	0.89002	0.97972	-0.03	0.45152	0.87443	1.0254	0.0362	0.48487	0.97554	0.9815	-0.027
289.2164_3.85	C01227, 3beta-Hydroxyandrost-5-en-17-one	0.55449	0.83492	0.71111	-0.49186	0.48417	0.83827	1.3731	0.4574	0.33763	0.66415	1.308	0.3873	0.73791	0.9048	1.4159	0.5017	0.18194	0.61158	2.5978	1.3773	0.17988	0.62149	0.32569	-1.618	0.090136	0.65597	2.772	1.4709	0.22311	0.99459	0.43534	-1.2
283.2641_9.01	C01530, Octadecanoic acid	0.040804	0.47954	1.402	0.48749	0.56968	0.92433	0.94851	-0.0763	0.08759	0.47625	1.4322	0.5182	0.16983	0.85896	0.75903	-0.398	0.35846	0.6134	0.80488	-0.313	0.29652	0.72481	1.3361	0.418	0.58067	0.97448	0.87436	-0.194	0.5273	0.97554	1.0925	0.1276
307.2634_7.02	C01530, Octadecanoic acid	0.30034	0.71962	0.20656	-2.2754	0.29699	0.81752	1.7503	0.8076	0.29685	0.65851	0.18404	-2.442	0.2748	0.76936	1.4806	0.5662	0.38912	0.68147	0.18273	-2.452	0.4694	0.76195	1.8091	0.8553	0.49196	0.87923	0.34113	-1.552	0.87952	0.99502	0.65323	-0.614
178.051_1.88	C01586, Hippurate	0.29543	0.61744	0.69929	-0.51603	0.96937	0.98574	0.42977	-1.2184	0.46657	0.66657	0.58909	-0.763	0.60065	0.90908	1.9268	0.9462	0.027523	0.40888	0.17557	-2.51	0.50747	0.79144	2.9058	1.539	0.29549	0.81662	0.57689	-0.794	0.56236	0.97554	0.86471	-0.21
303.2324_6.69	C01595, Linoleate	0.22429	0.69542	0.35695	-1.4862	0.24563	0.81752	2.1669	1.1156	0.50192	0.73945	0.48843	-1.034	0.12926	0.68575	1.4964	0.5815	0.72048	0.85602	0.58695	-0.769	0.85638	0.94631	1.1689	0.2252	0.93125	0.99973	0.8438	-0.245	0.75565	0.99459	0.72099	-0.472
263.2374_8.05	C01595, Linoleate	0.78748	0.91692	0.95981	-0.059184	0.39572	0.82217	1.1633	0.2182	0.14757	0.62084	1.2148	0.2807	0.56399	0.84508	1.0545	0.0765	0.3656	0.66039	1.1922	0.2536	0.16353	0.62149	0.75844	-0.399	0.85426	0.99047	0.97076	-0.043	0.75767	0.99459	1.0502	0.0707
281.248_8.05	C01595, Linoleate	0.79871	0.91877	0.96173	-0.056295	0.40252	0.82217	1.1678	0.2238	0.13777	0.62084	1.2302	0.2989	0.61027	0.86077	1.051	0.0718	0.35548	0.65986	1.2081	0.2728	0.17858	0.62149	0.7484	-0.418	0.8198	0.98561	0.96365	-0.053	0.7204	0.99459	1.0589	0.0825
245.2269_8.05	C01595, Linoleate	0.8364	0.92812	0.96873	-0.045841	0.46172	0.83804	1.1573	0.2108	0.13035	0.62084	1.2374	0.3073	0.56275	0.84508	1.0563	0.079	0.40989	0.69856	1.1846	0.2443	0.17883	0.62149	0.75465	-0.406	0.84164	0.98947	0.96514	-0.051	0.77894	0.99459	1.0542	0.0762
280.2366_8.04	C01595, Linoleate	0.85662	0.91434	1.0288	0.040925	0.34652	0.90573	1.2379	0.3079	0.037614	0.42827	1.4479	0.534	0.64874	0.90908	0.9304	-0.104	0.60613	0.74753	1.1578	0.2113	0.46746	0.7647	0.80563	-0.312	0.70447	0.99561	0.93734	-0.093	0.70477	0.97554	1.0928	0.128
279.2329_8.04	C01595, Linoleate	0.97667	0.97667	1.0038	0.0054016	0.29172	0.90573	1.2607	0.3342	0.059427	0.43102	1.383	0.4678	0.74435	0.90954	0.94586	-0.08	0.69965	0.80244	1.1292	0.1753	0.4647	0.76434	0.7982	-0.325	0.62536	0.99561	0.93067	-0.104	0.84703	0.97554	1.0556	0.0781
305.248_6.85	C01712, (9E)-Octadecenoic acid	0.1739	0.6945	0.21447	-2.2211	0.24594	0.81752	2.7103	1.4385	0.3496	0.67009	0.29555	-1.759	0.24684	0.76287	1.4083	0.494	0.47208	0.72021	0.32211	-1.634	0.64765	0.85884	1.5418	0.6246	0.62465	0.91673	0.58228	-0.78	0.81857	0.99491	0.62902	-0.669
281.2486_8.52	C01712, (9E)-Octadecenoic acid	0.2665	0.58983	1.2319	0.30092	0.39792	0.90573	1.1416	0.191	0.018042	0.32936	1.6467	0.7196	0.34788	0.85896	0.84572	-0.242	0.16723	0.40888	1.3917	0.4768	0.52172	0.79715	0.86373	-0.211	0.96804	0.99561	1.0067	0.0096	0.57507	0.97554	1.1571	0.2105
283.2636_8.53	C01712, (9E)-Octadecenoic acid	0.40873	0.76975	1.1484	0.19965	0.33929	0.82008	1.1504	0.2021	0.087827	0.62084	1.9292	0.948	0.56707	0.84582	0.72115	-0.472	0.3141	0.63885	1.2683	0.3429	0.88738	0.96198	0.943	-0.085	0.61269	0.91673	1.0655	0.0915	0.21904	0.99459	1.2316	0.3006
128.0353_0.44	C01879, 5-Oxoproline	0.039149	0.47954	2.3317	1.2214	0.83745	0.97304	0.96098	-0.0574	0.16947	0.47823	1.4394	0.5255	0.013338	0.85896	1.2491	0.3209	0.081094	0.40888	1.9456	0.9603	0.43237	0.73945	0.80513	-0.313	0.15767	0.68442	1.5316	0.6151	0.34998	0.97554	1.1838	0.2434
167.09_0.64	C02076, Sedoheptulose	0.814	0.92593	0.71911	-0.47571	0.88113	0.97539	0.864	-0.2109	0.56135	0.77072	0.5515	-0.859	0.20752	0.74816	1.4718	0.5576	0.52638	0.75094	1.2144	0.2803	0.045168	0.6184	0.43851	-1.189	0.70907	0.94875	0.62654	-0.675	0.39186	0.99459	1.2813	0.3576
83.0861_8.52	C02373, 4-Methylpentanal	0.10199	0.69216	1.3121	0.39188	0.20398	0.81752	1.1396	0.1885	0.059248	0.62084	2.1905	1.1312	0.59497	0.85408	0.70611	-0.502	0.38893	0.68147	1.2302	0.2989	0.78989	0.91913	0.91756	-0.124	0.3382	0.82966	1.1273	0.1729	0.19926	0.99459	1.154	0.2067
83.0861_8.05	C02373, 4-Methylpentanal	0.79594	0.91877	0.9491	-0.075362	0.12054	0.81752	1.2963	0.3744	0.16572	0.6295	1.4471	0.5332	0.93277	0.97398	0.96972	-0.044	0.43569	0.70823	1.1608	0.2152	0.21582	0.64161	0.78759	-0.344	0.83891	0.9891	0.95089	-0.073	0.36906	0.99459	1.1834	0.243
858.5245_12.07	C02737, Phosphatidylserine	0.13822	0.6945	1.3442	0.42675	0.7785	0.94466	0.91453	-0.1289	0.019691	0.62084	1.3583	0.4418	0.8012	0.92766	0.97974	-0.03	0.8411	0.91748	1.0253	0.0361	0.4881	0.76818	1.1634	0.2183	0.11296	0.65597	1.2408	0.3113	0.76016	0.99459	0.96311	-0.054
837.5464_12.14	C02737, Phosphatidylserine	0.14733	0.6945	1.4051	0.49067	0.55374	0.85991	0.83581	-0.2588	0.025427	0.62084	1.4757	0.5614	0.6311	0.86287	0.92168	-0.118	0.98913	0.99254	1.0106	0.0152	0.71524	0.88845	1.0964	0.1328	0.084527	0.65597	1.3843	0.4691	0.60437	0.99459	0.89129	-0.166
835.5294_12.07	C02737, Phosphatidylserine	0.26143	0.69775	1.279	0.35501	0.32665	0.81752	1.196	0.2582	0.073988	0.62084	1.3892	0.4742	0.83672	0.93342	1.0105	0.0151	0.73123	0.8613	1.0388	0.0549	0.23318	0.64469	1.2266	0.2947	0.11894	0.66197	1.3665	0.4504	0.73293	0.99459	0.92502	-0.112
836.5425_12.14	C02737, Phosphatidylserine	0.26997	0.69775	1.2991	0.37746	0.79789	0.94855	0.90113	-0.1502	0.039118	0.62084	1.4149	0.5007	0.61314	0.86077	0.9376	-0.093	0.69342	0.84198	0.92851	-0.107	0.35192	0.70998	1.2451	0.3163	0.081684	0.65597	1.3727	0.457	0.41289	0.99459	0.84723	-0.239
181.0627_2.52	C02909, (2-Naphthyl)methanol	0.79431	0.91877	1.0407	0.057499	0.57922	0.87199	1.1065	0.146	0.32886	0.6606	1.2876	0.3646	0.022617	0.63307	1.6525	0.7246	0.28816	0.63316	1.462	0.548	0.73291	0.89346	0.90467	-0.145	0.11723	0.65793	1.7464	0.8044	0.2625	0.99459	1.2855	0.3623
322.2715_5.75	C02934, 3-Dehydrosphinganine	0.014342	0.5528	2.0444	1.0316	0.013626	0.81752	0.55122	-0.8593	0.12448	0.62084	1.4436	0.5297	0.4201	0.80811	0.85168	-0.232	0.89142	0.94812	1.0184	0.0263	0.27039	0.66615	1.2395	0.3098	0.37071	0.85006	1.1914	0.2526	0.064461	0.99459	1.347	0.4297
282.2797_5.76	C02934, 3-Dehydrosphinganine	0.023569	0.5873	1.7742	0.82716	0.013358	0.81752	0.62517	-0.6777	0.1125	0.62084	1.4073	0.4929	0.441	0.80811	0.88824	-0.171	0.78613	0.89158	1.0598	0.0837	0.45697	0.75661	1.1224	0.1666	0.43566	0.86047	1.1447	0.195	0.070057	0.99459	1.3525	0.4357
300.2903_5.76	C02934, 3-Dehydrosphinganine	0.025902	0.59035	1.827	0.86949	0.012815	0.81752	0.61505	-0.7012	0.11952	0.62084	1.4247	0.5106	0.42688	0.80811	0.88309	-0.179	0.76309	0.88111	1.0682	0.0952	0.4598	0.75767	1.1275	0.1731	0.4264	0.86047	1.1624	0.2171	0.083514	0.99459	1.3596	0.4432
301.2927_5.76	C02934, 3-Dehydrosphinganine	0.031568	0.61892	1.8368	0.87717	0.036115	0.81752	0.65399	-0.6127	0.11289	0.62084	1.4409	0.5269	0.23775	0.75876	0.83823	-0.255	0.72651	0.85968	1.1061	0.1455	0.51482	0.78178	1.1083	0.1483	0.38665	0.86047	1.1792	0.2378	0.054917	0.99459	1.3668	0.4509
168.0623_5.61	C02946, 4-Acetamidobutanoate	0.22531	0.69542	1.1164	0.15887	0.68013	0.91676	0.97003	-0.0439	0.551	0.76452	1.0469	0.0662	0.02604	0.63307	1.2023	0.2658	0.13987	0.61158	1.1634	0.2183	0.60887	0.83247	0.94727	-0.078	0.06969	0.65597	1.1719	0.2288	0.73743	0.99459	1.0185	0.0265
329.2481_6.77	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	0.17044	0.6945	0.26952	-1.8915	0.20183	0.81752	2.6656	1.4145	0.48292	0.72797	0.43566	-1.199	0.30883	0.78345	1.3658	0.4497	0.47093	0.7197	0.39487	-1.341	0.67517	0.87002	1.3615	0.4452	0.93791	0.99973	0.80491	-0.313	0.67642	0.99459	0.71205	-0.49
136.0761_0.62	C03758, Dopamine	0.94628	0.97523	1.0391	0.055315	0.10755	0.81752	1.5803	0.6602	0.68549	0.84989	1.072	0.1003	0.10962	0.67902	1.6947	0.7611	0.034987	0.61158	2.4482	1.2917	0.076412	0.6184	0.59204	-0.756	0.48486	0.87694	1.4959	0.581	0.77185	0.99459	1.1366	0.1848
309.0437_0.43	C03838, 5'-Phosphoribosylglycinamide	0.51575	0.81721	1.0939	0.12946	0.39339	0.82217	0.88013	-0.1842	0.95069	0.98528	0.9992	-0.001	0.64212	0.86656	1.1713	0.2281	0.016706	0.61158	2.143	1.0997	0.082462	0.6184	0.67505	-0.567	0.094411	0.65597	1.575	0.6553	0.23706	0.99459	1.206	0.2702
263.1034_2.06	C04148, alpha-N-Phenylacetyl-L-glutamine	0.47768	0.73149	1.2758	0.35135	0.9677	0.98574	1.0971	0.1337	0.24487	0.48315	1.529	0.6126	0.85064	0.93578	0.89719	-0.157	0.038793	0.40888	2.0141	1.0101	0.054681	0.71367	0.56824	-0.815	0.066445	0.68442	1.7279	0.789	0.58032	0.97554	0.91224	-0.133
530.3584_7.01	C04230, 1-Acyl-sn-glycero-3-phosphocholine	0.84454	0.93364	1.019	0.027167	0.36381	0.82217	1.3479	0.4307	0.65502	0.82778	1.0576	0.0808	0.3352	0.78861	1.4339	0.52	0.072499	0.61158	1.8641	0.8985	0.11513	0.6184	0.74265	-0.429	0.72241	0.95483	1.1911	0.2524	0.86674	0.99502	0.85683	-0.223
301.2168_6.32	C04686, (13E)-(15S)-15-Hydroxy-9-oxoprosta-11,13-dienoate	0.045258	0.63665	0.29492	-1.7616	0.1376	0.81752	2.513	1.3294	0.14269	0.62084	0.42426	-1.237	0.03757	0.63307	1.9868	0.9905	0.27243	0.63193	0.5017	-0.995	0.85113	0.94385	0.95225	-0.071	0.53281	0.88973	0.72139	-0.471	0.9851	0.99664	0.91044	-0.135
321.2428_6.98	C04805, 5(S)-HETE	0.18043	0.6945	0.3299	-1.5999	0.066283	0.81752	2.348	1.2314	0.89427	0.95668	0.65746	-0.605	0.14117	0.69111	1.9033	0.9285	0.64603	0.81445	0.99647	-0.005	0.18943	0.63008	0.4821	-1.053	0.68373	0.94319	0.57284	-0.804	0.2539	0.99459	0.61632	-0.698
359.2203_6.16	C04849, (5Z,9E,14Z)-(8xi,11R,12S)-11,12-Epoxy-8-hydroxyicosa-5,9,14-trienoic acid	0.14895	0.6945	0.18441	-2.439	0.28291	0.81752	2.9283	1.5501	0.30943	0.65851	0.24483	-2.03	0.015617	0.63307	2.0861	1.0608	0.46699	0.7197	0.32079	-1.64	0.92448	0.97466	1.1253	0.1703	0.55068	0.89538	0.68972	-0.536	0.99153	0.99685	0.49238	-1.022
562.403_10.59	C05200, 3-Hexaprenyl-4,5-dihydroxybenzoate	0.87442	0.94757	0.99112	-0.012864	0.97852	0.99844	0.99679	-0.0046	0.68182	0.84775	0.97718	-0.033	0.042529	0.63307	1.1659	0.2215	0.043891	0.61158	1.1527	0.205	0.16703	0.62149	0.89665	-0.157	0.24523	0.76073	1.0857	0.1186	0.85935	0.99491	0.98446	-0.023
313.0318_0.43	C05382, D-Sedoheptulose 7-phosphate	0.30849	0.71962	0.83532	-0.25959	0.47988	0.83827	1.0963	0.1327	0.078774	0.62084	0.72977	-0.454	0.31591	0.78345	1.1467	0.1975	0.4498	0.71706	1.0984	0.1354	0.022001	0.6184	0.75494	-0.406	0.46116	0.86437	0.88112	-0.183	0.10627	0.99459	1.2781	0.3539
347.2202_8.04	C05472, Urocortisol	0.61442	0.81171	1.0719	0.10013	0.43803	0.90573	1.1381	0.1866	0.015598	0.32936	1.3336	0.4153	0.29397	0.85896	0.90831	-0.139	0.52201	0.70762	1.1271	0.1726	0.44218	0.74705	0.86242	-0.214	0.9295	0.99561	0.98961	-0.015	0.8796	0.97554	1.0289	0.0411
349.2356_8.52	C05476, Tetrahydrocorticosterone	0.22931	0.57493	1.1688	0.22502	0.51539	0.92005	1.0775	0.1077	0.019115	0.32936	1.4057	0.4913	0.44672	0.8592	0.91422	-0.129	0.11202	0.40888	1.3093	0.3889	0.31921	0.72481	0.85592	-0.224	0.94827	0.99561	1.0066	0.0095	0.72082	0.97554	1.0714	0.0996
150.0541_0.43	C05578, 5,6-Dihydroxyindole	0.68924	0.88554	0.96959	-0.044558	0.48061	0.83827	0.82779	-0.2727	0.97611	0.99041	0.76866	-0.38	0.33773	0.78861	1.14	0.1891	0.46307	0.71875	1.2228	0.2901	0.046371	0.6184	0.5644	-0.825	0.85731	0.99047	0.70334	-0.508	0.19802	0.99459	1.2758	0.3514
167.0708_5.61	C05581, 3-Methoxy-4-hydroxyphenylacetaldehyde	0.521	0.81982	1.0287	0.040873	0.95793	0.99502	0.99735	-0.0038	0.89802	0.95891	0.99352	-0.009	0.010846	0.63307	1.1428	0.1926	0.015876	0.61158	1.1819	0.2411	0.20375	0.6388	0.91181	-0.133	0.04238	0.65597	1.1318	0.1787	0.9389	0.99664	0.99391	-0.009
149.0603_0.64	C05581, 3-Methoxy-4-hydroxyphenylacetaldehyde	0.73269	0.90189	0.69291	-0.52927	0.84519	0.96491	0.85239	-0.2304	0.48386	0.72797	0.52808	-0.921	0.17497	0.71797	1.4438	0.5299	0.52309	0.74878	1.1934	0.2551	0.027976	0.6184	0.41474	-1.27	0.59355	0.91423	0.58354	-0.777	0.29344	0.99459	1.3132	0.3931
183.988_12.93	C05698, Selenohomocysteine	0.024685	0.5873	0.83127	-0.26662	0.24541	0.81752	1.0853	0.118	0.039049	0.62084	0.86257	-0.213	0.10085	0.67902	1.0959	0.1321	0.79647	0.89622	1.0211	0.0301	0.07876	0.6184	0.83886	-0.254	0.92899	0.99973	0.99236	-0.011	0.29423	0.99459	0.94033	-0.089
183.9881_0.1	C05698, Selenohomocysteine	0.034116	0.63301	0.80404	-0.31467	0.14048	0.81752	1.1838	0.2434	0.008699	0.57762	0.8508	-0.233	0.38484	0.80053	1.0962	0.1326	0.080858	0.61158	1.1289	0.1749	0.065159	0.6184	0.76969	-0.378	0.44415	0.86047	0.93185	-0.102	0.72632	0.99459	1.0391	0.0553
591.3154_3.08	C05791, D-Urobilinogen	0.065821	0.66599	0.45492	-1.1363	0.32646	0.81752	1.6266	0.7018	0.022376	0.62084	0.42883	-1.222	0.10657	0.67902	2.0828	1.0586	0.49109	0.72637	1.5248	0.6086	0.10109	0.6184	0.36469	-1.455	0.27093	0.77439	0.67679	-0.563	0.88471	0.99502	1.1341	0.1815
571.2882_7.52	C05791, D-Urobilinogen	0.53979	0.76642	1.2374	0.30729	0.82565	0.97304	0.99958	-0.0006	0.038416	0.42827	1.5791	0.6592	0.40322	0.85896	1.182	0.2412	0.12714	0.40888	1.5526	0.6347	0.30317	0.72481	0.74144	-0.432	0.26076	0.80092	1.7132	0.7767	0.28582	0.97554	1.4205	0.5064
393.2211_8.45	C05963,	0.000797	0.31434	1.3576	0.44108	0.30706	0.81752	0.92506	-0.1124	0.076288	0.62084	1.6085	0.6857	0.81954	0.92769	0.86535	-0.209	0.62087	0.80147	0.96241	-0.055	0.6166	0.8391	1.0642	0.0898	0.55196	0.89579	1.0443	0.0625	0.2564	0.99459	1.1599	0.214
381.0792_0.4	C06373, beta-D-Gal-(1->4)-D-Glc	0.64055	0.87494	0.45711	-1.1294	0.23449	0.81752	0.59106	-0.7586	0.87389	0.94569	0.34385	-1.54	0.58297	0.85299	0.8068	-0.31	0.57394	0.76985	0.48756	-1.036	0.56602	0.81289	0.88351	-0.179	0.8236	0.98643	0.235	-2.089	0.092959	0.99459	1.4304	0.5165
365.1058_0.41	C06373, beta-D-Gal-(1->4)-D-Glc	0.93035	0.97072	0.30504	-1.7129	0.19561	0.81752	0.57353	-0.8021	0.69279	0.8553	0.23521	-2.088	0.40489	0.80644	0.75091	-0.413	0.97621	0.98898	0.30972	-1.691	0.63816	0.85344	0.91752	-0.124	0.53808	0.88973	0.19734	-2.341	0.51563	0.99459	1.1293	0.1754
280.2333_6.42	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	0.088277	0.6793	0.086321	-3.5341	0.10849	0.81752	3.0082	1.5889	0.28528	0.65851	0.1669	-2.583	0.55657	0.84322	1.0932	0.1286	0.20263	0.61515	0.11049	-3.178	0.49285	0.76968	2.5776	1.366	0.52992	0.88861	0.31002	-1.69	0.52056	0.99459	0.56841	-0.815
280.2366_7.64	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	0.1051	0.69216	0.68067	-0.55498	0.1185	0.81752	1.6927	0.7593	0.49832	0.73763	1.1445	0.1947	0.70887	0.8894	1.1462	0.1969	0.56926	0.76843	0.86954	-0.202	0.3692	0.71302	0.73646	-0.441	0.050253	0.65597	0.57531	-0.798	0.43049	0.99459	1.2277	0.296

330.2512_6.77	C06429, (4Z,7Z,10Z,13Z,16Z,19Z)-Docosahexaenoic acid	0.13821	0.6945	0.26307	-1.9265	0.21668	0.81752	2.8062	1.4886	0.46689	0.72754	0.45206	-1.145	0.24208	0.76013	1.4366	0.5227	0.43022	0.70477	0.39193	-1.351	0.72679	0.89238	1.3813	0.466	0.83085	0.9885	0.78108	-0.356	0.6846	0.99459	0.67012	-0.578
155.0475_0.41	C06608, Diethylphosphoric acid	0.6795	0.88235	0.81523	-0.29473	0.26039	0.81752	0.8072	-0.309	0.51957	0.74679	0.75164	-0.412	0.99741	0.9993	1.0052	0.0074	0.77811	0.8877	1.0035	0.005	0.022875	0.6184	0.65971	-0.6	0.4724	0.86713	0.73686	-0.441	0.72711	0.99459	1.0792	0.11
401.2669_7.53	C13856, 2-Arachidonoylglycerol	0.69351	0.88674	1.0052	0.0075443	0.17072	0.81752	1.68	0.7485	0.80397	0.91268	0.84341	-0.246	0.50227	0.82022	1.3619	0.4457	0.36377	0.6602	1.3177	0.398	0.65622	0.861	1.1989	0.2618	0.50873	0.88344	1.1866	0.2468	0.40604	0.99459	1.3585	0.442
379.2847_7.53	C13856, 2-Arachidonoylglycerol	0.76475	0.90944	0.93392	-0.098628	0.16038	0.81752	1.666	0.7364	0.94113	0.98158	0.73553	-0.443	0.398	0.80644	1.4529	0.5389	0.3905	0.68214	1.2684	0.3431	0.61817	0.84037	1.2185	0.2851	0.53913	0.88973	1.1587	0.2125	0.4548	0.99459	1.2791	0.3551
277.2167_6.31	C14765, 13-OxoODE	0.071558	0.67661	0.28175	-1.8275	0.21108	0.81752	1.61	0.687	0.094186	0.62084	0.30466	-1.715	0.29548	0.77679	1.2317	0.3006	0.51098	0.73895	0.52713	-0.924	0.57305	0.81585	0.80772	-0.308	0.4632	0.86437	0.55304	-0.855	0.67684	0.99459	0.78058	-0.357
319.2278_6.68	C14771, 14,15-EET	0.18322	0.57493	0.36064	-1.4714	0.24136	0.90573	2.2477	1.1684	0.40884	0.64095	0.50444	-0.987	0.24325	0.85896	1.3993	0.4847	0.51942	0.70762	0.55082	-0.86	0.82515	0.93373	1.2016	0.265	0.79373	0.99561	0.79612	-0.329	0.72759	0.97554	0.71034	-0.493
320.2311_6.68	C14771, 14,15-EET	0.19176	0.57493	0.34781	-1.5236	0.24087	0.90573	2.2898	1.1952	0.42555	0.66026	0.48837	-1.034	0.24648	0.85896	1.406	0.4916	0.53788	0.70762	0.53689	-0.897	0.79554	0.91151	1.2304	0.2992	0.80206	0.99561	0.7928	-0.335	0.73669	0.97554	0.69885	-0.517
301.2167_6.68	C14771, 14,15-EET	0.19316	0.57493	0.32427	-1.6247	0.29882	0.90573	2.365	1.2419	0.43817	0.66276	0.46596	-1.102	0.2083	0.85896	1.4652	0.5511	0.52892	0.70762	0.50522	-0.985	0.83907	0.94239	1.2338	0.3031	0.8325	0.99561	0.75874	-0.398	0.69768	0.97554	0.70714	-0.5
343.225_6.69	C14779, 9(S)-HETE	0.22645	0.69542	0.33753	-1.5669	0.26883	0.81752	2.2161	1.0882	0.44996	0.71993	0.44881	-1.156	0.23282	0.75876	1.392	0.4772	0.59961	0.78696	0.49312	-1.02	0.80058	0.92227	1.3225	0.4033	0.84807	0.99047	0.78349	-0.352	0.70807	0.99459	0.68084	-0.555
295.2277_6.42	C14826, 12(13)-EpOME	0.046576	0.47954	0.088772	-3.4937	0.13532	0.90573	3.1817	1.6698	0.20226	0.47823	0.1861	-2.426	0.79444	0.91782	0.96567	-0.05	0.084683	0.40888	0.11752	-3.089	0.57033	0.80977	2.4212	1.2757	0.44541	0.87443	0.32647	-1.615	0.47132	0.97554	0.50578	-0.983
296.2311_6.42	C14826, 12(13)-EpOME	0.047658	0.47954	0.078474	-3.6716	0.14992	0.90573	3.3258	1.7337	0.19808	0.47823	0.16594	-2.591	0.75329	0.90954	0.98039	-0.029	0.084651	0.40888	0.10357	-3.271	0.66571	0.84666	2.4654	1.3018	0.43186	0.87443	0.29842	-1.745	0.43355	0.97554	0.47508	-1.074
261.2197_7.64	C14826, 12(13)-EpOME	0.18128	0.6945	0.71861	-0.47671	0.13805	0.81752	1.6035	0.6813	0.15054	0.62084	1.734	0.7941	0.77185	0.91931	0.83357	-0.263	0.8268	0.90976	0.96686	-0.049	0.45154	0.75373	0.75625	-0.403	0.084617	0.65597	0.61643	-0.698	0.31361	0.99459	1.2991	0.3775
259.2051_7.97	C16300, Stearidonic acid	0.17172	0.6945	1.5316	0.61508	0.65425	0.90563	0.93339	-0.0994	0.19165	0.63877	1.6264	0.7017	0.29826	0.77863	1.2542	0.3268	0.13118	0.61158	2.0389	1.0278	0.12738	0.6184	0.58015	-0.785	0.2881	0.78518	1.3452	0.4278	0.5999	0.99459	1.1075	0.1473
472.3421_6.08	c226crn, cervonyl carnitine	0.42135	0.77297	0.97696	-0.033629	0.33659	0.82008	0.73308	-0.448	0.19209	0.63886	1.6193	0.6953	0.2705	0.76647	1.3742	0.4586	0.12071	0.61158	3.4518	1.7873	0.40308	0.73062	0.49699	-1.009	0.023395	0.65597	0.9116	3.3091	0.28162	0.99459	0.36426	-1.457
473.345_6.08	c226crn, cervonyl carnitine	0.6849	0.88387	0.88439	-0.17724	0.64154	0.89898	0.93489	-0.0971	0.18718	0.63877	1.6127	0.6895	0.22159	0.75098	1.3771	0.4617	0.07276	0.61158	3.6615	1.8725	0.34884	0.70998	0.47745	-1.067	0.014318	0.65597	10.014	3.324	0.29084	0.99459	0.36918	-1.438
97.1016_8.05	CE2061,	0.65506	0.87642	0.9347	-0.09742	0.29352	0.81752	1.1849	0.2447	0.084482	0.62084	1.485	0.5705	0.62515	0.86115	0.86614	-0.207	0.43805	0.70823	1.1359	0.1838	0.10202	0.6184	0.76337	-0.39	0.83773	0.9891	0.96173	-0.056	0.71804	0.99459	1.0447	0.0631
133.1015_8.05	CE2061,	0.8893	0.95098	0.96562	-0.050467	0.51715	0.84766	1.1303	0.1767	0.21668	0.63886	1.243	0.3138	0.28229	0.76936	1.1978	0.2604	0.2045	0.61539	1.3069	0.3861	0.22551	0.64161	0.75887	-0.398	0.95852	0.99995	0.97035	-0.043	0.39525	0.99459	1.1409	0.1902
169.1227_8.05	CE2061,	0.95332	0.97714	0.98896	-0.016016	0.55665	0.85991	1.1175	0.1603	0.07124	0.62084	1.3007	0.3793	0.74351	0.90774	1.0286	0.0407	0.28599	0.63316	1.258	0.3311	0.15217	0.6184	0.71015	-0.494	0.73233	0.95781	0.94482	-0.082	0.85413	0.99491	1.0501	0.0706
94.0658_0.61	CE2172,	0.60121	0.85873	1.2907	0.36812	0.34623	0.82008	1.2256	0.2935	0.75951	0.89549	1.039	0.0552	0.085436	0.66832	1.8681	0.9016	0.047183	0.61158	2.6504	1.4062	0.11053	0.6184	0.60564	-0.723	0.3933	0.86047	1.6565	0.7282	0.8552	0.99491	1.1172	0.1599
166.0867_0.64	CE2172,	0.7454	0.90331	0.70362	-0.50713	0.92866	0.98864	0.89063	-0.1671	0.51645	0.74539	0.55758	-0.843	0.23528	0.75876	1.405	0.4905	0.54102	0.75936	1.172	0.229	0.039515	0.6184	0.46694	-1.099	0.64429	0.92511	0.62386	-0.681	0.37257	0.99459	1.265	0.3392
429.2994_8.04	CE2204, 25-hydroxyvitamin D3-26,23-lactone	0.34852	0.73608	1.3244	0.40536	0.23801	0.81752	1.2612	0.3348	0.4376	0.71503	1.1491	0.2005	0.29061	0.77329	1.4118	0.4976	0.25038	0.62664	1.5392	0.6222	0.97259	0.98838	1.0207	0.0296	0.64619	0.92627	0.76846	-0.38	0.005377	0.99459	1.9794	0.985
1070.4642_11.94	CE2257, tetracosanoyl-CoA	0.1742	0.6945	1.2266	0.2947	0.39867	0.82217	0.91247	-0.1322	0.20085	0.63886	1.1968	0.2592	0.66728	0.87579	0.96013	-0.059	0.56011	0.76528	1.1031	0.1416	0.99314	0.99638	0.98725	-0.019	0.22214	0.73427	1.1703	0.2269	0.31625	0.99459	1.1342	0.1817
332.266_7.14	CE2510,	0.38702	0.75984	0.2596	-1.9456	0.17175	0.81752	2.4609	1.2992	0.53964	0.75521	0.29397	-1.766	0.057006	0.63845	1.8772	0.9086	0.81946	0.90587	0.41148	-1.281	0.82183	0.93288	1.2912	0.3687	0.90725	0.99877	0.79727	-0.327	0.87489	0.99502	0.65021	-0.621
324.2083_8.6	CE2540, timnodonate	0.004182	0.45674	4.992	2.3196	0.012986	0.81752	0.20123	-2.3131	0.24312	0.64836	3.0919	1.6285	0.29546	0.77679	0.28259	-1.823	0.16045	0.61158	1.5645	0.6457	0.53697	0.79558	1.0387	0.0548	0.25377	0.76893	1.6271	0.7023	0.85381	0.99491	1.2826	0.3591
155.1073_8.05	CE2577,	0.71515	0.89943	1.037	0.052423	0.5823	0.87343	1.1369	0.1851	0.035365	0.62084	1.3832	0.468	0.64347	0.86712	1.0477	0.0673	0.15379	0.61158	1.2833	0.3599	0.09951	0.6184	0.71893	-0.476	0.67642	0.94164	0.95249	-0.07	0.30014	0.99459	1.1422	0.1918
300.0469_0.44	CE3075, sorbitol 3-phosphate	0.06417	0.5046	1.5983	0.67651	0.68988	0.96194	0.9404	-0.0887	0.23481	0.48308	1.2723	0.3474	0.34251	0.85896	1.1562	0.2094	0.025034	0.40888	1.8939	0.9214	0.38528	0.72481	0.86679	-0.206	0.31576	0.81662	1.1864	0.2466	0.1532	0.97554	1.406	0.4916
283.0198_0.46	CE3075, sorbitol 3-phosphate	0.68381	0.88387	1.0312	0.044373	0.066775	0.81752	0.9038	-0.1459	0.31599	0.65851	0.81905	-0.288	0.039039	0.63307	1.4177	0.5035	0.3617	0.6602	1.155	0.2079	0.395	0.72704	0.92669	-0.11	0.94125	0.99973	0.95557	-0.066	0.050763	0.99459	1.3345	0.4163
325.2135_6.69	CE5013,	0.13555	0.6945	0.35134	-1.509	0.2379	0.81752	1.8362	0.8767	0.32851	0.6606	0.48241	-1.052	0.33827	0.78861	1.2332	0.3024	0.44905	0.71706	0.50448	-0.987	0.94129	0.98213	1.2426	0.3133	0.59743	0.91423	0.67822	-0.56	0.7725	0.99459	0.76999	-0.377
267.21_6.69	CE5013,	0.14706	0.6945	0.33721	-1.5683	0.1976	0.81752	2.1954	1.1345	0.35535	0.67093	0.46457	-1.106	0.11651	0.68134	1.505	0.5898	0.60319	0.78851	0.56458	-0.825	0.93194	0.97704	1.1402	0.1893	0.8293	0.98844	0.83575	-0.259	0.69289	0.99459	0.68516	-0.545
304.2359_6.68	CE5013,	0.22572	0.69542	0.32723	-1.6116	0.24354	0.81752	2.3042	1.2043	0.51862	0.74646	0.4607	-1.118	0.13134	0.68575	1.5147	0.599	0.72252	0.8565	0.55189	-0.858	0.81327	0.92936	1.2208	0.2878	0.92526	0.99973	0.82138	-0.284	0.78244	0.99459	0.714	-0.486
285.2214_6.68	CE5013,	0.2343	0.69542	0.32982	-1.6002	0.26767	0.81752	2.2144	1.1469	0.50419	0.73945	0.4505	-1.15	0.10949	0.67902	1.54	0.6229	0.69664	0.84298	0.54172	-0.884	0.86668	0.9521	1.1952	0.2572	0.90772	0.99877	0.79615	-0.329	0.77272	0.99459	0.71771	-0.479
325.2144_8.05	CE5013,	0.33089	0.72721	1.1236	0.16813	0.52542	0.8499	1.1173	0.1601	0.00366	0.56421	1.3688	0.4529	0.97188	0.98843	0.99833	-0.002	0.11005	0.61158	1.3113	0.391	0.26537	0.66219	0.797	-0.327	0.81117	0.98358	1.0293	0.0416	0.69995	0.99459	1.0915	0.1263
180.0662_2.53	CE5536, adrenochrome	0.38372	0.75835	1.3499	0.4328	0.98494	0.99844	0.9593	-0.0599	0.2087	0.63886	1.492	0.5772	0.028089	0.63307	1.8201	0.8641	0.15016	0.61158	1.7819	0.8334	0.40547	0.7318	0.7692	-0.379	0.059372	0.65597	1.8393	0.8791	0.13719	0.99459	1.44	0.5261
415.3602_6.55	CE5655, 13'-hydroxy-gama-tocopherol	0.35509	0.74217	1.4444	0.53046	0.59906	0.87862	1.196	0.2582	0.11076	0.62084	2.1023	1.072	0.43303	0.80811	1.2224	0.2897	0.43359	0.70674	1.3638	0.4477	0.76249	0.9084	0.86505	-0.209	0.013682	0.65597	2.9907	1.5805	0.32019	0.99459	0.78094	-0.357
447.238_12.2	CE5708, 15-oxo-Prostaglandin E2 glyceryl ester	0.69909	0.89059	1.0338	0.047914	0.37181	0.82217	1.0893	0.1234	0.32268	0.6606	1.1255	0.1706	0.93373	0.97398	0.99788	-0.003	0.94204	0.97323	1.0037	0.0054	0.77049	0.91239	1.0351	0.0497	0.30839	0.80568	1.1773	0.2355	0.9126	0.99664	0.97712	-0.033
431.2443_4.65	CE5730,	0.053659	0.63928	2.9134	1.5427	0.33786	0.82008	0.56757	-0.8171	0.043873	0.62084	2.4036	1.2652	0.62052	0.86115	1.8299	0.8718	0.011337	0.61158	5.7344	2.5196	0.15784	0.61879	0.44313	-1.174	0.023589	0.65597	11.159	3.4802	0.51557	0.99459	0.30479	-1.714
445.3686_9.77	CE5838,	0.001781	0.39478	2.1134	1.0796	0.2091	0.81752	0.80155	-0.3191	0.000538	0.26436	2.2452	1.1668	0.19264	0.74315	0.78739	-0.345	0.007054	0.61158	1.8294	0.8714	0.16318	0.62149	1.1973	0.2598	0.005006	0.65597	1.7314	0.7919	0.97315	0.99664	1.0262	0.0373
442.3445_5.61	CE5843, 13'-carboxy-alpha-tocopherol	0.45163	0.78862	1.2267	0.29476	0.48771	0.83827	1.5725	0.653	0.3516	0.67009	2.3372	1.2248	0.19954	0.74393	1.7179	0.7806	0.069009	0.61158	3.6629	1.873	0.1468	0.6184	0.45272	-1.143	0.040943	0.65597	3.4876	1.8022	0.58516	0.99459	0.9212	-0.118
85.1014_8.52	CE6506,	0.081603	0.67661	1.411	0.49673	0.92398	0.98721	1.0269	0.0383	0.033748	0.62084	2.2122	1.1455	0.43347	0.80811	0.6742	-0.569	0.17419	0.61158	1.354	0.4372	0.35877	0.70998	0.80533	-0.312	0.80707	0.9829	0.95107	-0.072	0.10671	0.99459	1.3227	0.4035
121.1017_8.52	CE6506,	0.32946	0.72668	1.203	0.26662	0.39785	0.82217	1.1171	0.1598	0.10295	0.62084	2.2116	1.1451	0.71066	0.89079	0.71361	-0.487	0.31129	0.6384	1.3246	0.4056	0.56327	0.81221	0.85227	-0.231	0.89011	0.99877	0.98373	-0.024	0.04613	0.99459	1.4038	0.4893
139.1113_8.53	CE6506,	0.56582	0.83928	1.1105	0.15121	0.36882	0.82217	1.1323	0.1792	0.1225	0.62084	2.1414	1.0986	0.63168	0.86289	0.66384	-0.591	0.50907	0.73838	1.1652	0.2206	0.94266	0.98239	0.96396	-0.053	0.68599	0.94382	1.0353	0.05	0.15379	0.99459	1.2802	0.3564
139.112_8.06	CE6506,	0.83787	0.92888	0.96166	-0.0564	0.27326	0.81752	1.214	0.2798	0.1106	0.62084	1.5947	0.6733	0.56567	0.84582	0.7954	-0.33	0.17428	0.61158	1.6681	0.7382	0.77073	0.91239	0.81838	-0.289	0.91488	0.99951	0.99787	-0.003	0.65174	0.99459	1.0594	0.0832
312.1715_7.36	CE7110, 5,6-epoxy,18R-HEPE	0.43944	0.71407	0.60307	-0.72961	0.20098	0.90573	1.5695	0.6503	0.11076	0.47625	0.43277	-1.208	0.000387	0.11642	1.4476	0.5337	0.88057	0.9205	0.75655	-0.402	0.53598	0.80121	0.83059	-0.268	0.57049	0.97448	0.64831	-0.625	0.5464	0.97554	1.2076	0.2722
474.3566_6.21	clpndcrn, clupanodonyl carnitine	0.21062	0.69542	1.5748	0.65515	0.64669	0.90063	0.74339	-0.4278	0.029806	0.62084	2.6075	1.3827	0.15048	0.70436	1.4095	0.4952	0.022037	0.61158	5.0752	2.3435	0.50419	0.77506	0.65892	-0.602	0.002161	0.65597	10.877	3.4432	0.15663	0.99459	0.35984	-1.475
451.3602_6.3	dlnlcgcrn, dihomo-gamma-linolenyl carnitine	0.3666	0.74608	1.4296	0.51563	0.7906	0.94794	1.2507	0.3227	0.12874	0.62084	1.709	0.7731	0.25434	0.76376	1.4451	0.5311	0.078685	0.61158	3.0212	1.5951	0.35977	0.70998	0.69771	-0.519	0.019206	0.65597	4.4803	2.1636	0.27519	0.99459	0.63336	-0.659
398.327_6.21	hdd2crn, trans-Hexadec-2-enoyl carnitine	0.27403	0.70069	1.5433	0.62602	0.51886	0.84766	1.5601	0.6417	0.14487	0.62084	3.3413	1.7404	0.28918	0.77329	1.7966	0.8453	0.11589	0.61158	2.8387	1.5052	0.20287	0.63855	0.48303	-1.05	0.04097	0.65597	3.1198	1.6414	0.81513	0.99459	1.1706	0.2273
414.3584_6.55	hpdcacrn, heptadecanoyl carnitine	0.3478	0.73601	1.4248	0.51076	0.59709	0.87696	1.1999	0.263	0.15093	0.62084	2.193	1.1329	0.60696	0.8602	1.1027	0.1411	0.47058	0.7197	1.3547	0.438	0.88355	0.96011	0.88619	-0.174	0.047526	0.65597	2.8083	1.4897	0.50455	0.99459	0.81007	-0.304
446.3258_5.84	lneldcrn, Linoelaidyl carnitine	0.26395	0.69775	1.3582	0.44171	0.68311	0.91676	0.72701	-0.4599	0.038079	0.62084	2.6212	1.3902	0.96453	0.98602	1.1094	0.1497	0.060024	0.61158	3.2831	1.715	0.27036	0.66615	0.60107	-0.734	0.014335	0.65597	10.738	3.4246	0.40763	0.99459	0.38871	-1.363
425.3461_6.33	lneldcrn, Linoelaidyl carnitine	0.73448	0.90189	1.1547	0.2075	0.49042	0.83849	1.716	0.7791	0.24461	0.64961	3.6583	1.8712	0.51914	0.82172	1.0952	0.1312	0.077993	0.61158	4.1328	2.0471	0.21596	0.64161	0.50925	-0.974	0.044207	0.65597	3.9844	1.9943	0.77068	0.99459	1.0442	0.0624
424.3428_6.12	lneldcrn, Linoelaidyl carnitine	0.91614	0.96473	0.77838	-0.36145	0.3538	0.8216	1.4854	0.5709	0.28286	0.65851	1.6713	0.7409	0.88673	0.95722	1.0537	0.0754	0.27095	0.63193	1.7451	0.8033	0.31974	0.69605	0.75992	-0.396	0.042147	0.65597	3.726	1.8976	0.049168	0.99459	0.54574	-0.874
425.346_6.12	lneldcrn, Linoelaidyl carnitine	0.93646	0.97203	0.73369	-0.44676	0.33187	0.81752	1.5664	0.6475	0.28934	0.65851	1.68	0.7485	0.88872	0.95877	1.0588	0.0825	0.28769	0.63316	1.7239	0.7856	0.36398	0.70998	0.75549	-0.405	0.04549	0.65597	3.8983	1.9628	0.047363	0.99459	0.53319	-0.907
427.3615_6.43	odecrn, octadecenoyl carnitine	0.85042	0.93562	0.94741	-0.077936	0.43607	0.83068	1.6079	0.6852	0.26675	0.65839	1.9784	0.9843	0.7778	0.91995	1.0274	0.039	0.15739	0.61158	2.2109	1.1447	0.89482	0.96515	1.0052	0.0074	0.040343	0.65597	3.4965	1.8059	0.2448	0.99459	0.69297	-0.529
426.3583_6.43	odecrn, octadecenoyl carnitine	0.86338	0.94171	0.94821	-0.076716	0.42694	0.82768	1.597	0.6754	0.26126	0.65789	1.9542	0.9666	0.77948	0.92069	1.0368	0.0522	0.15318	0.61158	2.1803	1.1245	0.93047	0.97667	1.0175	0.025	0.036707	0.65597	3.5167	1.8142	0.24465	0.99459	0.67828	-0.56
218.1381_0.46	pcrn, propionyl-carnitine	0.015077	0.55658	0.32465	-1.623	0.32403	0.81752	1.2012	0.2645	0.17282	0.63219	0.58909	-0.763	0.819	0.92766	1.6156	0.692	0.11644	0.61158	0.48441	-1.046	0.54697	0.8023	0.56336	-0.828	0.011411	0.65597	3.4253	1.7762	0.12595	0.99459	0.41635	-1.264
450.3583_6.3	stcrn, stearoylcarnitine	0.32347	0.724	1.4104	0.49607	0.7701	0.94011	1.2291	0.2977	0.14287	0.62084	1.8346	0.8755	0.45328	0.80811	1.3028	0.3817	0.11497	0.61158	3.0915	1.6283	0.36516	0.70998	0.68912	-0.537	0.039953	0.65597	4.2227	2.0782	0.31135	0.99459	0.67233	-0.573
428.374_6.8	stcrn, stearoylcarnitine	0.45878	0.79384	1.2331	0.30229	0.63357	0.89501	1.3438	0.4263	0.21424	0.63886	1.8667	0.9005	0.34801	0.79179	1.3112	0.3909	0.31069	0.6384	1.5508	0.633	0.75262	0.90461	1.0124	0.0178	0.04379	0.65597	2.4345	1.2836	0.43694	0.99459	0.84074	-0.25
429.3773_6.8	stcrn, stearoylcarnitine	0.46238	0.79436	1.2453	0.31647	0.66097	0.91036	1.3552	0.4385	0.21105	0.63886	1.9538	0.9663	0.35417	0.7927	1.3161	0.3963	0.30934	0.6384	1.5837	0.6633	0.74488	0.89969	1.008	0.0115	0.03881	0.65597	2.5259	1.3368	0.45898	0.99459	0.84755	-0.239
447.3299_6.07	tmndncrn, Timnodonyl carnitine	0.31277	0.71962	1.0849	0.11754	0.84054	0.96351	1.6756	0.7447	0.27288	0.65839	1.1848	0.2447	0.021897	0.63307	4.2531	2.0885	0.049557	0.61158	3.9444	1.9798	0.10274	0.6184	0.32661	-1.614	0.042647	0.65597	5.8766	2.555	0.47078	0.99459	0.44826	-1.158

Supplementary Table 5. Comparative metabolomics data of spleen tissue between "irradiated vs naïve" and "GT3 vs irradiated" treatment groups for 4.0 and 5.8 Gy exposure to PBI (LINAC) and TBI (Cobalt-60).

		PBI 4 Gy Irradiated vs. Naïve				PBI 4 Gy Irradiated vs. GT3				TBI 4 Gy Irradiated vs. Naïve			
mz_RT	EmpiricalCompound	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)
784.1507_2.21	C00016, FAD	0.042889	0.30518	2.299	1.201	0.95944	0.99953	0.98181	-0.0265	0.039647	0.43922	2.2397	1.163
399.145_0.4	C00019, S-Adenosyl-L-methionine	0.16981	0.54848	1.5963	0.67472	0.80501	0.99977	1.0694	0.0968	0.027037	0.30434	1.979	0.985
346.0553_0.44	C00020, AMP	0.19063	0.37853	2.4892	1.3157	0.81192	0.99953	0.827	-0.274	0.002486	0.25534	4.4912	2.167
348.0712_2.26	C00020, AMP	0.051705	0.45103	1.6506	0.72301	0.65174	0.99977	1.0686	0.0957	0.013911	0.28672	1.9409	0.957
154.9965_0.11	C00036, Oxaloacetate	0.037508	0.45103	1.2735	0.34884	0.81619	0.99977	0.96645	-0.0492	0.12195	0.52091	1.2058	0.27
88.0397_0.42	C00041, L-Alanine	0.11878	0.31361	1.6085	0.68568	0.75256	0.99953	0.88865	-0.1703	0.072915	0.43922	1.6351	0.709
90.0557_0.42	C00041, L-Alanine	0.36482	0.69323	1.1416	0.19111	0.96598	0.99977	1.0262	0.0373	0.15943	0.5222	1.2286	0.297
74.0185_0.41	C00121, D-Ribose	0.039622	0.30518	2.3704	1.2452	0.54333	0.99953	0.74608	-0.4226	0.071891	0.43922	1.7161	0.779
195.0502_0.42	C00124, D-Galactose	0.005096	0.30518	3.1482	1.6545	0.55456	0.99953	0.79658	-0.3281	0.010859	0.41565	2.3132	1.21
215.0322_0.41	C00124, D-Galactose	0.024184	0.30518	2.4047	1.2658	0.94624	0.99953	0.92949	-0.1055	0.040412	0.43922	2.2248	1.154
226.9887_0.42	C00129, Isopentenyl diphosphate	0.011645	0.30518	0.71584	-0.48229	0.76679	0.99953	1.097	0.1336	0.14467	0.43922	0.78273	-0.353
154.0612_0.38	C00135, L-Histidine	0.037423	0.30518	2.2741	1.1853	0.66557	0.99953	0.82378	-0.2797	0.095261	0.43922	1.7509	0.808
116.0713_0.43	C00148, L-Proline	0.034088	0.45103	1.5825	0.66219	0.73799	0.99977	0.91083	-0.1348	0.019411	0.30434	1.5213	0.605
136.0437_6.41	C00155, L-Homocysteine	0.68105	0.88147	0.86098	-0.21595	0.61365	0.99977	0.80911	-0.3056	0.29545	0.6367	1.3228	0.404
298.0979_1.1	C00170, 5'-Methylthioadenosine	0.043538	0.45103	2.5835	1.3693	0.82455	0.99977	1.1723	0.2294	0.032903	0.31729	3.0193	1.594
369.3543_9.89	C00187, Cholesterol	0.038933	0.45103	0.70535	-0.5036	0.19256	0.99977	1.1792	0.2378	0.33051	0.67103	0.85093	-0.233
606.0739_0.49	C00203, UDP-N-acetyl-D-galactosamine	0.017886	0.30518	3.7176	1.8944	0.89489	0.99953	0.77624	-0.3654	0.00229	0.25534	2.8575	1.515
607.0766_0.48	C00203, UDP-N-acetyl-D-galactosamine	0.030437	0.30518	3.6264	1.8585	0.85196	0.99953	0.73072	-0.4526	0.0035	0.26368	2.7153	1.441
269.2264_7.53	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.34893	0.67841	1.3146	0.39465	0.84507	0.99977	0.99885	-0.0017	0.0169	0.28672	1.8281	0.87
287.2372_7.54	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.52698	0.80448	1.1876	0.24804	0.67591	0.99977	1.0769	0.1068	0.018911	0.30434	1.8269	0.869
306.2516_7.97	C00219, (5Z,8Z,11Z,14Z)-Icosatetraenoic acid	0.07134	0.45103	1.4875	0.57286	0.77018	0.99977	0.96177	-0.0562	0.15161	0.5222	1.4042	0.49
101.0239_0.43	C00232, Succinate semialdehyde	0.019437	0.30518	2.5372	1.3432	0.70164	0.99953	0.85196	-0.2312	0.042358	0.43922	1.8681	0.902
129.055_1.96	C00233, 4-Methyl-2-oxopentanoate	0.028226	0.30518	2.353	1.2345	0.27951	0.99953	0.7324	-0.4493	0.016296	0.43922	2.6063	1.382
255.2317_6.33	C00249, Hexadecanoic acid	0.16386	0.34739	1.5965	0.67493	0.5301	0.99953	1.1048	0.1438	0.030215	0.43922	2.482	1.312
222.9976_0.38	C00279, D-Erythrose 4-phosphate	0.03059	0.45103	1.4142	0.50001	0.59166	0.99977	0.9097	-0.1365	0.057126	0.39598	1.2313	0.3
307.0445_0.43	C00294, Inosine	0.44784	0.76616	1.0948	0.13071	0.62893	0.99977	1.064	0.0894	0.97025	0.99292	1.0133	0.019
322.2714_7.54	C00319, Sphingosine	0.095888	0.46239	0.45201	-1.1456	0.93284	0.99977	0.96471	-0.0518	0.12746	0.52091	0.48555	-1.042
300.29_7.54	C00319, Sphingosine	0.12174	0.50863	0.46082	-1.1177	0.80977	0.99977	0.92205	-0.1171	0.15455	0.5222	0.4866	-1.039
588.0752_0.51	C00325, GDP-L-fucose	0.080106	0.30518	2.493	1.3179	0.92479	0.99953	0.80595	-0.3112	0.030166	0.43922	2.1941	1.134
140.0113_0.42	C00346, Ethanolamine phosphate	0.040054	0.30518	1.6154	0.69188	0.85759	0.99953	0.94851	-0.0763	0.12343	0.43922	1.3676	0.452
282.0831_0.44	C00387, Guanosine	0.045059	0.30518	1.5036	0.58846	0.76925	0.99953	0.95242	-0.0703	0.81764	0.87328	1.0209	0.03
159.092_1.07	C00390, Ubiquinol	0.16371	0.34739	1.677	0.74585	0.6971	0.99953	0.88215	-0.1809	0.26438	0.49675	1.4465	0.533
86.0241_0.45	C00439, N-Formimino-L-glutamate	0.01782	0.30518	3.1497	1.6552	0.45204	0.99953	0.68996	-0.5354	0.093574	0.43922	2.0073	1.005
584.2592_8.73	C00486, Bilirubin	0.29817	0.49044	2.9213	1.5466	0.79765	0.99953	0.63083	-0.6647	0.27495	0.50193	1.4082	0.494
583.2553_8.73	C00486, Bilirubin	0.22712	0.42	2.9565	1.5639	0.79968	0.99953	0.67807	-0.5605	0.17608	0.44351	1.5185	0.603
607.2535_8.73	C00486, Bilirubin	0.021758	0.45103	2.4719	1.3056	0.95755	0.99977	0.96957	-0.0446	0.057174	0.39598	1.5488	0.631
585.2712_8.73	C00486, Bilirubin	0.025231	0.45103	2.4204	1.2752	0.96365	0.99977	0.9713	-0.042	0.066811	0.41966	1.5349	0.618
586.2749_8.73	C00486, Bilirubin	0.029085	0.45103	2.5583	1.3552	0.99552	0.99977	0.93875	-0.0912	0.099683	0.49814	1.4964	0.582
583.2566_5.22	C00500, Biliverdin	0.30673	0.64424	0.77533	-0.36713	0.61866	0.99977	1.2401	0.3105	0.68441	0.88887	0.9784	-0.032
584.2589_4.96	C00500, Biliverdin	0.71939	0.89818	1.0393	0.055599	0.14989	0.99977	1.528	0.6117	0.31035	0.6409	1.2788	0.355
583.2561_4.96	C00500, Biliverdin	0.73834	0.90677	1.1083	0.14835	0.13269	0.99977	1.4913	0.5766	0.2878	0.62986	1.301	0.38
292.2345_6.48	C00523, Androsterone	0.06315	0.45103	2.0495	1.0353	0.50971	0.99977	1.1668	0.2226	0.16461	0.52463	1.5072	0.592
271.2059_4.56	C00523, Androsterone	0.021531	0.30518	2.9575	1.5644	0.60763	0.99953	0.88671	-0.1735	0.026824	0.43922	2.7908	1.481
375.215_4.88	C00584, Prostaglandin E2	0.000398	0.36012	5.6938	2.5094	0.43663	0.99977	0.79358	-0.3336	0.001115	0.19996	3.9503	1.982
333.2066_4.56	C00584, Prostaglandin E2	0.021287	0.30518	2.9747	1.5728	0.59107	0.99953	0.86591	-0.2077	0.027439	0.43922	2.6962	1.431
317.212_4.56	C00584, Prostaglandin E2	0.022035	0.45103	2.3088	1.2072	0.49137	0.99977	0.89422	-0.1613	0.026726	0.30434	2.2085	1.143
352.2205_4.56	C00584, Prostaglandin E2	0.021346	0.30518	3.0153	1.5923	0.55294	0.99953	0.85432	-0.2272	0.028842	0.43922	2.6803	1.422
375.2149_5.37	C00584, Prostaglandin E2	0.32715	0.65829	1.5658	0.6469	0.8163	0.99977	0.96049	-0.0582	0.30132	0.63766	1.3736	0.458
335.2225_4.56	C00584, Prostaglandin E2	0.022107	0.45103	2.3142	1.2105	0.54333	0.99977	0.91011	-0.1359	0.03049	0.30434	2.1246	1.087
353.2328_3.94	C00584, Prostaglandin E2	0.097254	0.4642	2.0885	1.0625	0.7911	0.99977	0.8472	-0.2392	0.49353	0.79174	1.7206	0.783
409.2964_6.41	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	0.77295	0.91954	0.92482	-0.11275	0.62411	0.99977	0.79146	-0.3374	0.2153	0.57473	1.3775	0.462
391.2853_9.04	C00695, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholanate	0.015004	0.45103	2.0481	1.0343	0.92886	0.99977	0.96503	-0.0514	0.28067	0.62356	1.1023	0.141
370.2959_5.5	C00836, Sphinganine	0.3499	0.67841	1.718	0.78069	0.35992	0.99977	1.2792	0.3552	0.011329	0.27494	2.9429	1.557
302.306_5.91	C00836, Sphinganine	0.63182	0.85648	0.89717	-0.15655	0.8457	0.99977	1.1323	0.1793	0.01588	0.28672	2.0562	1.04
324.2901_7.19	C00836, Sphinganine	0.54264	0.81135	0.73317	-0.44777	0.27064	0.99977	0.82539	-0.2769	0.36982	0.6977	0.66501	-0.589
220.1187_0.8	C00864, Pantothenate	0.050366	0.45103	2.4954	1.3193	0.86329	0.99977	0.93978	-0.0896	0.05713	0.39598	2.2028	1.139
218.1027_0.63	C00864, Pantothenate	0.066735	0.30518	2.2734	1.1849	0.74275	0.99953	0.85202	-0.231	0.048466	0.43922	2.2762	1.187
138.0199_0.55	C00870, 4-Nitrophenol	0.73046	0.83783	0.97795	-0.032165	0.97227	0.99953	0.94008	-0.0892	0.57921	0.71598	1.0048	0.007
297.1095_2.64	C00921, Dihydropteroate	0.036933	0.45103	2.3256	1.2176	0.9115	0.99977	0.98859	-0.0166	0.045623	0.3697	2.0378	1.027
135.0302_0.43	C01013, 3-Hydroxypropanoate	0.056078	0.30518	1.7057	0.77037	0.49967	0.99953	0.83003	-0.2688	0.5257	0.67735	1.1541	0.207
146.0454_0.42	C01110, 5-Amino-2-oxopentanoic acid	0.070371	0.30518	1.6922	0.75893	0.70805	0.99953	0.87765	-0.1883	0.17297	0.44351	1.4022	0.488
404.2501_5.05	C01120, Sphinganine 1-phosphate	0.073306	0.45103	1.8945	0.92182	0.54694	0.99977	0.90582	-0.1427	0.089709	0.47402	1.7671	0.821
142.9982_0.44	C01127, 4-Hydroxy-2-oxoglutarate	0.11387	0.31269	0.82665	-0.27464	0.97793	0.99953	1.0193	0.0276	0.14487	0.43922	0.80358	-0.315
194.0198_0.44	C01194, 1-Phosphatidyl-D-myo-inositol	0.015634	0.30518	2.1925	1.1326	0.43776	0.99953	0.80737	-0.3087	0.030745	0.43922	1.838	0.878
271.2064_4.56	C01227, 3beta-Hydroxyandrost-5-en-17-one	0.015058	0.45103	2.5076	1.3263	0.53993	0.99977	0.90674	-0.1412	0.016959	0.28672	2.3945	1.26
289.2167_4.56	C01227, 3beta-Hydroxyandrost-5-en-17-one	0.024666	0.45103	2.3196	1.2139	0.56607	0.99977	0.91479	-0.1285	0.030309	0.30434	2.1785	1.123
289.2171_3.86	C01227, 3beta-Hydroxyandrost-5-en-17-one	0.36792	0.69692	1.5505	0.63272	0.66155	0.99977	0.98403	-0.0232	0.17483	0.52924	1.55	0.632
307.2637_7.03	C01530, Octadecanoic acid	0.98629	0.99295	0.68536	-0.54506	0.57902	0.99977	0.93633	-0.0949	0.76561	0.92099	0.57838	-0.79
151.024_0.44	C01620,	0.6239	0.75081	0.74367	-0.42727	0.015705	0.99953	0.46025	-1.1195	0.16468	0.43922	0.5907	-0.76
361.2016_3.86	C01780, Aldosterone	0.2467	0.59425	1.4444	0.5305	0.5965	0.99977	1.1015	0.1395	0.10285	0.50823	1.7908	0.841
128.0347_0.45	C01879, 5-Oxoproline	0.007696	0.30518	2.6862	1.4256	0.37145	0.99953	0.76531	-0.3859	0.054111	0.43922	1.6763	0.745
375.2149_4.56	C02198, Thromboxane A2	0.082094	0.45103	1.755	0.81151	0.59836	0.99977	0.9121	-0.1327	0.078445	0.45265	1.7773	0.83
110.0206_8.71	C02218, 2-Aminoacrylate	0.24256	0.59377	1.0615	0.086123	0.16444	0.99977	0.89657	-0.1575	0.46953	0.77409	1.0362	0.051
208.0002_0.39	C02532, D-O-Phosphoserine	0.12599	0.51134	1.3068	0.38606	0.28602	0.99977	0.89304	-0.1632	0.17982	0.5298	1.2447	0.316
214.0514_1.39	C02712, N-Acetylmethionine	0.064083	0.45103	1.9752	0.98203	0.42254	0.99977	0.76156	-0.393	0.057789	0.39598	1.8395	0.879
835.5299_12.06	C02737, Phosphatidylserine	0.086619	0.45633	0.55628	-0.84612	0.61683	0.99977	0.86861	-0.2032	0.12332	0.52091	0.59695	-0.744
322.2714_5.77	C02934, 3-Dehydrosphinganine	0.74639	0.90981	0.92093	-0.11883	0.97482	0.99977	1.0076	0.011	0.034788	0.32439	1.8797	0.911
401.346_6.34	C02990, L-Palmitoylcarnitine	0.27919	0.62696	1.5168	0.60107	0.66248	0.99977	1.035	0.0497	0.025807	0.30434	2.0923	1.065
400.3427_6.34	C02990, L-Palmitoylcarnitine	0.30119	0.64213	1.4632	0.54917	0.62559	0.99977	1.0521	0.0733	0.025654	0.30434	2.0099	1.007
308.2646_7.03	C03242, (8Z,11Z,14Z)-Icosatrienoic acid	0.82155	0.93956	0.62951	-0.6677	0.89631	0.99977	1.0377	0.0534	0.69808	0.89092	0.56815	-0.816
324.0929_0.43	C03410, N-Glycoloyl-neuraminate	0.026852	0.30518	2.7657	1.4676	0.97454	0.99953	0.97505	-0.0365	0.020774	0.43922	3.19	1.674
139.0507_0.44	C03680, 4-Imidazolone-5-propanoate	0.043257	0.45103	1.2874	0.36449	0.8084	0.99977	0.97664	-0.0341	0.038891	0.34374	1.2695	0.344
322.9936_0.61	C03785, D-Tagatose 1,6-bisphosphate	0.012786	0.45103	3.9462	1.9805	0.98857	0.99977	1.0033	0.0047	0.015282	0.28672	3.4964	1.806
339.9919_0.53	C03785, D-Tagatose 1,6-bisphosphate	0.017022	0.30518	3.8777	1.9552	0.82971	0.99953	0.89017	-0.1679	0.017038	0.43922	3.5253	1.818
338.9882_0.53	C03785, D-Tagatose 1,6-bisphosphate	0.027287	0.30518	3.5145	1.8133	0.89546	0.99953	0.91492	-0.1283	0.034169	0.43922	3.0365	1.602
378.96_0.53	C03785, D-Tagatose 1,6-bisphosphate	0.020125	0.45103	4.0907	2.0323	0.93577	0.99977	1.0248	0.0353	0.022081	0.30434	3.4358	1.781
362.9868_0.53	C03785, D-Tagatose 1,6-bisphosphate	0.029002	0.45103	3.2325	1.6926	0.56562	0.99977	1.2611	0.3347	0.017716	0.29402	3.7691	1.914
112.0399_0.46	C03912, (S)-1-Pyrroline-5-carboxylate	0.000813	0.30518	2.8973	1.5347	0.27472	0.99953	0.73823	-0.4379	0.005685	0.33873	2.7676	1.469
318.2506_7.47	C04042, 20alpha-Hydroxy-4-pregnen-3-one	0.72005	0.89818	1.0262	0.037299	0.75041	0.99977	0.92126	-0.1183	0.46977	0.77409	0.89256	-0.164
508.3766_7.01	C04230, 1-Acyl-sn-glycero-3-phosphocholine	0.53093	0.80561	1.0903	0.12477	0.45534	0.99977	0.87781	-0.188	0.35014	0.687	1.2074	0.272
509.3751_7.6	C04230, 1-Acyl-sn-glycero-3-phosphocholine	0.38843	0.71103	1.1811	0.2401	0.83533	0.99977	0.95029	-0.0736	0.005132	0.23802	1.659	0.73
509.3802_7.01	C04230, 1-Acyl-sn-glycero-3-phosphocholine	0.55217	0.81135	1.0887	0.12256	0.41741	0.99977	0.86103	-0.2159	0.34923	0.687	1.219	0.286
508.3763_7.6	C04230, 1-Acyl-sn-glycero-3-phosphocholine	0.73832	0.90677	1.0555	0.077982	0.79806	0.99977	0.93047	-0.104	0.035918	0.33078	1.5422	0.625
532.3733_7.62	C04598, 2-Acetyl-1-alkyl-sn-glycero-3-phosphocholine	0.041968	0.45103	1.7069	0.77141	0.25338	0.99977	0.79193	-0.3366	0.001741	0.19996	2.7876	1.479
321.2434_6.99	C04805, 5(S)-HETE	0.13157	0.51134	1.6973	0.7632	0.61997	0.99977	0.8424	-0.2474	0.15566	0.5222	1.5691	0.65
265.2166_4.55	C04849, (5Z,9E,14Z)-(8xi,11R,12S)-11,12-Epoxy-8-hydroxyicosa-5,9,14-trienoic acid	0.018684	0.45103	2.5247	1.3361	0.62506	0.99977	0.9067	-0.1413	0.021434	0.30434	2.3437	1.229
648.8542_11.89	C04884, N-Acetyl-D-galactosaminyl-(N-acetylneuraminyl)-D-galactosyl-D-glucosylceramide	0.11981	0.31484	1.6872	0.75465	0.75332	0.99953	0.85102	-0.2327	0.54752	0.69128	1.1913	0.252
127.0503_0.4	C05100, 3-Ureidoisobutyrate	0.030605	0.30518	2.3726	1.2465	0.57663	0.99953	0.76143	-0.3932	0.060288	0.43922	1.6449	0.718
102.0555_0.42	C05145, 3-Aminoisobutyric acid	0.06507	0.30518	1.7305	0.79116	0.65359	0.99953	0.86511	-0.2091	0.19293	0.4519	1.4172	0.503
363.2151_6.43	C05474, 3alpha,11beta,21-Trihydroxy-20-oxo-5beta-pregnan-18-al	0.61592	0.74597	1.0093	0.013307	0.53038	0.99953	0.78898	-0.3419	0.69084	0.80149	0.87793	-0.188
373.2352_6.96	C05476, Tetrahydrocorticosterone	0.83646	0.9416	0.58307	-0.77827	0.90721	0.99977	0.97756	-0.0327	0.69291	0.88962	0.48003	-1.059
317.2481_7.47	C05479, 5beta-Pregnane-3,20-dione	0.59727	0.83681	1.0984	0.13535	0.91021	0.99977	0.85967	-0.2181	0.42314	0.73416	0.95434	-0.067
319.2643_7.71	C05480, 3alpha-Hydroxy-5beta-pregnane-20-one	0.6981	0.88869	0.89003	-0.16807	0.88428	0.99977	0.88574	-0.175	0.59655	0.8496	0.66946	-0.579
334.21_4.56	C05954, Prostaglandin B2	0.022487	0.30518	2.9463	1.5589	0.56849	0.99953	0.87592	-0.1911	0.026465	0.43922	2.8074	1.489
315.1961_4.56	C05954, Prostaglandin B2	0.020215	0.30518	2.9834	1.5769	0.54752	0.99953	0.86072	-0.2164	0.029956	0.43922	2.6716	1.418
393.2274_4.54	C05954, Prostaglandin B2	0.15349	0.34215	1.6135	0.69015	0.72012	0.99953	0.91305	-0.1312	0.20109	0.45453	1.4977	0.583
299.2013_4.56	C05955, Prostaglandin C2	0.021899	0.45103	2.3915	1.2579	0.45989	0.99977	0.87593	-0.1911	0.024677	0.30434	2.2986	1.201
336.2258_4.56	C05955, Prostaglandin C2	0.03546	0.45103	2.2376	1.162	0.8095	0.99977	0.96219	-0.0556	0.039814	0.34794	2.1018	1.072
377.23_4.49	C05959, 11-epi-Prostaglandin F2alpha	0.029719	0.45103	2.479	1.3098	0.58156	0.99977	0.85186	-0.2313	0.094126	0.48281	1.6404	0.714
369.2277_4.38	C05959, 11-epi-Prostaglandin F2alpha	0.086798	0.30518	2.2933	1.1974	0.68312	0.99953	1.0472	0.0666	0.30372	0.53045	1.3628	0.447
319.2266_4.49	C05959, 11-epi-Prostaglandin F2alpha	0.027392	0.45103	2.1394	1.0972	0.61216	0.99977	0.90817	-0.139	0.090651	0.47452	1.6096	0.687
377.2304_4.91	C05959, 11-epi-Prostaglandin F2alpha	0.21294	0.57667	1.5678	0.64877	0.6099	0.99977	1.0703	0.098	0.52789	0.81593	1.0788	0.109
353.2325_4.92	C05959, 11-epi-Prostaglandin F2alpha	0.78576	0.88	0.85458	-0.22671	0.2978	0.99953	1.433	0.519	0.96631	0.9732	0.7443	-0.426
393.2254_4.34	C05963,	0.1556	0.5332	1.6332	0.70774	0.68297	0.99977	0.88581	-0.1749	0.42412	0.73416	1.1984	0.261
351.2171_4.56	C05963,	0.020861	0.30518	2.9575	1.5644	0.58006	0.99953	0.86207	-0.2141	0.029157	0.43922	2.6276	1.394
393.2255_3.93	C05963,	0.1451	0.52528	1.9349	0.95222	0.86505	0.99977	0.95785	-0.0621	0.27171	0.61595	1.751	0.808

	TBI 4 Gy Irradiated vs. GT3				PBI 5.8 Gy Irradiated vs. Naïve				PBI 5.8 Gy Irradiated vs. GT3				TBI 5.8 Gy Irradiated vs. Naïve				TBI 5.8 Gy Irradiated vs. GT3			
mz_RT	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)	p-value	FDR	FC	Log2(FC)
784.1507_2.21	0.38955	0.98029	0.77397	-0.3697	0.11822	0.32434	1.7507	0.8079	0.69819	0.91314	0.94426	-0.0827	0.08725	0.69603	1.9983	0.999	0.1602	0.71979	1.6534	0.725
399.145_0.4	0.59094	0.97009	0.88776	-0.1718	0.46815	0.83016	1.2391	0.3093	0.65042	0.9855	1.0862	0.1193	0.055971	0.61039	1.8017	0.849	0.36935	0.94956	1.3078	0.387
346.0553_0.44	0.10486	0.98029	0.4221	-1.2444	0.006113	0.29355	3.7451	1.905	0.9621	0.9906	1.0051	0.0073	0.038179	0.69603	2.9107	1.541	0.082589	0.71979	2.1038	1.073
348.0712_2.26	0.75092	0.99411	0.97823	-0.0318	0.06874	0.62891	1.7195	0.782	0.93506	0.9855	0.9966	-0.0049	0.065855	0.61039	1.6735	0.743	0.40214	0.94956	1.1696	0.226
154.9965_0.11	0.83596	0.99411	0.96226	-0.0555	0.041518	0.60576	1.2033	0.267	0.87545	0.9855	0.99032	-0.014	0.012769	0.61039	1.2783	0.354	0.9249	0.98189	0.99574	-0.006
88.0397_0.42	0.44917	0.98029	0.83448	-0.2611	0.16447	0.36973	1.6715	0.7411	0.51983	0.83492	0.76564	-0.3853	0.22501	0.69603	1.4321	0.518	0.18613	0.71979	1.5857	0.665
90.0557_0.42	0.70189	0.98329	0.95813	-0.0617	0.37561	0.78447	1.1225	0.1667	0.21762	0.9855	0.88568	-0.1752	0.033221	0.61039	1.417	0.503	0.71165	0.94956	1.0932	0.129
74.0185_0.41	0.47643	0.98029	0.83897	-0.2533	0.029295	0.29355	2.0614	1.0436	0.18827	0.67289	0.67588	-0.5652	0.17111	0.69603	1.6645	0.735	0.2637	0.71979	1.5829	0.663
195.0502_0.42	0.58252	0.98029	0.92792	-0.1079	0.002657	0.29355	3.0373	1.6028	0.025189	0.67289	0.61377	-0.7042	0.007992	0.68829	2.9397	1.556	0.48187	0.71979	1.2357	0.305
215.0322_0.41	0.4206	0.98029	0.73527	-0.4437	0.016246	0.29355	2.4325	1.2825	0.025042	0.67289	0.8209	-0.2847	0.032269	0.69603	2.677	1.421	0.51156	0.72933	1.2341	0.303
226.9887_0.42	0.35869	0.98029	1.2067	0.2711	0.058674	0.29355	0.76654	-0.3836	0.91387	0.9799	1.0672	0.0938	0.025687	0.69603	0.71211	-0.49	0.42726	0.71979	0.85405	-0.228
154.0612_0.38	0.5711	0.98029	0.82722	-0.2737	0.054811	0.29355	1.8262	0.8689	0.092606	0.67289	0.66931	-0.5793	0.20731	0.69603	1.6137	0.69	0.22077	0.71979	1.6375	0.712
116.0713_0.43	0.30788	0.97009	0.8281	-0.2721	0.04195	0.60576	1.3899	0.475	0.17925	0.9855	0.87304	-0.1959	0.19061	0.6618	1.2648	0.339	0.35449	0.94956	1.2478	0.319
136.0437_6.41	0.85036	0.99411	1.0593	0.0832	0.7128	0.91322	1.274	0.3494	0.44864	0.9855	0.62109	-0.6871	0.53698	0.79123	1.2457	0.317	0.58888	0.94956	0.81873	-0.289
298.0979_1.1	0.47011	0.97009	0.68998	-0.5354	0.20058	0.69627	1.6749	0.7441	0.76961	0.9855	1.2761	0.3517	0.078272	0.61256	2.4226	1.277	0.27828	0.94956	1.7494	0.807
369.3543_9.89	0.16585	0.97009	1.2509	0.323	0.6127	0.8803	0.90942	-0.137	0.67711	0.9855	1.0577	0.0809	0.47181	0.77066	0.89558	-0.159	0.43501	0.94956	0.72116	-0.472
606.0739_0.49	0.35901	0.98029	0.7496	-0.4158	0.003397	0.29355	2.8326	1.5021	0.75605	0.92734	0.92987	-0.1049	0.007644	0.68829	3.6884	1.883	0.25254	0.71979	2.1162	1.082
607.0766_0.48	0.42154	0.98029	0.76908	-0.3788	0.004025	0.29355	2.8502	1.5111	0.77101	0.93585	0.94816	-0.0768	0.010355	0.68829	3.4343	1.78	0.19639	0.71979	2.3566	1.237
269.2264_7.53	0.33406	0.97009	0.84049	-0.2507	0.17813	0.69604	1.3771	0.4616	0.31148	0.9855	1.2286	0.2971	0.63762	0.83358	1.2465	0.318	0.14942	0.94956	1.5253	0.609
287.2372_7.54	0.20364	0.97009	0.76592	-0.3847	0.20365	0.69627	1.3303	0.4118	0.66047	0.9855	1.1469	0.1978	0.59851	0.81529	1.3286	0.41	0.34165	0.94956	1.2896	0.367
306.2516_7.97	0.7667	0.99411	1.0314	0.0446	0.27324	0.7329	1.2455	0.3167	0.33017	0.9855	0.87799	-0.1877	0.19454	0.6618	1.4344	0.52	0.64282	0.94956	0.85599	-0.224
101.0239_0.43	0.34797	0.98029	0.79615	-0.3289	0.030231	0.29355	2.1316	1.092	0.19534	0.67289	0.81516	-0.2948	0.072811	0.69603	2.18	1.124	0.36457	0.71979	1.4297	0.516
129.055_1.96	0.15372	0.98029	0.65057	-0.6202	0.10793	0.31861	2.1385	1.0966	0.34529	0.74666	0.63114	-0.664	0.070325	0.69603	2.1647	1.114	0.097742	0.71979	1.9183	0.94
255.2317_6.33	0.65996	0.98029	1.0165	0.0237	0.24818	0.42881	1.4268	0.5128	0.70606	0.91449	1.3425	0.4249	0.081436	0.69603	3.2848	1.716	0.92744	0.96769	0.69267	-0.53
222.9976_0.38	0.87401	0.99411	0.9836	-0.0239	0.006604	0.54972	1.4393	0.5254	0.52204	0.9855	0.94124	-0.0874	0.13163	0.6618	1.2003	0.263	0.53178	0.94956	1.165	0.22
307.0445_0.43	0.64717	0.97009	1.0491	0.0692	0.34354	0.76538	1.1278	0.1735	0.39109	0.9855	1.1531	0.2056	0.20506	0.66365	1.2317	0.301	0.72701	0.94956	0.93463	-0.098
322.2714_7.54	0.69107	0.98329	1.0647	0.0904	0.13903	0.65986	0.44931	-1.1542	0.27559	0.9855	1.1954	0.2575	0.19544	0.6618	0.53633	-0.899	0.99839	0.99875	1.0092	0.013
300.29_7.54	0.39403	0.97009	1.1659	0.2214	0.38086	0.78447	0.57682	-0.7938	0.97911	0.99454	0.98952	-0.0152	0.30788	0.6878	0.58917	-0.763	0.8233	0.96811	0.94801	-0.077
588.0752_0.51	0.36158	0.98029	0.76066	-0.3947	0.036004	0.29355	2.1722	1.1191	0.45855	0.80586	0.83158	-0.2661	0.056563	0.69603	2.4575	1.297	0.24558	0.71979	1.7922	0.842
140.0113_0.42	0.53105	0.98029	0.88955	-0.1689	0.1546	0.36407	1.3168	0.397	0.64866	0.89655	0.94182	-0.0865	0.14815	0.69603	1.4103	0.496	0.242	0.71979	1.399	0.484
282.0831_0.44	0.84694	0.98687	1.1438	0.1939	0.1702	0.36987	1.2756	0.3512	0.52434	0.83492	0.92504	-0.1124	0.28789	0.73423	1.3448	0.427	0.96301	0.98693	0.99409	-0.009
159.092_1.07	0.39941	0.98029	0.76327	-0.3897	0.29386	0.46573	1.3528	0.436	0.039689	0.67289	0.62629	-0.6751	0.41907	0.79812	1.281	0.357	0.32386	0.71979	1.6378	0.712
86.0241_0.45	0.46694	0.98029	0.71651	-0.4809	0.019829	0.29355	2.5919	1.374	0.29021	0.73016	0.75539	-0.4047	0.32481	0.75833	1.5544	0.636	0.099398	0.71979	1.9881	0.991
584.2592_8.73	0.17195	0.98029	2.0989	1.0696	0.005298	0.29355	3.0786	1.6223	0.062197	0.67289	0.5056	-0.9839	0.31222	0.75139	2.1584	1.11	0.73098	0.84613	0.86367	-0.211
583.2553_8.73	0.19941	0.98029	1.9502	0.9636	0.006732	0.29355	2.9888	1.5796	0.045259	0.67289	0.51352	-0.9615	0.40988	0.79768	2.1351	1.094	0.98647	0.99438	0.99561	-0.006
607.2535_8.73	0.26702	0.97009	1.609	0.6862	0.008515	0.54972	2.5136	1.3298	0.043144	0.9855	0.52061	-0.9417	0.14452	0.6618	2.0671	1.048	0.8086	0.96615	0.86386	-0.211
585.2712_8.73	0.26304	0.97009	1.6371	0.7111	0.012313	0.54972	2.451	1.2934	0.059831	0.9855	0.53346	-0.9065	0.15895	0.6618	2.0217	1.016	0.85016	0.96957	0.87192	-0.198
586.2749_8.73	0.22427	0.97009	1.7416	0.8005	0.013874	0.54972	2.5394	1.3445	0.062388	0.9855	0.52645	-0.9256	0.19346	0.6618	2.068	1.048	0.87962	0.97468	0.86465	-0.21
583.2566_5.22	0.38606	0.97009	1.219	0.2857	0.44661	0.81856	1.22	0.2869	0.90447	0.9855	0.99886	-0.0016	0.20344	0.66365	0.64044	-0.643	0.62959	0.94956	1.0071	0.01
584.2589_4.96	0.5512	0.97009	0.8808	-0.1831	0.48661	0.83676	1.2114	0.2767	0.4535	0.9855	0.79501	-0.331	0.37763	0.72422	0.74452	-0.426	0.70235	0.94956	0.87441	-0.194
583.2561_4.96	0.91582	0.99411	0.96554	-0.0506	0.5075	0.84618	1.1712	0.228	0.53302	0.9855	0.85472	-0.2265	0.24519	0.66365	0.70907	-0.496	0.63661	0.94956	0.91914	-0.122
292.2345_6.48	0.22222	0.97009	0.74877	-0.4174	0.13105	0.65101	1.6983	0.7641	0.53215	0.9855	0.92145	-0.118	0.81834	0.93053	0.82262	-0.282	0.4293	0.94956	1.6628	0.734
271.2059_4.56	0.043787	0.98029	0.35649	-1.4881	0.2081	0.39169	1.9376	0.9543	0.47056	0.81057	0.64298	-0.6372	0.60709	0.86837	1.0839	0.116	0.14559	0.71979	2.8456	1.509
375.215_4.88	0.10719	0.97009	0.57733	-0.7925	0.01565	0.55512	2.5183	1.3325	0.75116	0.9855	0.97038	-0.0434	0.097108	0.64461	1.8292	0.871	0.19503	0.94956	1.6443	0.718
333.2066_4.56	0.048803	0.98029	0.38168	-1.3896	0.19029	0.38536	2.0356	1.0255	0.4481	0.79993	0.61475	-0.7019	0.53345	0.84009	1.1516	0.204	0.17693	0.71979	2.6228	1.391
317.212_4.56	0.05469	0.97009	0.48426	-1.0461	0.20151	0.69627	1.6442	0.7174	0.41087	0.9855	0.72006	-0.4738	0.72724	0.87999	0.89602	-0.158	0.29876	0.94956	1.7809	0.833
352.2205_4.56	0.047422	0.98029	0.37686	-1.4079	0.20539	0.39169	2.0062	1.0045	0.43629	0.79709	0.58605	-0.7709	0.50239	0.83023	1.1674	0.223	0.22316	0.71979	2.5635	1.358
375.2149_5.37	0.70393	0.98333	1.1297	0.1759	0.20771	0.69627	1.7577	0.8137	0.88803	0.9855	1.2134	0.2791	0.68167	0.85975	1.4034	0.489	0.28027	0.94956	1.572	0.653
335.2225_4.56	0.057323	0.97009	0.47355	-1.0784	0.216	0.69627	1.6071	0.6844	0.40769	0.9855	0.7192	-0.4755	0.85994	0.9425	0.84517	-0.243	0.29157	0.94956	1.8589	0.894
353.2328_3.94	0.80693	0.99411	0.75063	-0.4138	0.23388	0.70528	1.6663	0.7367	0.64012	0.9855	0.90803	-0.1392	0.18907	0.6618	1.9056	0.93	0.4665	0.94956	0.67539	-0.566
409.2964_6.41	0.91999	0.99411	1.0311	0.0442	0.68272	0.9033	1.301	0.3796	0.40811	0.9855	0.60319	-0.7293	0.48701	0.77672	1.2182	0.285	0.57457	0.94956	0.85167	-0.232
391.2853_9.04	0.29664	0.97009	2.0395	1.0282	0.88091	0.95614	1.008	0.0115	0.58153	0.9855	1.0845	0.117	0.75204	0.89487	1.0448	0.063	0.2705	0.94956	1.5234	0.607
370.2959_5.5	0.27384	0.97009	0.83543	-0.2594	0.061243	0.62891	2.2176	1.149	0.87202	0.9855	1.1327	0.1798	0.028657	0.61039	4.8993	2.293	0.70064	0.94956	0.62545	-0.677
302.306_5.91	0.5548	0.97009	1.1412	0.1905	0.21054	0.69627	1.3902	0.4753	0.7914	0.9855	1.1433	0.1932	0.038942	0.61039	1.8677	0.901	0.23227	0.94956	0.65168	-0.618
324.2901_7.19	0.39115	0.97009	1.1298	0.1761	0.97245	0.99281	0.89615	-0.1582	0.89022	0.9855	0.93816	-0.0921	0.61654	0.82373	0.75317	-0.409	0.73359	0.94956	1.1677	0.224
220.1187_0.8	0.51435	0.97009	0.83285	-0.2639	0.091739	0.65101	2.4677	1.3032	0.60575	0.9855	0.78508	-0.3491	0.36257	0.71369	1.2157	0.282	0.055078	0.94956	2.1478	1.103
218.1027_0.63	0.37489	0.98029	0.75316	-0.409	0.12591	0.33089	2.4057	1.2665	0.59229	0.86081	0.69023	-0.5348	0.35282	0.76818	1.1998	0.263	0.05595	0.71979	2.3394	1.226
138.0199_0.55	0.34011	0.98029	0.81647	-0.2925	0.76214	0.81555	1.14	0.189	0.71135	0.91604	0.72123	-0.4715	0.56858	0.85439	0.57065	-0.809	0.002631	0.71979	2.5936	1.375
297.1095_2.64	0.65642	0.97393	0.91645	-0.1259	0.054877	0.62891	2.0965	1.068	0.043956	0.9855	0.85679	-0.223	0.036719	0.61039	2.0264	1.019	0.4374	0.94956	1.2947	0.373
135.0302_0.43	0.87965	0.98687	0.94867	-0.076	0.25199	0.43153	1.2525	0.3248	0.30291	0.73584	0.86341	-0.2119	0.35957	0.77563	1.3832	0.468	0.60748	0.77303	1.2138	0.28
146.0454_0.42	0.46693	0.98029	0.83499	-0.2602	0.14657	0.35579	1.3907	0.4758	0.4133	0.7921	0.86637	-0.207	0.31065	0.75139	1.3648	0.449	0.29943	0.71979	1.5011	0.586
404.2501_5.05	0.16208	0.97009	0.68566	-0.5444	0.1756	0.69517	1.7708	0.8244	0.47288	0.9855	0.76333	-0.3896	0.97119	0.98718	0.78414	-0.351	0.22295	0.94956	1.5406	0.624
142.9982_0.44	0.34021	0.98029	1.1906	0.2517	0.051267	0.29355	0.76776	-0.3813	0.90593	0.9799	1.0312	0.0444	0.11275	0.69603	0.73105	-0.452	0.99314	0.995	0.96807	-0.047
194.0198_0.44	0.43237	0.98029	0.8412	-0.2495	0.031497	0.29355	1.9098	0.9334	0.036158	0.67289	0.74131	-0.4318	0.13022	0.69603	1.6287	0.704	0.31461	0.71979	1.405	0.491
271.2064_4.56	0.081944	0.97009	0.53647	-0.8984	0.12939	0.65101	1.9161	0.9381	0.21005	0.9855	0.58121	-0.7829	0.45075	0.76636	1.046	0.065	0.28012	0.94956	1.741	0.8
289.2167_4.56	0.042234	0.97009	0.47487	-1.0744	0.18449	0.69604	1.7341	0.7942	0.40289	0.9855	0.70169	-0.5111	0.62551	0.82837	0.94338	-0.084	0.44279	0.94956	1.6689	0.739
289.2171_3.86	0.42635	0.97009	0.84851	-0.237	0.6171	0.88039	1.1025	0.1408	0.49219	0.9855	0.79876	-0.3242	0.14716	0.6618	2.918	1.545	0.32959	0.94956	0.41481	-1.27
307.2637_7.03	0.018831	0.97009	0.65644	-0.6073	0.96549	0.9918	0.6945	-0.526	0.86559	0.9855	0.97196	-0.041	0.28984	0.68423	0.39453	-1.342	0.53382	0.94956	1.235	0.304
151.024_0.44	0.80332	0.98029	1.0581	0.0815	0.015669	0.29355	0.24639	-2.021	0.73451	0.92634	1.2348	0.3043	0.02417	0.69603	0.30738	-1.702	0.63127	0.78973	1.2432	0.314
361.2016_3.86	0.76288	0.99411	1.0796	0.1105	0.62585	0.8848	1.0218	0.0312	0.63142	0.9855	0.93579	-0.0957	0.29091	0.68423	1.4855	0.571	0.41253	0.94956	0.71102	-0.492
128.0347_0.45	0.43333	0.98029	0.86241	-0.2136	0.1084	0.31861	1.755	0.8115	0.564	0.85108	0.82246	-0.282	0.1759	0.69603	1.5056	0.59	0.13592	0.71979	1.8549	0.891
375.2149_4.56	0.043203	0.97009	0.47332	-1.0791	0.25214	0.72067	1.5182	0.6024	0.49745	0.9855	0.7971	-0.3272	0.99315	0.99646	0.81061	-0.303	0.78192	0.96458	1.3909	0.476
110.0206_8.71	0.64525	0.97009	1.0221	0.0316	0.17028	0.68914	1.0779	0.1082	0.4642	0.9855	0.94664	-0.0791	0.71165	0.87189	1.0329	0.047	0.1996	0.94956	0.87271	-0.196
208.0002_0.39	0.81717	0.99411	0.98078	-0.028	0.40186	0.793	1.1472	0.1981	0.63055	0.9855	1.0819	0.1136	0.11121	0.65959	1.3761	0.461	0.79236	0.96615	1.0693	0.097
214.0514_1.39	0.28542	0.97009	0.76246	-0.3913	0.2204	0.69627	1.5466	0.6291	0.52931	0.9855	0.81379	-0.2973	0.5039	0.77672	1.1772	0.235	0.043823	0.94956	2.1027	1.072
835.5299_12.06	0.18375	0.97009	1.342	0.4244	0.51491	0.84957	0.76377	-0.3888	0.80811	0.9855	0.93931	-0.0903	0.41268	0.74728	0.79659	-0.328	0.19842	0.94956	0.51216	-0.965
322.2714_5.77	0.75983	0.99411	1.0454	0.0641	0.39431	0.79065	1.2643	0.3384	0.36725	0.9855	1.3194	0.3999	0.23646	0.66365	1.2893	0.367	0.73566	0.95037	0.94958	-0.075
401.346_6.34	0.653	0.97201	0.99508	-0.0071	0.39428	0.79065	1.2974	0.3757	0.39346	0.9855	1.5571	0.6389	0.093377	0.63788	3.2819	1.715	0.72644	0.94956	0.58042	-0.785
400.3427_6.34	0.65515	0.97385	0.99164	-0.0121	0.42205	0.80142	1.2572	0.3303	0.39612	0.9855	1.5213	0.6053	0.08678	0.62698	3.2021	1.679	0.68607	0.94956	0.57718	-0.793
308.2646_7.03	0.031012	0.97009	0.6404	-0.643	0.90252	0.96215	0.67579	-0.5653	0.66325	0.9855	0.88387	-0.1781	0.22876	0.66365	0.36907	-1.438	0.46215	0.94956	1.3325	0.414
324.0929_0.43	0.79111	0.98029	0.95573	-0.0653	0.12084	0.32434	1.6434	0.7167	0.43503	0.79709	1.2206	0.2876	0.00325	0.68829	3.2002	1.678	0.80955	0.89773	1.0166	0.024
139.0507_0.44	0.12244	0.97009	0.86714	-0.2057	0.97994	0.99281	1.0001	8E-05	0.61854	0.9855	1.0994	0.1367	0.31637	0.6878	1.1868	0.247	0.66261	0.94956	0.91202	-0.133
322.9936_0.61	0.30674	0.97009	0.78067	-0.3572	0.087354	0.65101	2.2904	1.1956	0.66101	0.9855	0.94818	-0.0768	0.02711	0.61039	3.7996	1.926	0.41304	0.94956	1.967	0.976
339.9919_0.53	0.21858	0.98029	0.65767	-0.6046	0.098783	0.3087	2.3876	1.2556	0.54939	0.84695	0.78262	-0.3536	0.05801	0.69603	2.7229	1.445	0.29206	0.71979	2.3456	1.23
338.9882_0.53	0.3071	0.98029	0.7286	-0.4568	0.12895	0.33575	2.2017	1.1386	0.57575	0.85797	0.82041	-0.2856	0.069391	0.69603	2.8089	1.49	0.24869	0.71979	2.0743	1.053
378.96_0.53	0.15094	0.97009	0.6908	-0.5337	0.14106	0.66086	2.0637	1.0452	0.82314	0.9855	0.97815	-0.0319	0.044407	0.61039	3.3617	1.749	0.37896	0.94956	2.008	1.006
362.9868_0.53	0.15831	0.97009	0.618	-0.6943	0.16344	0.6851	1.8851	0.9146	0.94572	0.99005	1.0883	0.1221	0.03491	0.61039	3.8745	1.954	0.37757	0.94956	1.7796	0.832
112.0399_0.46	0.23361	0.98029	0.62467	-0.6788	0.012563	0.29355	2.2403	1.1637	0.097692	0.67289	0.60858	-0.7165	0.028156	0.69603	2.1637	1.114	0.30102	0.71979	1.5984	0.677
318.2506_7.47	0.47494	0.97009	1.4061	0.4917	0.35702	0.77469	1.1945	0.2565	0.48615	0.9855	0.86386	-0.2111	0.91175	0.96347	0.69494	-0.525	0.22624	0.94956	1.7807	0.832
508.3766_7.01	0.82469	0.99411	0.93658	-0.0945	0.036983	0.60576	1.5424	0.6252	0.78359	0.9855	0.97713	-0.0334	0.60379	0.81677	0.89611	-0.158	0.13391	0.94956	1.3104	0.39
509.3751_7.6	0.95778	0.99411	1.0005	0.0006	0.040534	0.60576	1.4453	0.5314	0.64017	0.9855	1.1302	0.1766	0.0481	0.61039	1.6374	0.711	0.60654	0.94956	0.85279	-0.23
509.3802_7.01	0.89907	0.99411	0.94817	-0.0768	0.042238	0.60576	1.5747	0.6551	0.83255	0.9855	0.98484	-0.022	0.5829	0.80795	0.88028	-0.184	0.16375	0.94956	1.3089	0.388
508.3763_7.6	0.87906	0.99411	1.0403	0.057	0.12519	0.65101	1.4065	0.4921	0.68253	0.9855	1.0903	0.1248	0.31394	0.6878	1.3758	0.46	0.55738	0.94956	0.7847	-0.35
532.3733_7.62	0.75638	0.99411	1.0224	0.0319	0.052684	0.62891	1.8009	0.8487	0.13852	0.9855	0.70888	-0.4964	0.02577	0.61039	2.3823	1.252	0.86719	0.97158	0.9821	-0.026
321.2434_6.99	0.94251	0.99411	1.0136	0.0194	0.056475	0.62891	2.1234	1.0864	0.12509	0.9855	0.5977	-0.7425	0.35415	0.71258	1.5314	0.615	0.732	0.94956	1.0214	0.031
265.2166_4.55	0.076534	0.97009	0.53016	-0.9155	0.16865	0.68809	1.7627	0.8178	0.42592	0.9855	0.72274	-0.4685	0.71691	0.87441	0.92255	-0.116	0.38801	0.94956	1.7963	0.845
648.8542_11.89	0.78638	0.98029	0.90544	-0.1433	0.1053	0.31322	1.5374	0.6205	0.20079	0.67724	0.8323	-0.2648	0.17519	0.69603	1.622	0.698	0.57765	0.759	1.1849	0.245
127.0503_0.4	0.57051	0.98029	0.88924	-0.1694	0.051665	0.29355	1.9488	0.9626	0.38937	0.78569	0.77356	-0.3704	0.34758	0.76818	1.5269	0.611	0.18932	0.71979	1.838	0.878
102.0555_0.42	0.51084	0.98029	0.83265	-0.2642	0.16064	0.3682	1.3951	0.4804	0.43716	0.79709	0.86842	-0.2035	0.32239	0.75581	1.3869	0.472	0.29728	0.71979	1.5429	0.626
363.2151_6.43	0.020869	0.98029	0.63344	-0.6587	0.54743	0.64439	1.1314	0.1781	0.20787	0.67724	0.65117	-0.6189	0.86913	0.98606	1.0279	0.04	0.60524	0.77193	0.95209	-0.071
373.2352_6.96	0.19776	0.97009	2.2334	1.1593	0.55677	0.86034	0.94	-0.0893	0.42615	0.9855	0.83513	-0.2599	0.96553	0.98718	0.7734	-0.371	0.94987	0.98527	0.93885	-0.091
317.2481_7.47	0.60003	0.97009	1.3142	0.3942	0.32276	0.755	1.2811	0.3574	0.37604	0.9855	0.81815	-0.2896	0.8569	0.94232	0.73984	-0.435	0.23072	0.94956	1.7458	0.804
319.2643_7.71	0.97278	0.99638	1.096	0.1322	0.43384	0.81	0.97631	-0.0346	0.45207	0.9855	0.80817	-0.3073	0.96067	0.98574	0.55996	-0.837	0.38522	0.94956	1.3544	0.438
334.21_4.56	0.049666	0.98029	0.37186	-1.4272	0.18444	0.38256	2.0852	1.0602	0.38209	0.78311	0.57791	-0.7911	0.5771	0.85694	1.116	0.158	0.17252	0.71979	2.7504	1.46
315.1961_4.56	0.048463	0.98029	0.37905	-1.3995	0.20835	0.39169	1.949	0.9627	0.47891	0.81373	0.63772	-0.649	0.5439	0.84009	1.1516	0.204	0.17051	0.71979	2.5722	1.363
393.2274_4.54	0.042181	0.98029	0.50221	-0.9936	0.35683	0.49765	1.3013	0.3799	0.66966	0.90095	0.86424	-0.2105	0.4974	0.83023	1.3107	0.39	0.40072	0.71979	1.8864	0.916
299.2013_4.56	0.051004	0.97009	0.47878	-1.0626	0.21356	0.69627	1.6693	0.7393	0.44867	0.9855	0.71691	-0.4801	0.68077	0.85975	0.91	-0.136	0.36126	0.94956	1.7822	0.834
336.2258_4.56	0.072585	0.97009	0.51425	-0.9595	0.2616	0.7252	1.5428	0.6256	0.60801	0.9855	0.79212	-0.3362	0.71187	0.87189	0.86469	-0.21	0.33878	0.94956	1.8113	0.857
377.23_4.49	0.25622	0.97009	0.76112	-0.3938	0.07248	0.63469	2.0402	1.0287	0.11918	0.9855	0.66606	-0.5863	0.90796	0.96155	0.86936	-0.202	0.72534	0.94956	1.483	0.569
369.2277_4.38	0.23878	0.98029	0.62402	-0.6803	0.16364	0.36973	1.6459	0.7189	0.023292	0.67289	0.59927	-0.7387	0.93603	0.99216	0.89858	-0.154	0.31011	0.71979	2.0146	1.011
319.2266_4.49	0.29263	0.97009	0.76192	-0.3923	0.17401	0.69337	1.5164	0.6006	0.20522	0.9855	0.71316	-0.4877	0.83102	0.9349	0.81604	-0.293	0.33897	0.94956	1.8241	0.867
377.2304_4.91	0.71854	0.98447	1.1172	0.1599	0.19487	0.69604	1.4947	0.5799	0.010893	0.9855	0.54227	-0.8829	0.76583	0.9043	0.89566	-0.159	0.66228	0.94956	1.2119	0.277
353.2325_4.92	0.98143	0.99995	1.0301	0.0428	0.59836	0.68126	0.97195	-0.0411	0.046449	0.67289	0.63937	-0.6453	0.7527	0.94439	0.80459	-0.314	0.59456	0.76673	1.646	0.719
393.2254_4.34	0.92185	0.99411	0.94712	-0.0784	0.04292	0.60576	2.1329	1.0928	0.012817	0.9855	0.60193	-0.7323	0.38757	0.72805	0.75134	-0.412	0.98309	0.99297	1.0675	0.094
351.2171_4.56	0.048981	0.98029	0.38447	-1.3791	0.19851	0.38922	2.0136	1.0098	0.42798	0.79709	0.58842	-0.7651	0.5321	0.84009	1.1308	0.177	0.17807	0.71979	2.6278	1.394
393.2255_3.93	0.58429	0.97009	0.72015	-0.4736	0.2151	0.69627	1.8655	0.8996	0.51599	0.9855	0.72257	-0.4688	0.48146	0.77413	1.3867	0.472	0.63331	0.94956	0.67665	-0.564

378.2409_5.91	C06124, Sphingosine 1-phosphate	0.019951	0.30518	1.6992 ↑	0.76488	0.95402	0.99953	1.0954 ↑	0.1315	4.35E-05	0.049133	3.3813 ↑	1.758	0.30497	0.98029	0.8678 ↓	-0.2046	0.000935	0.29355	4.1235 ↑	2.0439	0.10767	0.67289	0.55226 ↓	-0.8566	0.003194	0.68829	2.0052 ↑	1.004	0.6542	0.80307	0.98257 ↓	-0.025
370.0536_0.43	C06376, N-Acetyl-D-galactosamine 6-phosphate	0.46884	0.77455	1.2015 ↑	0.26489	0.82897	0.99977	0.91359 ↓	-0.1304	0.29877	0.63766	1.1705 ↑	0.227	0.84247	0.99411	0.98515 ↓	-0.0216	0.47687	0.83145	1.1097 ↑	0.1502	0.96725	0.99454	1.0626 ↑	0.0877	0.49173	0.77672	0.86335 ↓	-0.212	0.16807	0.94956	1.407 ↑	0.493
258.0404_1.33	C06377, D-Galactosamine 6-phosphate	0.050749	0.30518	1.8671 ↑	0.90077	0.41058	0.99953	0.74563 ↓	-0.4235	0.048816	0.43922	1.65 ↑	0.722	0.25024	0.98029	0.72988 ↓	-0.4543	0.066256	0.29355	1.73 ↑	0.7908	0.287	0.73016	0.74206 ↓	-0.4304	0.31315	0.75139	1.3103 ↑	0.39	0.075814	0.71979	1.8083 ↑	0.855
243.2107_6.43	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	0.86218	0.95256	0.58717 ↓	-0.76816	0.29209	0.99977	0.80184 ↓	-0.3186	0.94861	0.98736	0.70064 ↓	-0.513	0.02508	0.97009	0.54875 ↓	-0.8658	0.79256	0.93743	0.84877 ↓	-0.2366	0.30608	0.9855	0.68702 ↓	-0.5416	0.55064	0.79627	0.57543 ↓	-0.797	0.72626	0.94956	0.93978 ↓	-0.09
261.2217_6.43	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	0.91407	0.97254	0.59249 ↓	-0.75514	0.29034	0.99977	0.80752 ↓	-0.3084	0.94477	0.98564	0.69361 ↓	-0.528	0.041405	0.97009	0.57785 ↓	-0.7912	0.80338	0.94099	0.83189 ↓	-0.2655	0.3884	0.9855	0.72707 ↓	-0.4598	0.63083	0.83033	0.61054 ↓	-0.712	0.8335	0.96811	0.85838 ↓	-0.22
280.2353_6.43	C06426, (6Z,9Z,12Z)-Octadecatrienoic acid	0.8967	0.9667	0.62899 ↓	-0.66889	0.30826	0.99977	0.81897 ↓	-0.2881	0.96298	0.99148	0.72171 ↓	-0.471	0.043055	0.97009	0.58829 ↓	-0.7654	0.80483	0.94099	0.86909 ↓	-0.2024	0.37823	0.9855	0.72106 ↓	-0.4718	0.62306	0.82713	0.6322 ↓	-0.662	0.81127	0.96615	0.89953 ↓	-0.153
243.0201_12.07	C07047, Ifosfamide	0.26664	0.61297	1.1354 ↑	0.1832	0.84604	0.99977	1.0131 ↑	0.0188	0.086264	0.46444	1.1654 ↑	0.221	0.94427	0.99411	0.99771 ↓	-0.0033	0.065576	0.62891	1.141 ↑	0.1903	0.97185	0.99454	0.99728 ↓	-0.0039	0.002669	0.4653	1.2422 ↑	0.313	0.1817	0.94956	0.89796 ↓	-0.155
466.2522_4.66	C11135, Androsterone glucuronide	0.021356	0.30518	5.5478 ↑	2.4719	0.30177	0.99953	0.55229 ↓	-0.8565	0.020964	0.43922	4.1664 ↑	2.059	0.3013	0.98029	2.2735 ↑	1.1849	0.017982	0.29355	8.7063 ↑	3.1221	0.26867	0.71927	0.49967 ↓	-1.0009	0.02113	0.69603	11.636 ↑	3.541	0.92593	0.96734	0.7964 ↓	-0.328
465.2489_4.66	C11135, Androsterone glucuronide	0.027233	0.30518	5.09 ↑	2.3477	0.34697	0.99953	0.63535 ↓	-0.6544	0.025873	0.43922	4.0549 ↑	2.02	0.27021	0.98029	2.7463 ↑	1.4575	0.023821	0.29355	7.916 ↑	2.9848	0.25844	0.71096	0.51762 ↓	-0.95	0.023787	0.69603	10.761 ↑	3.428	0.93679	0.97295	0.79817 ↓	-0.325
300.2904_5.77	C12144, Phytosphingosine	0.77496	0.91954	1.0456 ↑	0.064328	0.77414	0.99977	1.1449 ↑	0.1953	0.001864	0.19996	2.4658 ↑	1.302	0.81371	0.99411	1.0291 ↑	0.0414	0.053327	0.62891	1.6125 ↑	0.6893	0.64869	0.9855	1.2156 ↑	0.2817	0.023298	0.61039	1.8338 ↑	0.875	0.36465	0.94956	0.75155 ↓	-0.412
282.2798_5.77	C12144, Phytosphingosine	0.70622	0.89277	1.066 ↑	0.092199	0.82218	0.99977	1.116 ↑	0.1583	0.001222	0.19996	2.3789 ↑	1.25	0.91109	0.99411	1.0087 ↑	0.0125	0.053645	0.62891	1.5757 ↑	0.656	0.67569	0.9855	1.1765 ↑	0.2345	0.022008	0.61039	1.8121 ↑	0.858	0.36775	0.94956	0.75909 ↓	-0.398
318.3004_5.6	C12144, Phytosphingosine	0.75641	0.91225	1.1269 ↑	0.17238	0.73352	0.99977	1.2819 ↑	0.3583	0.010425	0.27494	2.2969 ↑	1.2	0.63722	0.97009	1.1533 ↑	0.2058	0.10673	0.65101	1.5234 ↑	0.6073	0.43093	0.9855	1.3813 ↑	0.4661	0.18074	0.6618	2.1248 ↑	1.087	0.61621	0.94956	0.67549 ↓	-0.566
380.2901_7.52	C13856, 2-Arachidonoylglycerol	0.52476	0.80332	1.1894 ↑	0.2502	0.79463	0.99977	1.0794 ↑	0.1103	0.004926	0.23589	1.9825 ↑	0.987	0.093711	0.97009	0.68844 ↓	-0.5386	0.11574	0.65101	1.4507 ↑	0.5368	0.87838	0.9855	1.0647 ↑	0.0905	0.51178	0.78062	1.4159 ↑	0.502	0.38623	0.94956	1.252 ↑	0.324
379.2847_7.53	C13856, 2-Arachidonoylglycerol	0.63933	0.85893	1.1689 ↑	0.2252	0.78281	0.99977	1.0521 ↑	0.0732	0.015033	0.28672	1.7844 ↑	0.835	0.25845	0.97009	0.7754 ↓	-0.367	0.19806	0.69627	1.3398 ↑	0.422	0.62027	0.9855	1.1752 ↑	0.2329	0.63901	0.83404	1.3252 ↑	0.406	0.35722	0.94956	1.2702 ↑	0.345
401.2672_7.53	C13856, 2-Arachidonoylglycerol	0.64122	0.85893	1.1809 ↑	0.23989	0.76708	0.99977	1.0421 ↑	0.0595	0.002666	0.19996	1.8121 ↑	0.858	0.077098	0.97009	0.75642 ↓	-0.4027	0.29723	0.74539	1.2371 ↑	0.307	0.43508	0.9855	1.2706 ↑	0.3455	0.46197	0.76952	1.2977 ↑	0.376	0.40746	0.94956	1.1829 ↑	0.242
361.2745_7.29	C13856, 2-Arachidonoylglycerol	0.054424	0.45103	1.6246 ↑	0.70008	0.86638	0.99977	0.9957 ↓	-0.0062	0.010457	0.27494	1.9052 ↑	0.93	0.96258	0.99411	1.1183 ↑	0.1614	0.44185	0.81508	1.2197 ↑	0.2866	0.52514	0.9855	0.84352 ↓	-0.2455	0.58273	0.80795	1.1454 ↑	0.196	0.15744	0.94956	1.3597 ↑	0.443
319.2274_6.69	C14779, 9(S)-HETE	0.31611	0.50232	1.5263 ↑	0.61004	0.99292	0.99953	0.91546 ↓	-0.1274	0.55088	0.69243	1.0345 ↑	0.049	0.94189	0.99957	0.95163 ↓	-0.0715	0.30307	0.47041	1.4487 ↑	0.5348	0.37466	0.77809	0.82865 ↓	-0.2712	0.92912	0.99216	1.0919 ↑	0.127	0.32425	0.71979	1.5292 ↑	0.613
373.2156_7.86	C15492, all-trans-13,14-Dihydroretinol	0.15681	0.53491	1.5729 ↑	0.65339	0.93228	0.99977	0.93768 ↓	-0.0928	0.22671	0.58504	1.3785 ↑	0.463	0.62023	0.97009	1.0918 ↑	0.1267	0.65832	0.89744	1.0337 ↑	0.0479	0.79413	0.9855	0.94788 ↓	-0.0772	0.27323	0.67908	2.0862 ↑	1.061	0.48332	0.94956	0.51952 ↓	-0.945
311.236_7.86	C15492, all-trans-13,14-Dihydroretinol	0.20757	0.57649	1.4232 ↑	0.50914	0.82446	0.99977	0.94154 ↓	-0.0869	0.26761	0.61517	1.348 ↑	0.431	0.91986	0.99411	0.9551 ↓	-0.0663	0.77474	0.9316	0.93214 ↓	-0.1014	0.48673	0.9855	0.9328 ↓	-0.1004	0.1836	0.6618	2.1546 ↑	1.108	0.42288	0.94956	0.5422 ↓	-0.883
250.0914_0.43	C16255, [Dihydrolipoyllysine-residue acetyltransferase] S-acetyldihydrolipoyllysine	0.047986	0.45103	1.5751 ↑	0.65544	0.89935	0.99977	1.028 ↑	0.0399	0.071859	0.43187	1.5436 ↑	0.626	0.6205	0.97009	0.92328 ↓	-0.1152	0.33811	0.76538	1.2193 ↑	0.286	0.78147	0.9855	1.0376 ↑	0.0533	0.39797	0.73982	1.3011 ↑	0.38	0.44261	0.94956	1.2252 ↑	0.293
259.2051_7.97	C16300, Stearidonic acid	0.096834	0.46342	1.4649 ↑	0.55081	0.91863	0.99977	0.97695 ↓	-0.0336	0.16867	0.52533	1.4012 ↑	0.487	0.84232	0.99411	1.029 ↑	0.0413	0.30727	0.75014	1.2368 ↑	0.3067	0.38949	0.9855	0.8811 ↓	-0.1826	0.21111	0.66365	1.6085 ↑	0.686	0.59416	0.94956	0.7568 ↓	-0.402
278.2202_6.11	C16300, Stearidonic acid	0.27934	0.62696	0.1921 ↓	-2.3801	0.27058	0.99977	0.79443 ↓	-0.332	0.35871	0.69056	0.2224 ↓	-2.169	0.045935	0.97009	0.66817 ↓	-0.5817	0.5671	0.86511	0.29121 ↓	-1.7799	0.38884	0.9855	0.7095 ↓	-0.4951	0.12114	0.6618	0.13151 ↓	-2.927	0.88182	0.97478	1.041 ↑	0.058
277.2169_6.11	C16300, Stearidonic acid	0.32647	0.65829	0.21018 ↓	-2.2503	0.42011	0.99977	0.83173 ↓	-0.2658	0.42045	0.73205	0.24265 ↓	-2.043	0.004346	0.97009	0.6577 ↓	-0.6045	0.62447	0.88463	0.31681 ↓	-1.6583	0.40998	0.9855	0.71467 ↓	-0.4847	0.128	0.6618	0.13254 ↓	-2.916	0.80274	0.96615	1.1762 ↑	0.234
164.0719_0.62	C16591, 3-Carbamoyl-2-phenylpropionic acid	0.05336	0.45103	2.0301 ↑	1.0215	0.59659	0.99977	0.7981 ↓	-0.3254	0.037027	0.33592	1.7497 ↑	0.807	0.74639	0.99411	2.3661 ↑	1.2425	0.25985	0.72495	2.0595 ↑	1.0423	0.97982	0.99454	0.87444 ↓	-0.1936	0.026165	0.61039	7.3106 ↑	2.87	0.188	0.94956	5.1259 ↑	2.358
192.0658_0.62	C16591, 3-Carbamoyl-2-phenylpropionic acid	0.082804	0.45103	2.0673 ↑	1.0478	0.55268	0.99977	0.73414 ↓	-0.4459	0.050633	0.38975	1.7616 ↑	0.817	0.22799	0.97009	0.73865 ↓	-0.437	0.36647	0.77865	1.8675 ↑	0.9012	0.81676	0.9855	0.98538 ↓	-0.0212	0.044475	0.61039	1.9118 ↑	0.935	0.16821	0.94956	1.6024 ↑	0.68
305.2482_7.97	CE1754, 9-cis-retinol	0.080211	0.45103	1.4644 ↑	0.55029	0.83495	0.99977	0.9721 ↓	-0.0408	0.15776	0.5222	1.3879 ↑	0.473	0.81639	0.99411	1.0236 ↑	0.0336	0.28841	0.73856	1.235 ↑	0.3045	0.34061	0.9855	0.88158 ↓	-0.1818	0.19947	0.66323	1.4227 ↑	0.509	0.65094	0.94956	0.86081 ↓	-0.216
431.3153_6.28	CE2203, 25-hydroxyvitamin D3-26,23-lactol	0.10091	0.46736	1.8264 ↑	0.869	0.71709	0.99977	0.79859 ↓	-0.3245	0.16318	0.52463	1.6738 ↑	0.743	0.57577	0.97009	1.1734 ↑	0.2307	0.15308	0.67783	1.8729 ↑	0.9053	0.51001	0.9855	0.68301 ↓	-0.55	0.1062	0.64857	2.6908 ↑	1.428	0.85839	0.97128	0.68585 ↓	-0.544
334.2829_8.43	CE2414, (3S,7R,11R)-phytanate	0.43095	0.74852	1.1291 ↑	0.17516	0.82618	0.99977	1.0578 ↑	0.0811	0.51056	0.80593	1.1834 ↑	0.243	0.61672	0.97009	1.1121 ↑	0.1533	0.88317	0.95726	0.95423 ↓	-0.0676	0.64605	0.9855	1.1443 ↑	0.1944	0.31738	0.6878	1.3834 ↑	0.468	0.39642	0.94956	0.72797 ↓	-0.458
367.2252_6.62	CE2961, 4-hydroxy-all-trans-retinyl acetate	0.16991	0.54848	1.6138 ↑	0.69049	0.88015	0.99977	0.9492 ↓	-0.0752	0.28992	0.62986	1.3633 ↑	0.447	0.74307	0.99411	0.92573 ↓	-0.1113	0.31325	0.7514	1.3756 ↑	0.4601	0.80414	0.9855	1.0806 ↑	0.1118	0.46145	0.76936	1.4961 ↑	0.581	0.56603	0.94956	1.0807 ↑	0.112
309.2224_6.63	CE2961, 4-hydroxy-all-trans-retinyl acetate	0.24879	0.59552	1.4325 ↑	0.51852	0.89685	0.99977	0.95081 ↓	-0.0728	0.28434	0.62653	1.4255 ↑	0.511	0.86732	0.99411	0.92338 ↓	-0.115	0.32629	0.75628	1.344 ↑	0.4266	0.707	0.9855	1.1842 ↑	0.244	0.36686	0.71669	1.586 ↑	0.665	0.65714	0.94956	1.056 ↑	0.079
327.2325_6.63	CE2961, 4-hydroxy-all-trans-retinyl acetate	0.20263	0.57466	1.5413 ↑	0.62415	0.86009	0.99977	0.93199 ↓	-0.1016	0.34042	0.67598	1.2779 ↑	0.354	0.92164	0.99411	0.9965 ↓	-0.0051	0.35869	0.77469	1.2943 ↑	0.3722	0.59496	0.9855	1.161 ↑	0.2154	0.44047	0.76276	1.4662 ↑	0.552	0.62115	0.94956	1.0307 ↑	0.044
298.9941_0.46	CE3075, sorbitol 3-phosphate	0.30089	0.64213	1.6067 ↑	0.68413	0.97252	0.99977	0.93071 ↓	-0.1036	0.75886	0.92099	1.0245 ↑	0.035	0.67554	0.97801	0.87325 ↓	-0.1955	0.42016	0.80142	1.1908 ↑	0.2519	0.44753	0.9855	1.2096 ↑	0.2746	0.27445	0.67943	1.4101 ↑	0.496	0.56217	0.94956	1.2499 ↑	0.322
285.2219_7.49	CE5013,	0.45313	0.76641	1.1895 ↑	0.25033	0.93127	0.99977	0.95858 ↓	-0.061	0.43969	0.75109	1.1115 ↑	0.153	0.66302	0.97393	1.1686 ↑	0.2248	0.49417	0.84075	1.0998 ↑	0.1373	0.50011	0.9855	0.88696 ↓	-0.1731	0.53994	0.79346	1.0191 ↑	0.027	0.49629	0.94956	1.2052 ↑	0.269
269.2271_7.96	CE5014, anhydroretinol	0.12452	0.51134	1.3544 ↑	0.43765	0.47556	0.99977	0.92278 ↓	-0.116	0.16768	0.52533	1.3654 ↑	0.449	0.99609	0.99964	0.98811 ↓	-0.0173	0.41963	0.80142	1.1461 ↑	0.1967	0.61447	0.9855	0.94123 ↓	-0.0874	0.41266	0.74728	1.2986 ↑	0.377	0.71114	0.94956	0.84264 ↓	-0.247
270.2308_7.96	CE5014, anhydroretinol	0.12953	0.51134	1.3769 ↑	0.46144	0.47388	0.99977	0.903 ↓	-0.1472	0.23832	0.5914	1.3849 ↑	0.47	0.71575	0.98389	1.0369 ↑	0.0523	0.49051	0.83908	1.1155 ↑	0.1577	0.66683	0.9855	0.95222 ↓	-0.0706	0.31385	0.6878	1.3455 ↑	0.428	0.41194	0.94956	0.75805 ↓	-0.4
350.2108_7.96	CE5138, 12-oxo-20-hydroxy-leukotriene B4	0.070723	0.45103	1.4567 ↑	0.54268	0.6791	0.99977	0.95048 ↓	-0.0733	0.2604	0.60892	1.2637 ↑	0.338	0.7732	0.99411	1.0672 ↑	0.0939	0.44501	0.81646	1.1262 ↑	0.1714	0.44007	0.9855	0.87261 ↓	-0.1966	0.45431	0.76806	1.2894 ↑	0.367	0.70104	0.94956	0.82876 ↓	-0.271
222.1618_7.97	CE5325, 6(S)-hydroxy-tetradeca-4E,8Z-dienoate	0.036385	0.45103	1.5569 ↑	0.63871	0.5683	0.99977	0.93505 ↓	-0.0969	0.15673	0.5222	1.4045 ↑	0.49	0.55743	0.97009	1.0809 ↑	0.1122	0.32279	0.755	1.1946 ↑	0.2565	0.63321	0.9855	0.94081 ↓	-0.088	0.10496	0.64857	1.5495 ↑	0.632	0.4675	0.94956	0.81017 ↓	-0.304
455.2969_6.64	CE5560, glycolithocholate	0.049956	0.45103	0.71797 ↓	-0.47801	0.56351	0.99977	0.84823 ↓	-0.2375	0.015902	0.28672	0.74575 ↓	-0.423	0.18588	0.97009	1.3254 ↑	0.4064	0.003876	0.54972	0.6779 ↓	-0.5609	0.25973	0.9855	1.132 ↑	0.1789	0.77961	0.90988	0.97774 ↓	-0.032	0.18732	0.94956	0.73052 ↓	-0.453
376.2186_4.56	CE5828,	0.077074	0.45103	1.8049 ↑	0.85195	0.56162	0.99977	0.89723 ↓	-0.1564	0.065583	0.41724	1.8734 ↑	0.906	0.044592	0.97009	0.45939 ↓	-1.1222	0.2577	0.72495	1.5358 ↑	0.619	0.53037	0.9855	0.79566 ↓	-0.3298	0.94529	0.97884	0.81372 ↓	-0.297	0.74705	0.95329	1.3748 ↑	0.459
429.3726_9.7	CE5835,	0.38746	0.71087	1.259 ↑	0.33222	0.098028	0.99977	1.8279 ↑	0.8702	0.026609	0.30434	2.5464 ↑	1.348	0.40128	0.97009	0.71151 ↓	-0.491	0.53967	0.85588	1.1939 ↑	0.2557	0.3767	0.9855	1.2867 ↑	0.3637	0.013822	0.61039	3.6787 ↑	1.879	0.2375	0.94956	0.51588 ↓	-0.955
445.3682_9.77	CE5838,	0.70558	0.89273	1.0413 ↑	0.058404	0.37118	0.99977	1.1814 ↑	0.2405	0.024489	0.30434	1.6699 ↑	0.74	0.73983	0.99403	0.93218 ↓	-0.1013	0.046532	0.60576	1.525 ↑	0.6088	0.62483	0.9855	1.0739 ↑	0.1029	0.12287	0.6618	1.6448 ↑	0.718	0.12776	0.94956	0.49239 ↓	-1.022
139.112_8.06	CE6506,	0.90108	0.96794	0.94943 ↓	-0.074867	0.72263	0.99977	0.96926 ↓	-0.0451	0.99073	0.99567	1.0133 ↑	0.019	0.80637	0.99411	0.90563 ↓	-0.143	0.94365	0.98163	0.95315 ↓	-0.0692	0.77247	0.9855	0.97565 ↓	-0.0356	0.83826	0.93728	1.0025 ↑	0.004	0.63681	0.94956	0.9495 ↓	-0.075
441.3402_5.63	CE7144, 13'-hydroxy-alpha-tocotrienol	0.15136	0.52961	0.57371 ↓	-0.80161	0.15106	0.99977	1.7881 ↑	0.8384	0.038953	0.34374	2.4488 ↑	1.292	0.27454	0.97009	0.67517 ↓	-0.5667	0.17188	0.69251	0.52434 ↓	-0.9314	0.70342	0.9855	1.6533 ↑	0.7253	0.47458	0.77066	2.5819 ↑	1.369	0.58217	0.94956	0.41396 ↓	-1.272
399.3301_5.99	hdd2crn, trans-Hexadec-2-enoyl carnitine	0.44448	0.76227	1.5765 ↑	0.65675	0.3106	0.99977	1.3274 ↑	0.4086	0.027143	0.30434	2.5913 ↑	1.374	0.38014	0.97009	1.0245 ↑	0.035	0.31519	0.7514	1.3875 ↑	0.4725	0.54474	0.9855	1.7189 ↑	0.7815	0.1296	0.6618	3.9348 ↑	1.976	0.92202	0.98109	0.67884 ↓	-0.559
398.327_5.99	hdd2crn, trans-Hexadec-2-enoyl carnitine	0.43858	0.75633	1.5464 ↑	0.6289	0.30132	0.99977	1.2978 ↑	0.3761	0.029492	0.30434	2.5091 ↑	1.327	0.37186	0.97009	0.9704 ↓	-0.0434	0.31681	0.7514	1.3757 ↑	0.4601	0.59792	0.9855	1.6906 ↑	0.7576	0.12743	0.6618	3.5878 ↑	1.843	0.90007	0.97499	0.72196 ↓	-0.47
414.3585_6.57	hpdcacrn, heptadecanoyl carnitine	0.30085	0.64213	1.758 ↑	0.81396	0.61642	0.99977	1.0179 ↑	0.0256	0.033241	0.31729	2.7757 ↑	1.473	0.64833	0.97009	0.86484 ↓	-0.2095	0.8401	0.94564	1.0254 ↑	0.0362	0.26852	0.9855	1.7091 ↑	0.7733	0.075516	0.61256	2.9602 ↑	1.566	0.63862	0.94956	0.6105 ↓	-0.712
422.3273_5.9	lnlncacrn, alpha-linolenyl carnitine	0.78095	0.92215	0.85231 ↓	-0.23054	0.18225	0.99977	1.6211 ↑	0.697	0.035617	0.33041	2.4638 ↑	1.301	0.21757	0.97009	0.649 ↓	-0.6237	0.75584	0.92586	0.95943 ↓	-0.0598	0.64847	0.9855	2.221 ↑	1.1512	0.22795	0.66365	2.8127 ↑	1.492	0.87985	0.97468	0.61724 ↓	-0.696
279.2324_6.43	ocdcya, octadecadienoate (n-C18:2)	0.95255	0.98305	0.66002 ↓	-0.59941	0.27481	0.99977	0.81846 ↓	-0.289	0.9175	0.97805	0.74656 ↓	-0.422	0.037604	0.97009	0.61263 ↓	-0.7069	0.7785	0.9316	0.88483 ↓	-0.1765	0.33773	0.9855	0.72835 ↓	-0.4573	0.63205	0.83033	0.64598 ↓	-0.63	0.7535	0.95329	0.93035 ↓	-0.104
446.3263_6.11	tmndnccrn, Timnodonyl carnitine	0.66032	0.86881	1.121 ↑	0.16479	0.35434	0.99977	1.2022 ↑	0.2656	0.012969	0.28672	1.8089 ↑	0.855	0.44514	0.97009	0.89449 ↓	-0.1609	0.75438	0.92586	1.027 ↑	0.0385	0.52808	0.9855	1.297 ↑	0.3752	0.13263	0.6618	2.1475 ↑	1.103	0.56199	0.94956	0.63822 ↓	-0.648
372.3119_5.83	ttdcrn, tetradecanoyl carnitine	0.19755	0.56946	1.9553 ↑	0.96741	0.38194	0.99977	1.1933 ↑	0.255	0.030619	0.30434	2.3236 ↑	1.216	0.50284	0.97009	1.0613 ↑	0.0859	0.47618	0.83145	1.2925 ↑	0.3702	0.57851	0.9855	1.3919 ↑	0.4771	0.12189	0.6618	3.9816 ↑	1.993	0.93798	0.98244	0.60784 ↓	-0.718
373.3144_5.83	ttdcrn, tetradecanoyl carnitine	0.17488	0.55572	2.0511 ↑	1.0364	0.38667	0.99977	1.1935 ↑	0.2552	0.029959	0.30434	2.3631 ↑	1.241	0.55366	0.97009	1.1192 ↑	0.1625	0.53979	0.85588	1.3062 ↑	0.3854	0.60738	0.9855	1.4034 ↑	0.4889	0.14367	0.6618	4.3726 ↑	2.129	0.96625	0.98877	0.57609 ↓	-0.796
394.2951_5.5	ttdcrn, tetradecanoyl carnitine	0.36017	0.68947	1.3404 ↑	0.42268	0.36284	0.99977	1.2409 ↑	0.3114	0.014581	0.28672	2.4048 ↑	1.266	0.2475	0.97009	0.71839 ↓	-0.4772	0.69316	0.90602	0.99275 ↓	-0.0105	0.74117	0.9855	1.4596 ↑	0.5456	0.10571	0.64857	2.3116 ↑	1.209	0.85022	0.96957	0.80466 ↓	-0.314
427.3616_6.45	vacccrn, Vaccenyl carnitine	0.94449	0.98305	0.99103 ↓	-0.013006	0.35988	0.99977	1.2703 ↑	0.3452	0.024445	0.30434	2.3651 ↑	1.242	0.18491	0.97009	0.62911 ↓	-0.6686	0.1201	0.65101	1.8296 ↑	0.8716	0.57767	0.9855	1.7207 ↑	0.783	0.077998	0.61256	2.9829 ↑	1.577	0.78628	0.96615	0.72404 ↓	-0.466
426.3582_6.45	vacccrn, Vaccenyl carnitine	0.92253	0.97651	1.0039 ↑	0.0055913	0.36859	0.99977	1.2494 ↑	0.3212	0.023889	0.30434	2.3057 ↑	1.205	0.18871	0.97009	0.63956 ↓	-0.6449	0.12134	0.65101	1.7866 ↑	0.8372	0.53856	0.9855	1.7595 ↑	0.8152	0.072129	0.61256	2.9718 ↑	1.571	0.75136	0.95329	0.71343 ↓	-0.487

Supplementary Table 6. Metabolomic pathway analysis results for the effects of radiation and GT3 treatment at SD30 in jejunum tissue. Analysis was performed with Mummichog software, version 2.06.

	Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3	
	PBI 4 Gy		PBI 4 Gy		TBI 4 Gy		TBI 4 Gy		PBI 5.8 Gy		PBI 5.8 Gy		TBI 5.8 Gy		TBI 5.8 Gy	
Pathway	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*
Aminosugars metabolism	-	-	-	-	-	-	-	-	2(7)	0.02604823	-	-	-	-	-	-
Androgen and estrogen biosynthesis and metabolism	-	-	-	-	-	-	-	-	-	-	-	-	1(3)	0.0227712	-	-
Arachidonic acid metabolism	-	-	-	-	5(15)	0.02789682	-	-	-	-	-	-	-	-	3(23)	0.02495589
Arginine and Proline Metabolism	-	-	3(4)	0.04092093	-	-	-	-	-	-	-	-	1(4)	0.03041761	-	-
Ascorbate (Vitamin C) and Aldarate Metabolism	-	-	4(5)	0.0053777	-	-	-	-	1(2)	0.02663642	-	-	-	-	-	-
Aspartate and asparagine metabolism	-	-	5(8)	0.03075372	-	-	-	-	-	-	-	-	1(8)	0.04982775	-	-
Bile acid biosynthesis	3(13)	2.70E-02	10(18)	0.00193261	6(13)	0.00378119	-	-	2(13)	0.02663642	-	-	-	-	-	-
Blood Group Biosynthesis	-	-	3(3)	0.01151164	-	-	-	-	1(1)	0.02335938	-	-	-	-	-	-
Butanoate metabolism	-	-	4(5)	0.0053777	-	-	-	-	-	-	-	-	1(4)	0.03041761	-	-
C21-steroid hormone biosynthesis and metabolism	-	-	-	-	4(10)	0.02226704	-	-	-	-	-	-	-	-	-	-
Carnitine shuttle	4(19)	0.01504075	10(19)	0.0025208	-	-	-	-	3(19)	0.04268549	-	-	-	-	-	-
Chondroitin sulfate degradation	1(1)	0.03150996	-	-	-	-	-	-	1(1)	0.01193177	-	-	-	-	-	-
De novo fatty acid biosynthesis	-	-	-	-	9(26)	0.00638602	-	-	-	-	-	-	-	-	3(26)	0.0313419
Dimethyl-branched-chain fatty acid mitochondrial beta-oxidation	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.00806655	-	-
Di-unsaturated fatty acid beta-oxidation	-	-	-	-	-	-	-	-	-	-	-	-	1(3)	0.0227712	-	-
Drug metabolism - other enzymes	-	-	2(2)	0.04041677	-	-	-	-	-	-	-	-	-	-	-	-
Fatty acid activation	-	-	-	-	9(25)	0.00495757	-	-	-	-	-	-	-	-	3(25)	0.0297454
Fatty Acid Metabolism	-	-	-	-	8(17)	0.00193261	-	-	-	-	-	-	-	-	2(17)	0.04789513
Fatty acid oxidation	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.00806655	-	-
Glutamate metabolism	-	-	2(3)	0.04571044	-	-	-	-	-	-	-	-	-	-	-	-
Glutathione Metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Glycerophospholipid metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4(25)	0.00613394
Glycine, serine, alanine and threonine metabolism	-	-	5(6)	0.00478951	-	-	-	-	-	-	-	-	1(6)	0.04100496	-	-
Glycosphingolipid biosynthesis - ganglioseries	-	-	3(3)	0.01151164	-	-	-	-	1(1)	0.02335938	-	-	-	-	-	-
Glycosphingolipid biosynthesis - globoseries	-	-	3(3)	0.01151164	-	-	-	-	1(1)	0.02335938	-	-	-	-	-	-
Glycosphingolipid biosynthesis - lactoseries	-	-	3(3)	0.01151164	-	-	-	-	1(1)	0.02335938	-	-	-	-	-	-
Glycosphingolipid biosynthesis - neolactoseries	-	-	3(3)	0.01151164	-	-	-	-	1(1)	0.02335938	-	-	-	-	-	-
Glycosphingolipid metabolism	5(15)	0.00151248	6(8)	5.55E-03	5(15)	0.0297454	-	-	-	-	-	-	1(8)	0.04982775	-	-
Glyoxylate and Dicarboxylate Metabolism	1(1)	0.03150996	-	-	-	-	-	-	1(1)	0.01193177	-	-	-	-	-	-
Heparan sulfate degradation	-	-	-	-	-	-	-	-	1(2)	0.02663642	-	-	-	-	-	-
Hyaluronan Metabolism	-	-	2(2)	0.01663726	-	-	-	-	1(2)	0.04386186	-	-	-	-	-	-
Keratan sulfate biosynthesis	-	-	2(2)	0.04041677	-	-	-	-	1(1)	0.02335938	-	-	-	-	-	-
Keratan sulfate degradation	-	-	-	-	-	-	-	-	1(1)	0.02335938	-	-	-	-	-	-
Linoleate metabolism	-	-	-	-	6(9)	5.04E-04	-	-	-	-	-	-	3(21)	0.01470465	-	-
Lysine metabolism	-	-	-	-	-	-	-	-	-	-	-	-	1(4)	0.03041761	-	-
Methionine and cysteine metabolism	-	-	5(8)	0.00731031	-	-	-	-	-	-	-	-	-	-	-	-
Mono-unsaturated fatty acid beta-oxidation	-	-	-	-	-	-	-	-	-	-	-	-	1(2)	0.01529283	-	-
N-Glycan biosynthesis	-	-	4(4)	0.0028569	-	-	-	-	1(2)	0.04386186	-	-	1(4)	0.03041761	-	-
N-Glycan Degradation	-	-	-	-	-	-	-	-	1(2)	0.04386186	-	-	-	-	-	-
O-Glycan biosynthesis	-	-	2(2)	0.04041677	-	-	-	-	1(1)	0.02335938	-	-	-	-	-	-
Omega-6 fatty acid metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1(3)	0.0363835
Pentose and Glucuronate Interconversions	2(2)	0.00361314	-	-	2(2)	1.23E-02	-	-	2(2)	3.36E-04	-	-	-	-	-	-
Pentose phosphate pathway	2(5)	0.02142677	-	-	-	-	-	-	2(5)	0.00596589	-	-	-	-	-	-
Phytanic acid peroxisomal oxidation	-	-	-	-	-	-	1(3)	0.01016721	-	-	-	-	-	-	1(3)	0.0363835
Propanoate metabolism	-	-	-	-	-	-	-	-	-	-	-	-	1(3)	0.0227712	-	-
Proteoglycan biosynthesis	-	-	2(2)	0.04041677	-	-	-	-	1(1)	0.02335938	-	-	-	-	-	-
Purine metabolism	-	-	5(11)	0.02672044	-	-	-	-	3(11)	0.00957903	-	-	2(11)	0.02478783	-	-
Pyrimidine metabolism	-	-	5(6)	0.00210066	-	-	1(7)	0.01478867	-	-	-	-	-	-	-	-
R Group Synthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.00806655	-	-
Saturated fatty acids beta-oxidation	3(6)	0.0025208	-	-	-	-	-	-	-	-	-	-	1(2)	0.01529283	-	-
Sialic acid metabolism	1(1)	0.02478783	-	-	-	-	1(1)	0.00327704	-	-	-	-	-	-	-	-
Squalene and cholesterol biosynthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(5)	0.0351231	-	-
Starch and Sucrose Metabolism	-	-	2(2)	0.04041677	-	-	-	-	-	-	-	-	-	-	-	-
TCA cycle	-	-	-	-	-	-	-	-	-	-	-	-	1(4)	0.03041761	-	-
Tryptophan metabolism	-	-	-	-	-	-	-	-	-	-	-	-	1(8)	0.04982775	-	-
Tyrosine metabolism	-	-	7(19)	0.04318965	-	-	-	-	-	-	-	-	-	-	-	-
Urea cycle/amino group metabolism	-	-	4(6)	0.03495505	-	-	-	-	-	-	-	-	1(6)	0.04100496	-	-
Valine, leucine and isoleucine degradation	-	-	3(4)	0.01319217	-	-	-	-	-	-	-	-	1(5)	0.0351231	-	-
Vitamin A (retinol) metabolism	-	-	-	-	-	-	-	-	4(19)	0.00932695	-	-	-	-	4(19)	0.00226872
Vitamin B1 (thiamin) metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Vitamin B2 (riboflavin) metabolism	-	-	-	-	-	-	-	-	-	-	-	-	1(3)	0.0227712	-	-
Vitamin B5 - CoA biosynthesis from pantothenate	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Vitamin B9 (folate) metabolism	-	-	2(2)	0.01663726	-	-	-	-	1(2)	0.04386186	-	-	1(2)	0.01529283	-	-
Vitamin D	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Vitamin D3 (cholecalciferol) metabolism	-	-	-	-	-	-	1(8)	0.02579615	-	-	-	-	-	-	-	-
Vitamin E metabolism	-	-	5(12)	0.03932443	-	-	-	-	-	-	-	-	-	-	-	-
Vitamin K metabolism	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.01193177	-	-
Xenobiotics metabolism	-	-	-	-	4(12)	0.04075288	-	-	-	-	-	-	-	-	-	-

Supplementary Table 7. Metabolomic pathway analysis results for the effects of radiation and GT3 treatment at SD30 in kidney tissue. Analysis was performed with Mummichog software, version 2.06.

	Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3	
	PBI 4 Gy		PBI 4 Gy		TBI 4 Gy		TBI 4 Gy		PBI 5.8 Gy		PBI 5.8 Gy		TBI 5.8 Gy		TBI 5.8 Gy	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***	***overlap size***	***p-value***	***overlap size***	***p-value***	***overlap size***	***p-value***	***overlap size***	***p-value***	***overlap size***	***p-value***	***overlap size***	***p-value***
3-oxo-10R-octadecatrienoate beta-oxidation	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.00428535
Alanine and Aspartate Metabolism	2(8)	0.01319217	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Androgen and estrogen biosynthesis and metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Arachidonic acid metabolism	-	-	-	-	-	-	-	-	-	-	-	-	5(11)	0.01529283	-	-
Arginine and Proline Metabolism	4(15)	9.24E-04	-	-	-	-	-	-	-	-	-	-	5(15)	0.00756239	-	-
Ascorbate (Vitamin C) and Aldarate Metabolism	-	-	-	-	-	-	-	-	2(5)	0.0281489	-	-	4(5)	0.00184858	-	-
Aspartate and asparagine metabolism	-	-	-	-	-	-	-	-	-	-	-	-	5(23)	0.04890345	-	-
Beta-Alanine metabolism	-	-	-	-	-	-	-	-	-	-	1(5)	0.03495505	2(5)	0.04243341	-	-
Biopterin metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1(7)	0.03066969
Blood Group Biosynthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.04755903	-	-
C21-steroid hormone biosynthesis and metabolism	2(10)	0.02999748	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Caffeine metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Carnitine shuttle	-	-	-	-	-	-	8(27)	0.00025208	-	-	-	-	-	-	-	-
Chondroitin sulfate degradation	-	-	-	-	-	-	-	-	-	-	-	-	2(2)	0.01714142	-	-
D4&E4-neuroprostanes formation	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1(2)	0.02907319
Drug metabolism - cytochrome P450	-	-	3(5)	0.00075624	2(8)	0.01621712	2(8)	0.04445005	-	-	-	-	-	-	-	-
Drug metabolism - other enzymes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1(4)	0.0164692
Dynorphin metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Fructose and mannose metabolism	-	-	-	-	-	-	-	-	-	-	-	-	2(2)	0.01714142	1(2)	0.00756239
Galactose metabolism	-	-	-	-	-	-	-	-	-	-	-	-	2(2)	0.01714142	-	-
Glutamate metabolism	2(7)	0.00991513	-	-	-	-	-	-	-	-	1(7)	0.04722292	-	-	-	-
Glutathione Metabolism	-	-	-	-	-	-	-	-	-	-	1(6)	0.04024872	-	-	-	-
Glycerophospholipid metabolism	-	-	-	-	-	-	-	-	-	-	-	-	6(15)	0.01663726	-	-
Glycine, serine, alanine and threonine metabolism	3(17)	0.00899084	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Glycosphingolipid biosynthesis - ganglioseries	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Glycosphingolipid biosynthesis - globoseries	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Glycosphingolipid biosynthesis - lactoseries	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.04755903	-	-
Glycosphingolipid biosynthesis - neolactoseries	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.04755903	-	-
Heparan sulfate degradation	-	-	-	-	-	-	-	-	-	-	-	-	2(2)	0.01714142	-	-
Hexose phosphorylation	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Keratan sulfate biosynthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.04755903	-	-
Linoleate metabolism	-	-	2(13)	0.03865221	-	-	-	-	-	-	-	-	-	-	-	-
N-Glycan biosynthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.04755903	-	-
O-Glycan biosynthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.04755903	-	-
Pentose and Glucuronate Interconversions	-	-	-	-	-	-	-	-	-	-	-	-	3(5)	0.02235106	-	-
Pentose phosphate pathway	-	-	-	-	-	-	-	-	-	-	-	-	3(5)	0.02235106	-	-
Phosphatidylinositol phosphate metabolism	-	-	-	-	-	-	-	-	-	-	1(4)	0.01806571	3(6)	0.00764642	-	-
Prostaglandin formation from arachidonate	2(12)	0.03285438	-	-	2(12)	0.03781195	-	-	-	-	-	-	-	-	-	-
Pyrimidine metabolism	2(12)	0.03285438	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Saturated fatty acids beta-oxidation	-	-	-	-	-	-	2(6)	0.02672044	-	-	-	-	-	-	-	-
Sialic acid metabolism	-	-	-	-	-	-	-	-	-	-	-	-	3(3)	0.00226872	1(3)	0.0408369
Starch and Sucrose Metabolism	-	-	-	-	1(1)	0.01579699	-	-	1(1)	0.02251912	-	-	1(1)	0.04755903	-	-
Urea cycle/amino group metabolism	5(19)	0.00067221	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Vitamin A (retinol) metabolism	-	-	-	-	-	-	-	-	-	-	1(7)	0.03058567	-	-	-	-
Vitamin B2 (riboflavin) metabolism	-	-	-	-	-	-	-	-	-	-	1(5)	0.03495505	-	-	-	-
Vitamin D3 (cholecalciferol) metabolism	-	-	-	-	-	-	2(7)	0.03562726	-	-	-	-	-	-	-	-
Vitamin E metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Vitamin K metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Xenobiotics metabolism	-	-	-	-	-	-	-	-	-	-	-	-	4(15)	0.03335854	-	-

Supplementary Table 8. Metabolomic pathway analysis results for the effects of radiation and GT3 treatment at SD30 in lung tissue. Analysis was performed with Mummichog software, version 2.06.

	Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3	
	PBI 4 Gy		PBI 4 Gy		TBI 4 Gy		TBI 4 Gy		PBI 5.8 Gy		PBI 5.8 Gy		TBI 5.8 Gy		TBI 5.8 Gy	
Pathway	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*
1- and 2-Methylnaphthalene degradation	-	-	-	-	-	-	1(1)	0.02999748	-	-	-	-	-	-	-	-
Alanine and Aspartate Metabolism	-	-	-	-	-	-	2(3)	0.00613394	2(3)	0.02083858	-	-	-	-	-	-
Alkaloid biosynthesis II	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.00462146	-	-
Aminosugars metabolism	-	-	-	-	-	-	-	-	3(3)	0.00117637	-	-	-	-	-	-
Androgen and estrogen biosynthesis and metabolism	2(5)	0.03066969	-	-	2(5)	0.01840181	-	-	2(5)	0.01579699	1(2)	0.0202504	1(2)	0.01117553	-	-
Arachidonic acid metabolism	7(20)	0.00142845	-	-	-	-	4(20)	0.0351231	-	-	1(9)	0.03772792	-	-	-	-
Arginine and Proline Metabolism	2(4)	8.23E-03	-	-	-	-	3(4)	0.00084027	2(4)	0.04478615	-	-	-	-	-	-
Ascorbate (Vitamin C) and Aldarate Metabolism	-	-	-	-	-	-	-	-	-	-	1(5)	0.03251828	-	-	-	-
Aspartate and asparagine metabolism	2(6)	0.01882195	-	-	-	-	3(6)	0.00243677	-	-	1(6)	0.03419881	-	-	-	-
Beta-Alanine metabolism	-	-	-	-	-	-	2(6)	0.0259642	-	-	-	-	-	-	-	-
C21-steroid hormone biosynthesis and metabolism	-	-	-	-	4(5)	0.00042013	-	-	3(14)	0.02638434	-	-	1(5)	0.02932527	-	-
Carbon fixation	-	-	-	-	-	-	1(1)	0.02999748	2(2)	0.00840266	-	-	-	-	-	-
Carnitine shuttle	-	-	-	-	-	-	-	-	-	-	-	-	17(31)	8.4027E-05	-	-
Chondroitin sulfate degradation	-	-	1(2)	0.02478783	-	-	-	-	-	-	-	-	-	-	-	-
CoA Catabolism	-	-	-	-	-	-	1(1)	0.02999748	-	-	-	-	-	-	1(1)	0.00999916
De novo fatty acid biosynthesis	2(9)	0.04856735	-	-	3(9)	0.02193093	-	-	-	-	-	-	-	-	-	-
Di-unsaturated fatty acid beta-oxidation	-	-	-	-	1(1)	0.03621544	-	-	-	-	-	-	-	-	-	-
Fatty acid activation	2(5)	0.01251996	-	-	3(5)	0.00462146	-	-	-	-	-	-	-	-	-	-
Fatty Acid Metabolism	2(3)	0.00487354	-	-	2(3)	0.01151164	-	-	-	-	-	-	-	-	-	-
Fructose and mannose metabolism	-	-	-	-	-	-	1(1)	0.02999748	-	-	-	-	-	-	-	-
Galactose metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Glutamate metabolism	-	-	-	-	-	-	-	-	-	-	1(6)	0.03419881	-	-	-	-
Glutathione Metabolism	2(4)	0.0082346	-	-	-	-	2(4)	0.01218385	-	-	1(4)	0.02966137	-	-	-	-
Glycine, serine, alanine and threonine metabolism	-	-	-	-	-	-	-	-	-	-	3(11)	0.02176288	-	-	-	-
Glycolysis and Gluconeogenesis	-	-	-	-	-	-	-	-	-	-	2(3)	0.00840266	-	-	-	-
Glycosphingolipid metabolism	4(14)	0.01840181	2(14)	0.03176204	-	-	-	-	-	-	-	-	-	-	-	-
Glycosylphosphatidylinositol(GPI)-anchor biosynthesis	-	-	-	-	-	-	1(1)	0.02999748	-	-	-	-	-	-	-	-
Glyoxylate and Dicarboxylate Metabolism	-	-	1(2)	0.02478783	-	-	-	-	-	-	-	-	-	-	-	-
Heparan sulfate degradation	-	-	1(2)	0.02478783	-	-	-	-	-	-	-	-	-	-	-	-
Hexose phosphorylation	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Histidine metabolism	-	-	-	-	-	-	-	-	-	-	1(4)	0.02966137	-	-	-	-
Leukotriene metabolism	5(19)	0.01604907	-	-	-	-	-	-	-	-	1(4)	0.02966137	-	-	-	-
Linoleate metabolism	-	-	-	-	-	-	-	-	-	-	1(3)	0.02361146	-	-	-	-
Methionine and cysteine metabolism	-	-	-	-	-	-	-	-	-	-	1(7)	0.03655155	-	-	-	-
N-Glycan Degradation	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Nitrogen metabolism	-	-	-	-	-	-	2(2)	0.00243677	2(2)	0.00840266	-	-	-	-	-	-
Nucleotide Sugar Metabolism	-	-	-	-	-	-	1(1)	0.02999748	-	-	-	-	-	-	-	-
Omega-3 fatty acid metabolism	2(5)	0.03066969	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Parathio degradation	-	-	-	-	-	-	-	-	-	-	1(1)	0.03235022	-	-	-	-
Pentose and Glucuronate Interconversions	-	-	1(2)	0.02478783	-	-	-	-	-	-	-	-	-	-	-	-
Pentose phosphate pathway	-	-	-	-	-	-	-	-	-	-	3(5)	0.00243677	-	-	-	-
Phosphatidylinositol phosphate metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Polyunsaturated fatty acid biosynthesis	1(1)	0.0202504	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Porphyrin metabolism	-	-	2(14)	0.03176204	1(1)	0.03621544	-	-	-	-	-	-	-	-	-	-
Prostaglandin formation from arachidonate	7(22)	0.00243677	-	-	4(22)	0.04663474	-	-	-	-	1(4)	0.02966137	-	-	-	-
Purine metabolism	-	-	-	-	-	-	2(5)	1.66E-02	3(5)	1.09E-02	5(9)	4.20E-04	-	-	-	-
Putative anti-Inflammatory metabolites formation from EPA	1(1)	0.03730779	1(1)	0.01151164	-	-	2(3)	0.00613394	-	-	1(3)	0.02361146	-	-	-	-
Pyrimidine metabolism	-	-	1(8)	0.02604823	-	-	2(8)	0.04302159	4(8)	0.00781447	-	-	-	-	-	-
Pyruvate Metabolism	-	-	-	-	-	-	-	-	-	-	1(3)	0.02361146	-	-	-	-
Saturated fatty acids beta-oxidation	1(1)	0.0202504	-	-	1(1)	0.03621544	-	-	-	-	-	-	-	-	-	-
Selenoamino acid metabolism	2(5)	0.03066969	-	-	2(5)	0.01840181	-	-	-	-	-	-	-	-	-	-
Sialic acid metabolism	-	-	-	-	-	-	-	-	2(3)	0.02083858	-	-	-	-	-	-
Starch and Sucrose Metabolism	-	-	-	-	-	-	-	-	2(3)	0.02083858	1(3)	0.02361146	-	-	-	-
Tryptophan metabolism	-	-	-	-	-	-	-	-	-	-	1(9)	0.03772792	-	-	-	-
Tyrosine metabolism	-	-	-	-	-	-	-	-	5(25)	0.01100748	6(25)	0.00739434	-	-	-	-
Urea cycle/amino group metabolism	-	-	-	-	-	-	2(6)	0.0259642	3(6)	0.01722544	6(21)	0.0028569	-	-	-	-
Vitamin B2 (riboflavin) metabolism	-	-	-	-	-	-	1(1)	0.02999748	-	-	-	-	-	-	-	-
Vitamin B3 (nicotinate and nicotinamide) metabolism	-	-	-	-	-	-	3(4)	0.00084027	2(4)	0.04478615	-	-	-	-	-	-
Vitamin B5 - CoA biosynthesis from pantothenate	-	-	-	-	-	-	1(1)	0.02999748	-	-	-	-	-	-	1(1)	0.00999916
Vitamin B6 (pyridoxine) metabolism	-	-	-	-	-	-	-	-	-	-	1(1)	0.03235022	-	-	-	-

Vitamin B9 (folate) metabolism	1(1)	0.0202504	-	-	-	-	1(1)	0.03125788	-	-	-	-	-	-	-	-
Vitamin D3 (cholecalciferol) metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2(10)	0.01294009
Vitamin E metabolism	-	-	-	-	-	-	-	-	-	-	-	-	3(8)	0.01209982	-	-
Xenobiotics metabolism	-	-	-	-	-	-	-	-	-	-	1(3)	0.02361146	-	-	-	-

Supplementary Table 9. Metabolomic pathway analysis results for the effects of radiation and GT3 treatment at SD30 in spleen tissue. Analysis was performed with Mummichog software, version 2.06.

	Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3		Irradiated vs. Naïve		Irradiated vs. GT3	
	PBI 4 Gy		PBI 4 Gy		TBI 4 Gy		TBI 4 Gy		PBI 5.8 Gy		PBI 5.8 Gy		TBI 5.8 Gy		TBI 5.8 Gy	
Pathway	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*	*overlap size*	*p-value*
3-oxo-10R-octadecatrienoate beta-oxidation	1(1)	0.03646752	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Alanine and Aspartate Metabolism	-	-	-	-	-	-	-	-	-	-	-	-	2(6)	0.02041845	-	-
Alkaloid biosynthesis II	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.02932527	-	-
Aminosugars metabolism	4(6)	0.01537686	-	-	3(6)	0.0338627	-	-	-	-	-	-	2(6)	0.02571213	-	-
Androgen and estrogen biosynthesis and metabolism	2(2)	0.02394757	-	-	2(2)	0.0161331	1(2)	0.03243425	-	-	-	-	-	-	-	-
Arachidonic acid metabolism	-	-	-	-	-	-	4(33)	0.03108982	-	-	-	-	-	-	-	-
Arginine and Proline Metabolism	6(11)	0.01352827	-	-	-	-	-	-	2(8)	0.01504075	-	-	-	-	-	-
Ascorbate (Vitamin C) and Aldarate Metabolism	-	-	1(7)	0.00243677	-	-	-	-	3(7)	0.03377867	2(7)	0.02823292	2(7)	0.03487102	-	-
Aspartate and asparagine metabolism	-	-	-	-	-	-	-	-	2(9)	0.01789766	-	-	-	-	-	-
Beta-Alanine metabolism	-	-	-	-	-	-	-	-	-	-	-	-	1(2)	0.04797916	-	-
Bile acid biosynthesis	3(11)	0.03646752	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Blood Group Biosynthesis	-	-	-	-	2(2)	0.0161331	-	-	2(2)	0.01033527	-	-	-	-	-	-
C21-steroid hormone biosynthesis and metabolism	3(12)	0.04797916	-	-	-	-	3(9)	0.00201664	-	-	1(12)	0.04579447	-	-	-	-
Carbon fixation	3(4)	0.00294093	-	-	-	-	-	-	2(4)	0.00470549	-	-	2(4)	0.00815058	-	-
Carnitine shuttle	-	-	-	-	10(23)	0.00193261	-	-	-	-	-	-	-	-	-	-
Chondroitin sulfate degradation	-	-	-	-	2(3)	0.03781195	-	-	2(3)	0.02865305	2(3)	0.00520965	2(3)	0.00638602	-	-
CoA Catabolism	-	-	-	-	2(2)	0.0161331	-	-	-	-	-	-	-	-	-	-
Di-unsaturated fatty acid beta-oxidation	-	-	-	-	2(3)	0.03781195	-	-	-	-	-	-	-	-	-	-
Drug metabolism - cytochrome P450	-	-	-	-	-	-	-	-	-	-	-	-	3(9)	0.00655407	-	-
Electron transport chain	-	-	-	-	-	-	-	-	-	-	1(1)	0.02646836	-	-	-	-
Fatty acid activation	-	-	-	-	-	-	4(25)	0.01151164	-	-	-	-	-	-	-	-
Fructose and mannose metabolism	-	-	-	-	3(6)	0.0338627	-	-	-	-	-	-	1(2)	0.04797916	-	-
Glutamate metabolism	4(7)	0.02579615	-	-	-	-	-	-	-	-	-	-	1(2)	0.04797916	-	-
Glutathione Metabolism	-	-	-	-	-	-	-	-	-	-	-	-	1(2)	0.04797916	-	-
Glycerophospholipid metabolism	-	-	-	-	-	-	-	-	-	-	-	-	6(34)	0.00815058	-	-
Glycine, serine, alanine and threonine metabolism	6(13)	0.02873708	-	-	-	-	-	-	5(13)	0.01504075	-	-	-	-	-	-
Glycolysis and Gluconeogenesis	3(8)	0.0173935	-	-	-	-	-	-	-	-	-	-	2(7)	0.03487102	-	-
Glycosphingolipid biosynthesis - ganglioseries	-	-	-	-	3(4)	0.0107554	-	-	3(4)	0.00495757	-	-	2(4)	0.01117553	-	-
Glycosphingolipid biosynthesis - globoseries	-	-	-	-	3(3)	0.00428535	-	-	3(3)	0.00184858	-	-	2(3)	0.00638602	-	-
Glycosphingolipid biosynthesis - lactoseries	-	-	-	-	2(2)	0.0161331	-	-	2(2)	0.01033527	-	-	-	-	-	-
Glycosphingolipid biosynthesis - neolactoseries	-	-	-	-	2(2)	0.0161331	-	-	2(2)	0.01033527	-	-	-	-	-	-
Glycosphingolipid metabolism	6(9)	0.00336106	-	-	6(9)	1.01E-03	-	-	5(9)	2.69E-03	-	-	4(13)	0.00378119	-	-
Heparan sulfate degradation	-	-	-	-	2(3)	0.03781195	-	-	2(3)	0.02865305	2(3)	0.00520965	2(3)	0.00638602	-	-
Histidine metabolism	3(5)	0.04066885	-	-	4(10)	0.02856903	-	-	-	-	-	-	-	-	-	-
Keratan sulfate biosynthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.02932527	-	-
Keratan sulfate degradation	2(2)	0.02394757	-	-	2(2)	0.0161331	-	-	2(2)	0.01033527	-	-	2(2)	0.00226872	-	-
Leukotriene metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Methionine and cysteine metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1(14)	0.0259642
Mono-unsaturated fatty acid beta-oxidation	-	-	-	-	2(2)	0.0161331	-	-	-	-	-	-	-	-	-	-
N-Glycan biosynthesis	3(5)	4.07E-02	-	-	3(5)	0.01974624	-	-	3(5)	0.01176372	-	-	3(5)	0.00168053	-	-
N-Glycan Degradation	-	-	-	-	-	-	-	-	-	-	1(1)	0.02646836	1(1)	0.02932527	-	-
O-Glycan biosynthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.02932527	-	-
Omega-3 fatty acid metabolism	-	-	-	-	-	-	2(8)	0.02058651	-	-	-	-	-	-	-	-
Omega-6 fatty acid metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Parathio degradation	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.0227712
Pentose and Glucuronate Interconversions	-	-	-	-	2(3)	0.03781195	-	-	2(3)	0.02865305	2(3)	0.00520965	2(3)	0.00638602	-	-
Pentose phosphate pathway	-	-	-	-	5(9)	0.00621796	-	-	4(9)	0.01537686	3(9)	0.0066381	4(9)	0.00134442	-	-
Phosphatidylinositol phosphate metabolism	4(8)	0.04436602	-	-	5(8)	0.00428535	-	-	3(8)	0.04495421	2(8)	0.0367196	2(8)	0.04545836	-	-
Phytanic acid peroxisomal oxidation	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Polyunsaturated fatty acid biosynthesis	-	-	-	-	-	-	1(2)	0.03503907	-	-	-	-	-	-	-	-
Porphyrin metabolism	-	-	-	-	-	-	-	-	3(8)	0.04495421	1(6)	0.02159482	2(8)	0.04545836	-	-
Propanoate metabolism	-	-	-	-	3(6)	0.0338627	-	-	1(3)	0.04478615	-	-	-	-	-	-
Prostaglandin formation from arachidonate	7(33)	0.02016637	-	-	10(33)	0.01604907	3(22)	0.03033359	-	-	2(33)	0.01470465	-	-	-	-
Prostaglandin formation from dihomo gama-linoleic acid	-	-	-	-	-	-	-	-	-	-	2(4)	0.00915889	-	-	-	-
Proteoglycan biosynthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.02932527	-	-
Purine metabolism	5(9)	0.01907403	-	-	-	-	-	-	-	-	2(9)	0.04688682	3(9)	0.00890681	-	-
Pyrimidine metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Pyruvate Metabolism	1(1)	0.03646752	-	-	-	-	-	-	1(1)	0.01478867	-	-	1(1)	0.02235106	-	-
Saturated fatty acids beta-oxidation	-	-	-	-	2(3)	0.03781195	-	-	-	-	-	-	-	-	-	-
Selenoamino acid metabolism	-	-	-	-	-	-	-	-	3(4)	0.00495757	-	-	-	-	-	-

Sialic acid metabolism	3(5)	0.04066885	-	-	-	-	-	-	3(5)	0.01176372	2(5)	0.0136123	-	-	-	-
Squalene and cholesterol biosynthesis	4(4)	0.00168053	-	-	3(4)	0.0107554	-	-	-	-	-	-	-	-	-	-
TCA cycle	1(1)	0.03646752	-	-	-	-	-	-	1(1)	0.01478867	-	-	1(1)	0.02235106	-	-
Tryptophan metabolism	-	-	-	-	-	-	-	-	-	-	-	-	3(15)	0.0272246	-	-
Ubiquinone Biosynthesis	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.02932527	-	-
Urea cycle/amino group metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Valine, leucine and isoleucine degradation	-	-	-	-	4(10)	0.03739182	-	-	-	-	-	-	-	-	-	-
Vitamin A (retinol) metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Vitamin B1 (thiamin) metabolism	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Vitamin B2 (riboflavin) metabolism	-	-	-	-	2(2)	0.0161331	-	-	-	-	-	-	-	-	-	-
Vitamin B5 - CoA biosynthesis from pantothenate	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Vitamin B9 (folate) metabolism	3(4)	0.01941013	-	-	-	-	-	-	-	-	1(3)	0.01008319	-	-	-	-
Vitamin E metabolism	-	-	-	-	4(8)	0.01117553	-	-	-	-	-	-	-	-	-	-
Vitamin H (biotin) metabolism	-	-	-	-	-	-	-	-	-	-	-	-	1(1)	0.02932527	-	-