

LPS effect- complete study plasma (identified and annotated metabolites)

CTL T0h vs CTL T12h

Peak id	Metabolite	Log fc	p	Adjusted p	Peak intensity CTL T0h	Peak intensity CTL T12h	Identification
1	Betaine	-0.98	0.0000	0.0000	1704046315	864408838	identified+fragment
4	Pterolactam	-0.50	0.0000	0.0000	358042565	253201284	annotated+fragment
5	Methionine sulfoxide	-0.93	0.0000	0.0000	1670841	878954	annotated
6	Hydroxypropyl-Valine	-0.92	0.0000	0.0000	868952	459394	annotated
8	4-Methylthio-2-oxobutanoic acid	-0.76	0.0000	0.0000	177030	104462	annotated
47	Hydroxypropyl-Glutamine	0.54	0.0000	0.0000	296972	431267	annotated
48	L-Glutamine	-0.66	0.0000	0.0000	157564731	99997618	identified+fragment
51	N-Nitrosoguvacoline	-0.67	0.0000	0.0000	7777423	4879346	annotated
61	Miraxanthin-I	-1.03	0.0000	0.0000	1346913	659162	annotated
73	(S)-2-Aminobutanoate	-0.49	0.0000	0.0000	131321504	93642603	annotated+fragment
99	L-Arginine	-0.51	0.0000	0.0000	57344499	40226320	identified+fragment
106	Northienamycin	-0.30	0.0000	0.0000	174243	141389	annotated
117	O-Desmethylcarvedilol	-0.91	0.0000	0.0000	76148	40538	annotated
136	Bentazone	-0.37	0.0000	0.0000	91233	70745	annotated
170	PC(18:1(9Z)/18:1(9Z))	-0.42	0.0000	0.0000	44872845	33505239	annotated
171	L-Acetopine	-3.12	0.0000	0.0000	46033555	5298638	annotated
173	Xanthopterin-B2	-0.42	0.0000	0.0000	57065	42632	annotated
174	L-Alloisoleucine	-0.48	0.0000	0.0000	37922822	27220535	annotated+fragment
175	PE(22:1(13Z)/15:0)	-0.25	0.0000	0.0000	25252349	21267610	annotated
177	3beta,6beta-Dihydroxynortropane	-0.52	0.0000	0.0000	23371266	16252669	annotated
235	PC(16:0/0:0)	-0.97	0.0000	0.0000	13097980	6706384	annotated
238	PE(20:4(5Z,8Z,11Z,14Z)/0:0)	-0.68	0.0000	0.0000	236263	147192	annotated
239	dCTP	-0.60	0.0000	0.0000	37346	24710	annotated
242	L-Valine	-0.29	0.0000	0.0000	23293168	19026420	identified+fragment
249	L-Methionine	-0.78	0.0000	0.0000	27563852	16059557	identified+fragment
256	3-Demethyldigicitrin	-0.78	0.0000	0.0000	428768	250036	annotated
263	beta-Alanine	-0.84	0.0000	0.0000	28674370	16069185	identified
291	L-Lysine	1.07	0.0000	0.0000	9706419	20441740	identified
299	Nalbuphine	1.19	0.0000	0.0000	176209	402759	annotated

301	Cilastatin	1.36	0.0000	0.0000	123141	315156	annotated
302	Metoxuron	0.33	0.0000	0.0000	129107	162764	annotated
308	(S)-lipoic acid	0.65	0.0000	0.0000	46189	72353	annotated
316	PC(P-18:0/0:0)	-0.77	0.0000	0.0000	67679	39583	annotated
320	L-Tyrosine	-0.64	0.0000	0.0000	17063947	10969979	identified+fragment
330	Hydroxypropyl-Serine	-1.36	0.0000	0.0000	594882	232374	annotated
337	Gamma-Glutamyltyrosine	-0.95	0.0000	0.0000	327618	169089	annotated+fragment
534	PE(24:1(15Z)/16:1(9Z))	-0.39	0.0000	0.0000	239572	183089	annotated
564	N-Methylnicotinate	-0.99	0.0000	0.0000	13808694	6974457	annotated+fragment
653	PC(18:0/0:0)	-1.55	0.0000	0.0000	6753844	2309389	annotated+fragment
662	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	-0.66	0.0000	0.0000	190766	120978	annotated
690	LysoPE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	-0.48	0.0000	0.0000	104799	74939	annotated
692	Ectoine	-0.58	0.0000	0.0000	13750108	9180409	annotated+fragment
696	N6-Acetyl-5S-hydroxy-L-lysine	-1.16	0.0000	0.0000	4030878	1810013	annotated
751	Hydroxypropyl-Proline	2.08	0.0000	0.0000	1361485	5770136	annotated
817	L-Theanine	-0.47	0.0000	0.0000	8980666	6497001	annotated
849	Neolinustatin	-0.49	0.0000	0.0000	398256	283546	annotated
929	(S)-2,3,4,5-Tetrahydropyridine-2-carboxylate	-3.12	0.0000	0.0000	9054823	1040978	annotated
932	Dihydroclavaminic acid	-2.13	0.0000	0.0000	115922	26469	annotated
933	Seriny-Tyrosine	-2.39	0.0000	0.0000	105472	20132	annotated
934	Pyroglutamylglycine	-2.93	0.0000	0.0000	113826	14963	annotated
965	Succinylproline	-1.53	0.0000	0.0000	27049	9397	annotated
969	Alanvl-Aspartate	-3.56	0.0000	0.0000	7612220	645907	annotated
970	Thionazin	-3.17	0.0000	0.0000	387545	42987	annotated
985	Histidinyl-Aspartate	-4.11	0.0000	0.0000	68927	3999	annotated
991	Bicozamycin	-3.41	0.0000	0.0000	40020	3778	annotated
993	gibberellin A2 O-beta-D-glucoside	3.46	0.0000	0.0000	45789	504605	annotated
1063	Aspartyl-Threonine	-0.58	0.0000	0.0000	119278	79617	annotated
1064	Tromethamine	2.24	0.0000	0.0000	244275	1153678	annotated+fragment
1107	Glutamylphenylalanine	-0.39	0.0000	0.0000	422898	321741	annotated+fragment
1216	2-Octenoylcarnitine	0.62	0.0000	0.0000	70377	108057	annotated
1220	L-Pipecolate	-0.63	0.0000	0.0000	3758433	2432000	annotated
1253	Choline sulfate	-0.81	0.0000	0.0000	2057506	1175988	annotated
1269	L-Glutamate	-0.76	0.0000	0.0000	4080611	2410382	identified+fragment
1270	L-Acetylcarnitine	-0.94	0.0000	0.0000	2642779	1382011	annotated
1276	PC(22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	-0.43	0.0000	0.0000	574523	425479	annotated
1283	3-Ureidopropionate	-1.10	0.0000	0.0000	2849243	1330976	annotated+fragment
1302	Isoleucyl-Serine	-3.06	0.0000	0.0000	2266946	271174	annotated
1310	L-2-Amino-3-(1-pyrazolyl)propanoic acid	-0.39	0.0000	0.0000	1482596	1131744	annotated+fragment

1364	L-phenylalanyl-L-hydroxyproline	0.74	0.0000	0.0000	553165	926406	annotated
1385	Melledonal B	0.39	0.0000	0.0000	13643	17896	annotated
1391	Isoleucyl-Aspartate	-0.55	0.0000	0.0000	139345	95467	annotated
1401	L-Ornithine	-0.50	0.0000	0.0000	1649963	1164798	identified+fragment
1407	5-Hydroxymethyl-2-furaldehyde	-1.29	0.0000	0.0000	1398399	572428	annotated
1436	Acetone cyanohydrin	0.59	0.0000	0.0000	770815	1157677	annotated
1452	alpha-linolenic acid	-1.11	0.0000	0.0000	1221065	565929	annotated
1528	L-isoleucyl-L-proline	0.59	0.0000	0.0000	658692	991845	annotated
1535	Hydroxypropyl-Hydroxyproline	-2.60	0.0000	0.0000	1524416	250935	annotated
1587	Hypoglycin B	-3.27	0.0000	0.0000	953523	98885	annotated
1591	L-cis-Cyclo(aspartylphenylalanyl)	-2.16	0.0000	0.0000	307593	68665	annotated
1595	Etoazole	-4.26	0.0000	0.0000	188279	9859	annotated
1601	Midodrine	-0.88	0.0000	0.0000	1496947	813912	annotated
1644	LysoPC(16:1(9Z))	-1.27	0.0000	0.0000	740361	306936	annotated
1694	N-Formyl-4-amino-5-aminomethyl-2-methylpyrimidine	-1.05	0.0000	0.0000	1197593	578627	annotated
1698	L-Histidine trimethylbetaine	-0.64	0.0000	0.0000	1186577	762434	annotated
1712	Cytidine	0.84	0.0000	0.0000	625725	1117303	identified
1785	PE(18:2(9Z,12Z)/0:0)	-0.84	0.0000	0.0000	1116525	624881	annotated
1807	DL-2-amino-octanoic acid	-0.49	0.0000	0.0000	881941	629346	annotated
1813	L-N2-(2-Carboxyethyl)arginine	-0.83	0.0000	0.0000	408866	229527	annotated
1854	PE(20:3(5Z,8Z,11Z)/16:1(9Z))	-0.30	0.0000	0.0000	1009085	820600	annotated
1910	N-Methylcalystegine B2	-0.45	0.0000	0.0000	376538	275525	annotated
1948	Sakacin P	-0.70	0.0000	0.0000	249517	153742	annotated
1983	Dinex	-1.15	0.0000	0.0000	345678	156197	annotated
1991	(S)-Spinacine	-1.47	0.0000	0.0000	108860	39214	annotated
2004	2,4-Diamino-6-nitrotoluene	-1.47	0.0000	0.0000	108860	39214	annotated
2010	2-Pyrroloylglycine	0.58	0.0000	0.0000	36273	54197	annotated
2098	N2-Acetyl-L-aminoadipate	-0.53	0.0000	0.0000	56961	39417	annotated
2100	2-Acetyl-1,5,6,7-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4H-	-0.33	0.0000	0.0000	54583	43329	annotated
2127	Porphobilinogen	-0.31	0.0000	0.0000	47121	37948	annotated
2152	4-Aminosalicylate	-0.44	0.0000	0.0000	25273	18605	annotated
2153	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:0)	0.40	0.0000	0.0000	705181	927386	annotated
2156	Gamma-Glutamyl Glutamine	-1.28	0.0000	0.0000	770025	317261	annotated
2179	PI(18:1(9Z)/18:2(9Z,12Z))	-0.61	0.0000	0.0000	110136	72068	annotated
2203	Butalbital	-1.29	0.0000	0.0000	602682	247210	annotated
2477	Alanyl-Proline	2.25	0.0000	0.0000	89889	426395	annotated
2517	N-Lignoceroylsphingosine	-0.65	0.0000	0.0000	368948	234658	annotated
2531	Glycyl-Aspartate	-3.80	0.0000	0.0000	536466	38391	annotated
2533	Lysyl-Asparagine	-3.16	0.0000	0.0000	336963	37572	annotated

2535	Alanyl-Threonine	-0.57	0.0000	0.0000	513882	346969	annotated
2543	L-Noradrenaline	-0.68	0.0000	0.0000	388359	241953	annotated
2585	N-Palmitoylsphingosine	-0.67	0.0000	0.0000	415193	260995	annotated
2586	(1xi,3S)-1,2,3,4-Tetrahydro-1-methyl-beta-carboline-1,3-dicarboxylic	0.26	0.0000	0.0000	83126	99806	annotated
2587	Ornaline	-0.79	0.0000	0.0000	97635	56603	annotated
2588	Glycerophosphocholine	-1.66	0.0000	0.0000	247444	78306	annotated
2594	Pirbuterol	0.24	0.0000	0.0000	362749	429485	annotated
2596	Daidzein 4'-O-glucuronide	-1.20	0.0000	0.0000	261165	114072	annotated
2604	Etrimfos	-0.48	0.0000	0.0000	82486	59341	annotated
2704	O-Ureido-L-serine	0.21	0.0000	0.0000	308340	357491	annotated
2730	Eosin	-0.75	0.0000	0.0000	103275	61385	annotated
2756	PE(20:0/14:1(9Z))	-0.65	0.0000	0.0000	269958	172606	annotated
2757	L-Cystine	-0.62	0.0000	0.0000	318502	206611	identified+fragment
2760	PE(20:3(5Z,8Z,11Z)/P-18:1(11Z))	0.38	0.0000	0.0000	292547	380555	annotated
2771	Threoninyl-Phenylalanine	-1.23	0.0000	0.0000	198336	84621	annotated
2776	PE(22:5(7Z,10Z,13Z,16Z,19Z)/P-18:0)	0.50	0.0000	0.0000	209573	295757	annotated
3082	Norambreinolide	-0.90	0.0000	0.0000	149875	80506	annotated
3095	N-gamma-L-Glutamyl-L-methionine	-0.94	0.0000	0.0000	326596	170105	annotated
3179	N-acetyl-L-2-aminoadipate(2-)	-1.34	0.0000	0.0000	243087	95971	annotated
3185	QH(2)	-0.70	0.0000	0.0000	41843	25788	annotated
3446	Isolinderanolide	-0.83	0.0000	0.0000	98872	55799	annotated
3462	PE(22:4(7Z,10Z,13Z,16Z)/P-18:0)	0.60	0.0000	0.0000	145554	220066	annotated
3463	N-Acetylhistidine	-1.00	0.0000	0.0000	198941	99703	annotated
3516	delta-Guanidinovaleric acid	-1.17	0.0000	0.0000	200482	88948	annotated
3539	PS(18:2(9Z,12Z)/18:0)	0.37	0.0000	0.0000	137358	177364	annotated
3599	PS(18:0/20:4(8Z,11Z,14Z,17Z))	0.33	0.0000	0.0000	121525	153043	annotated
3610	Homocysteine	-1.32	0.0000	0.0000	282690	113060	annotated
3616	(3S,5S)-Carbapenam-3-carboxylic acid	-1.26	0.0000	0.0000	322983	135137	annotated
3715	Normetanephine	-0.48	0.0000	0.0000	234624	168123	annotated
3757	Pseudoecgonine	-0.92	0.0000	0.0000	212518	112443	annotated
3762	Glyburide	1.08	0.0000	0.0000	83089	175097	annotated
3772	Metharbital	-0.67	0.0000	0.0000	171427	107380	annotated
3799	N-lactoyl-Methionine	-1.89	0.0000	0.0000	40847	11057	annotated
3801	Alanyl-Arginine	-0.95	0.0000	0.0000	195615	100968	annotated
3978	Aprobarbital	0.87	0.0000	0.0000	104568	191528	annotated
4082	(3S)-3-Hydroxy-L-enduracididine	-0.80	0.0000	0.0000	197370	113353	annotated
4177	(2R,2'S)-Isobuteine	-1.13	0.0000	0.0000	178834	81886	annotated
4196	Valyl-Valine	-0.58	0.0000	0.0000	116840	77936	annotated
4279	Etaconazole	-0.35	0.0000	0.0000	221517	174229	annotated

4393	LysoPC(22:5(4Z,7Z,10Z,13Z,16Z))	-0.63	0.0000	0.0000	139789	90345	annotated
4486	5'-O-beta-D-Glucosylpyridoxine	-0.73	0.0000	0.0000	168550	101784	annotated
4563	6-Hydroxy-9,9-dimethyl-5-(3-methyl-1-oxobutyl)-1-propyl-3H,9H-	-0.50	0.0000	0.0000	151010	106498	annotated
4683	5-L-Glutamyl-taurine	-0.67	0.0000	0.0000	138977	87521	annotated
4719	Diisopropyl sulfate	-0.85	0.0000	0.0000	177650	98776	annotated
4742	Talbutal	-0.70	0.0000	0.0000	163878	100998	annotated
4819	Glycerolphosphorylethanolamine	0.53	0.0000	0.0000	71269	102612	annotated
130	Cyclovariegatin	-0.50	0.0000	0.0001	175726	124506	annotated
230	Fenpiclonil	-0.75	0.0000	0.0001	177298	105575	annotated
842	1-[(5-Amino-5-carboxypentyl)amino]-1-deoxyfructose	-0.96	0.0000	0.0001	192059	98705	annotated
921	S-Methyl-1-thio-D-glycerate	-0.57	0.0000	0.0001	103545	69789	annotated
931	Prolyl-Valine	-0.67	0.0000	0.0001	132497	83381	annotated
1497	beta,beta-dimethyl acrylic acid	-0.71	0.0000	0.0001	121106	73845	annotated
1589	N-Methylcalystegine C1	-0.49	0.0000	0.0001	131055	93588	annotated
1936	Orthophosphate	0.29	0.0000	0.0001	127287	155154	annotated
2483	Polyethylene, oxidized	-0.53	0.0000	0.0001	76499	52948	annotated
2534	L-alpha-Amino-1H-pyrrole-1-hexanoic acid	-0.99	0.0000	0.0001	131798	66531	annotated
3602	5-Hydroxytryptophol	-1.62	0.0000	0.0001	97622	31809	annotated
3970	8-Oxodeoxycoformycin	-0.72	0.0000	0.0001	110384	66830	annotated
4111	apo-[3-methylcrotonoyl-CoA:carbon-dioxide ligase (ADP-forming)]	0.58	0.0000	0.0001	65499	97973	annotated
4182	Thymidine	0.60	0.0000	0.0001	82530	124742	annotated
4378	N-Acetyl-L-methionine	-0.80	0.0000	0.0001	66957	38559	annotated
4477	Isobutyryl-L-carnitine	-0.80	0.0000	0.0001	98238	56388	annotated
4516	5-Acetyl-2,4-dimethyloxazole	-0.35	0.0000	0.0001	98389	77221	annotated
4769	Cyclobassinone	-0.42	0.0000	0.0001	81943	61189	annotated
253	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	-0.82	0.0000	0.0002	57977	32918	annotated
1474	1,2-Dimethoxy-13-methyl-[1,3]benzodioxolo[5,6-c]phenanthridine	0.71	0.0000	0.0002	20522	33674	annotated
1762	(Indol-3-yl)acetamide	0.32	0.0000	0.0002	54188	67497	annotated
2114	Glycyl-Arginine	-0.55	0.0000	0.0002	58312	39740	annotated
2248	Heptyl p-hydroxybenzoate	-0.61	0.0000	0.0002	50612	33124	annotated
2287	trizma acetate	-0.91	0.0000	0.0002	42963	22930	annotated
2529	Geranyl acetoacetate	-0.53	0.0000	0.0002	61204	42259	annotated
3796	Cer(d14:2(4E,6E)/22:0(2OH))	-0.79	0.0000	0.0002	47480	27529	annotated
3840	3R-aminononanoic acid	-0.54	0.0000	0.0002	71312	49014	annotated
4144	Dambonitol	-0.62	0.0000	0.0002	52150	33977	annotated
4315	Anhalamine	-0.37	0.0000	0.0002	64827	50041	annotated
3640	Hydroxypropionylcarnitine	0.82	0.0000	0.0003	26549	47008	annotated
4534	3-Hydroxymelatonin	-1.26	0.0000	0.0003	55209	22998	annotated
137	Cysteineglutathione disulfide	-0.67	0.0001	0.0004	65142	40954	annotated

189	Allocystathionine	-0.75	0.0001	0.0004	59995	35691	annotated
1832	N-(1-Deoxy-1-fructosyl)histidine	-3.28	0.0001	0.0004	59419	6097	annotated
3779	Enilconazole	-0.51	0.0001	0.0004	41774	29374	annotated
4453	Hydroxymethyl indol-3-yl ketone	-0.55	0.0001	0.0004	25446	17410	annotated
4775	Glutathione	-0.79	0.0001	0.0004	24377	14068	annotated
2044	6-Imino-5-oxocyclohexa-1,3-dienecarboxylate	-1.08	0.0001	0.0005	29122	13730	annotated
2496	2-Hydroxynicotinic acid	-0.56	0.0001	0.0005	19270	13078	annotated
2947	3-Hydroxypropanoate	-0.63	0.0001	0.0005	73332037	47342233	annotated+fragment
1268	Sulfate	-1.22	0.0001	0.0006	23384987	10014954	annotated
1839	citrate	-1.30	0.0001	0.0006	4877544	1981169	identified+fragment
3615	Trimetaphosphoric acid	-0.53	0.0001	0.0006	543333	376112	annotated
4091	L-Homocysteic acid	-1.93	0.0001	0.0006	16524138	4323385	annotated
1007	Bromisovalum	0.11	0.0001	0.0008	140902	152076	annotated
4011	2-Methylcitric acid	-0.71	0.0001	0.0008	56878	34773	annotated
1052	Firocoxib	-0.79	0.0002	0.0009	98034	56511	annotated
1455	(S)-3-Hydroxybutanoate	-0.24	0.0002	0.0009	3315051	2812828	annotated
1624	Ethyl (±)-3-methylpentanoate	0.33	0.0001	0.0009	5465330	6872834	annotated
354	9-Octadecenoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester	-0.26	0.0002	0.0010	114180	95464	annotated
1036	Malate	-0.67	0.0002	0.0010	4091340	2567773	annotated+fragment
1594	D-Glucuronic acid	-0.35	0.0002	0.0010	576868	453190	annotated+fragment
1933	L-Serine	-0.37	0.0002	0.0010	4088694	3154451	identified+fragment
2471	Metsulfovax	-0.62	0.0002	0.0010	127608	83196	annotated
2532	trans-Grandmarin	-0.26	0.0002	0.0010	47896	40059	annotated
250	L-1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	-0.34	0.0002	0.0011	34565	27275	annotated
280	Methionyl-Cysteine	-0.35	0.0002	0.0011	23091	18151	annotated
1440	5-Hydroxyindoleacetic acid	-2.36	0.0002	0.0011	3119805	607914	annotated
2311	L-Tyrosine	-0.67	0.0002	0.0011	2904110	1821756	annotated+fragment
1599	GW 6471	-0.31	0.0002	0.0012	80304	64787	annotated
1697	Calabaxanthone	-0.53	0.0002	0.0012	49774	34445	annotated
4062	Dimethylenetriurea	0.62	0.0002	0.0012	178222	274750	annotated
843	5'-Oxoinosine	0.89	0.0002	0.0013	19898	36852	annotated
4734	Enalaprilate	1.66	0.0002	0.0013	6529	20689	annotated
3837	6-Galloylglucose	0.53	0.0002	0.0014	27561	39858	annotated
1074	Clidinium	1.30	0.0003	0.0015	13435	33109	annotated
1777	Isoeugenol acetate	0.63	0.0003	0.0016	27820	43071	annotated
4375	Cyclocommunin	1.70	0.0003	0.0016	8062	26264	annotated
161	Picrasin G	1.36	0.0003	0.0017	7783	20044	annotated
3802	N-Desalkyl flurazepam	0.67	0.0003	0.0017	10150	16138	annotated
1853	p,p'-Methoxychlor olefin	0.49	0.0003	0.0018	10091	14168	annotated

1695	L-Arabinose	-1.10	0.0004	0.0020	2015411	940050	annotated
1932	N-Formimino-L-glutamate	-1.40	0.0004	0.0020	355762	134385	annotated
3936	D-altro-D-manno-Heptose	-0.94	0.0004	0.0020	129273	67470	annotated
1279	Succinylacetone	-0.87	0.0004	0.0021	118590	64760	annotated
1048	Ovalitenin A	-0.98	0.0004	0.0022	79008	40189	annotated
1615	Dienestrol	-1.31	0.0004	0.0023	54656	22059	annotated
1982	Pseudouridine	1.10	0.0004	0.0023	1099719	2352998	annotated+fragment
3603	5-Sulfoxymethylfurfural	-0.53	0.0004	0.0023	1502369	1039739	annotated
241	Glycylproline	-0.24	0.0005	0.0024	169620	143623	annotated
1389	Loteprednol	0.15	0.0005	0.0024	106105	117614	annotated
184	Tizanidine	-0.46	0.0005	0.0025	21472	15597	annotated
4060	Tauro-b-muricholic acid	-0.68	0.0005	0.0025	869335	544425	annotated+fragment
114	Catechol sulfate	-0.70	0.0005	0.0026	917171	565528	annotated
281	N-Acetyl-L-glutamate 5-semialdehyde	-3.04	0.0006	0.0028	1758411	213624	annotated
1942	2-Oxoglutaramate	-2.12	0.0006	0.0028	1519381	350047	annotated
2438	Glutarylglucine	-2.93	0.0006	0.0029	1403951	184451	annotated
2547	L-gamma-glutamyl-L-isoleucine	-3.39	0.0006	0.0029	141972	13546	annotated
1513	D-Glucosamine	-1.00	0.0006	0.0030	1569767	787119	annotated
2707	(S)-17-Hydroxy-9,11,13,15-octadecatetraynoic acid	-0.37	0.0007	0.0033	30738	23785	annotated
1381	PI(18:2(9Z,12Z)/20:1(11Z))	-0.27	0.0007	0.0035	1058482	878282	annotated
1395	L-Aspartate	-1.25	0.0008	0.0039	429333	180189	identified+fragment
3536	Citramalate	-0.43	0.0008	0.0040	640205	476340	annotated
1383	2-Oxosuccinamate	-2.63	0.0009	0.0042	913517	147119	annotated
251	Homocysteinesulfinic acid	0.35	0.0009	0.0043	686588	874895	annotated
547	thymine	0.75	0.0010	0.0047	452429	760513	identified
3949	(3xi,6xi)-Cyclo(alanylvalyl)	0.12	0.0010	0.0049	235994	255938	annotated
1635	3,4-Dihydroxyphenylpropanoate	-0.59	0.0011	0.0054	518602	344663	annotated+fragment
89	Tiglylglycine	-2.37	0.0012	0.0055	724633	139983	annotated
4073	5,6-Dihydrothymine	-2.27	0.0012	0.0055	779146	161923	annotated
4560	Apigenin 7-sulfate	-0.56	0.0012	0.0055	422784	286245	annotated
1081	Aminoadipic acid	-0.74	0.0012	0.0058	485616	290464	annotated+fragment
1960	Quinic acid	-1.04	0.0013	0.0060	638741	309898	annotated+fragment
1921	D-Biopterin	-1.01	0.0013	0.0062	112925	56207	annotated
536	Acamprosate	-0.28	0.0014	0.0063	59858	49342	annotated
2258	Citraconic acid	-0.42	0.0014	0.0064	549824	409582	annotated+fragment
2464	N-Acetyl-L-aspartate	-0.47	0.0014	0.0067	315928	228091	annotated
1890	4-beta-Hydroxymethyl-4-alpha-methyl-5-alpha-cholest-7-en-3-beta-	-0.55	0.0015	0.0069	543493	370061	annotated+fragment
3792	Nevirapine	0.15	0.0015	0.0069	333739	371370	annotated
3832	Cysteine-S-sulfate	-1.85	0.0017	0.0079	414163	114905	annotated

2091	Ethyl 2-hydroxyisovalerate	-0.61	0.0018	0.0082	343105	225123	annotated
83	Metaldehyde	-0.65	0.0019	0.0087	111255	70716	annotated
1080	3-hydroxy-tetradecanedioic acid	-1.19	0.0019	0.0088	281163	122891	annotated
88	L-glycyl-L-hydroxyproline	-0.60	0.0020	0.0089	323355	213529	annotated
2466	L-trans-alpha-Amino-2-carboxycyclopropaneacetic acid	-1.10	0.0020	0.0091	307612	143704	annotated
4712	Citreovirone	-0.82	0.0022	0.0099	194197	110059	annotated
1719	Patulin	-0.59	0.0023	0.0103	259748	173083	annotated+fragment
324	4,5-Dihydrooorotic acid	-3.12	0.0025	0.0109	405568	46697	annotated
1551	3,6,8-Trimethylallantoin	-3.03	0.0025	0.0109	373951	45695	annotated
3164	Hydroiodic acid	-0.76	0.0030	0.0129	247448	145778	annotated
3131	1-Pyrenylsulfate	-3.31	0.0031	0.0132	350986	35408	annotated
11	trans-Aconitate	-0.52	0.0032	0.0137	300770	210474	annotated+fragment
1366	Ascorbic acid-2-sulfate	0.62	0.0033	0.0140	106562	164185	annotated
755	Ethyl 1-(ethylthio)propyl disulfide	-0.67	0.0034	0.0143	147300	92639	annotated
1317	Monomethyl sulfate	-0.75	0.0035	0.0146	248639	147582	annotated
2492	L-Quebrachitol	-1.07	0.0035	0.0146	282258	134686	annotated
1631	(2R)-1-O-beta-D-Galactopyranosylglycerol	-1.26	0.0036	0.0149	80693	33618	annotated
4809	4-Hydroxyphenylpyruvic acid	-0.64	0.0037	0.0156	269929	173553	annotated
3621	Pydanon	-0.70	0.0040	0.0167	26383	16275	annotated
2804	Ezetimibe	0.76	0.0041	0.0169	159122	270155	annotated
3092	2-Amino-1,7,9-trimethylimidazo[4,5-g]quinoxaline	0.36	0.0043	0.0177	126221	161938	annotated
4151	5-Hydroxy-7-tetracosanone	-0.57	0.0044	0.0181	134753	91062	annotated+fragment
4068	7-bromo-5-heptynoic acid	0.29	0.0044	0.0183	206599	252395	annotated
167	Malonate	-0.45	0.0045	0.0184	194194	142432	annotated+fragment
2440	3-Keto-scyllo-inosamine	-0.32	0.0045	0.0187	62579	50062	annotated
2722	8-Hydroxy-7-methylguanine	0.64	0.0046	0.0187	14309	22350	annotated
3962	alpha-15,16-DiHODE	-0.89	0.0046	0.0187	191730	103316	annotated
3278	Pemirolast	0.33	0.0046	0.0188	144631	182368	annotated
2548	Melatonin glucuronide	-0.74	0.0047	0.0190	30747	18422	annotated
3477	4-Hydroxy-estazolam	0.40	0.0047	0.0190	41029	54096	annotated
4485	5-Hydroxydantrolene	0.36	0.0048	0.0194	18807	24108	annotated
1722	TEPP	0.29	0.0048	0.0195	15016	18301	annotated
2622	Ethyl tiglate	-0.24	0.0049	0.0197	204556	173010	annotated
1728	Glycylprolylhydroxyproline	2.19	0.0053	0.0212	30394	139009	annotated
1515	alpha,alpha-Trehalose	-0.92	0.0056	0.0221	70653	37467	annotated+fragment
4793	Adefovir	-2.41	0.0059	0.0233	27493	5159	annotated
1884	Salsoline-1-carboxylate	-0.72	0.0060	0.0235	145264	88277	annotated
1070	Diethyl sulfate	-1.01	0.0061	0.0240	65518	32509	annotated
1632	3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid	-0.53	0.0063	0.0246	16392	11364	annotated

1577	Hexanoylglycine	-1.11	0.0066	0.0255	92138	42828	annotated
126	Orotate	-1.28	0.0070	0.0269	129917	53634	identified
807	L-gamma-glutamyl-L-leucine	-1.36	0.0071	0.0274	141972	55434	annotated
1370	Methyl 1-(propylsulfanyl)propyl disulfide	-0.76	0.0072	0.0275	72248	42624	annotated
1294	4-vinylphenol Sulfate	-0.75	0.0075	0.0288	59735	35493	annotated
2954	3-Sulfinoalanine	-0.77	0.0081	0.0308	72175	42338	annotated
1050	2-aminomuconic acid semialdehyde	-1.61	0.0083	0.0314	110493	36258	annotated
3995	Margrapine B	-3.96	0.0083	0.0315	45270	2900	annotated
2649	Dehydrocycloxanthohumol hydrate	-0.66	0.0086	0.0323	82100	52090	annotated
2633	4-Oxononanal	-0.31	0.0088	0.0330	77736	62731	annotated
1914	PG(18:1(9Z)/18:0)	0.42	0.0090	0.0335	44897	60150	annotated
1603	1-O-Methyl-myo-inositol	-0.61	0.0093	0.0344	76664	50397	annotated
1075	Ascorbalamic acid	-0.79	0.0095	0.0350	54912	31816	annotated
3871	L-N-Carboxymethylserine	1.00	0.0095	0.0350	19409	38920	annotated
2271	Galactaric acid	-0.51	0.0108	0.0395	41246	28965	annotated
1917	Phenindione	-0.78	0.0109	0.0397	59613	34617	annotated
2259	Phenylpyruvate	-0.82	0.0116	0.0420	38658	21941	annotated
994	2-Deoxy-D-ribitol	-0.39	0.0117	0.0423	34363	26152	annotated
1781	Histidiny-Glutamine	-0.98	0.0120	0.0434	25523	12968	annotated
1077	Steroid O-sulfate	-0.43	0.0124	0.0445	28367	21038	annotated
4441	Potassium 2-(1'-ethoxy) ethoxypropanoate	-1.16	0.0128	0.0458	22405	10040	annotated
1980	Benzoylmalic acid	-1.41	0.0132	0.0469	20823	7814	annotated
3784	(S)C(S)S-S-Methylcysteine sulfoxide	0.65	0.0134	0.0477	16910	26521	annotated

CTL T0h vs CTL T24h

Peak id	Metabolite	Log fc	p	Adjusted p	Peak intensity CTL T0h	Peak intensity CTL T24h	Identification
71	PE-NMe(18:1(9Z)/18:1(9Z))	0.24	0.0000	0.0000	54503658	64520086	annotated
173	beta-Alanine	-0.78	0.0000	0.0000	28674370	16692828	identified
235	L-Tyrosine	-0.97	0.0000	0.0000	17063947	8694339	identified+fragment
238	Hydroxypropyl-Serine	-0.93	0.0000	0.0000	594882	311966	annotated
239	Gamma-Glutamyltyrosine	-1.14	0.0000	0.0000	327618	148437	annotated+fragment
256	N6-Acetyl-5S-hydroxy-L-lysine	-8.27	0.0000	0.0000	4030878	13043	annotated
263	Hydroxypropyl-Proline	1.51	0.0000	0.0000	1361485	3890647	annotated
291	(S)-2,3,4,5-Tetrahydropyridine-2-carboxylate	-4.78	0.0000	0.0000	9054823	329549	annotated
299	Dihydroclavaminc acid	-3.89	0.0000	0.0000	115922	7838	annotated
302	Pyroglutamylglycine	-5.27	0.0000	0.0000	113826	2941	annotated
308	Succinylproline	-2.13	0.0000	0.0000	27049	6191	annotated
316	Alanyl-Aspartate	-8.93	0.0000	0.0000	7612220	15590	annotated
337	gibberellin A2 O-beta-D-glucoside	3.04	0.0000	0.0000	45789	375726	annotated
534	Tromethamine	2.22	0.0000	0.0000	244275	1136139	annotated+fragment
662	L-Glutamate	-0.72	0.0000	0.0000	4080611	2483110	identified+fragment
751	Isoleucyl-Serine	-11.89	0.0000	0.0000	2266946	597	annotated
817	Melledonal B	0.34	0.0000	0.0000	13643	17271	annotated
933	Hypoglycin B	-6.93	0.0000	0.0000	953523	7828	annotated
934	L-cis-Cyclo(aspartylphenylalanyl)	-4.70	0.0000	0.0000	307593	11807	annotated
1063	(S)-Spinacine	-1.38	0.0000	0.0000	108860	41808	annotated
1064	2,4-Diamino-6-nitrotoluene	-1.38	0.0000	0.0000	108860	41808	annotated
1102	2,3-Dehydrosalvipisone	1.14	0.0000	0.0000	84055	184856	annotated
1218	(S)-11,12,13-Trinor-7-calamenone	1.93	0.0000	0.0000	93148	353939	annotated
1223	PC(20:3(8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z))	-0.95	0.0000	0.0000	477366	246735	annotated
1253	Alanyl-Proline	1.97	0.0000	0.0000	89889	351029	annotated
1276	Alanyl-Threonine	-0.73	0.0000	0.0000	513882	309166	annotated
1356	Mammea B/AC cyclo D	0.68	0.0000	0.0000	127432	204602	annotated
1388	PC(20:3(8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	-0.83	0.0000	0.0000	376968	212123	annotated
1594	Alanyl-Arginine	-2.05	0.0000	0.0000	195615	47258	annotated
1595	Aprobarbital	0.66	0.0000	0.0000	104568	164900	annotated
1807	5-Hydroxytryptophol	-3.34	0.0000	0.0000	97622	9619	annotated

1832	apo-[3-methylcrotonoyl-CoA:carbon-dioxide ligase (ADP-	0.69	0.0000	0.0000	65499	105931	annotated
1921	Glycyl-Arginine	-1.12	0.0000	0.0000	58312	26804	annotated
1933	trizma acetate	-1.33	0.0000	0.0000	42963	17140	annotated
1960	Dambonitol	-1.11	0.0000	0.0000	52150	24204	annotated
2437	Phenylacetic acid	1.41	0.0000	0.0000	447073	1186380	annotated
2483	L-Tyrosine	-1.02	0.0000	0.0000	2904110	1430124	annotated+fragment
2496	Calabaxanthone	-0.86	0.0000	0.0000	49774	27457	annotated
2603	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	0.59	0.0000	0.0000	1198880	1806127	annotated
2633	Glycylproline	-1.93	0.0000	0.0000	169620	44394	annotated
2704	Tizanidine	-0.62	0.0000	0.0000	21472	13961	annotated
2756	2-Oxoglutaramate	-2.89	0.0000	0.0000	1519381	204277	annotated
2757	Glutaryl-glycine	-5.69	0.0000	0.0000	1403951	27236	annotated
2760	L-gamma-glutamyl-L-isoleucine	-7.99	0.0000	0.0000	141972	557	annotated
3081	Dodecanedioic acid	1.65	0.0000	0.0000	54745	172031	annotated
3082	2-Oxosuccinamate	-6.33	0.0000	0.0000	913517	11365	annotated
3102	Methyl benzoate	0.81	0.0000	0.0000	300493	527280	annotated
3179	Tiglylglycine	-4.10	0.0000	0.0000	724633	42162	annotated
3185	5,6-Dihydrothymine	-2.73	0.0000	0.0000	779146	117182	annotated
3465	Methyl benzoate	0.92	0.0000	0.0000	233220	442147	annotated
3520	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	3.11	0.0000	0.0000	36062	311256	annotated
3525	2,4,6-Triethyl-1,3,5-trioxane	1.02	0.0000	0.0000	177546	359150	annotated
3536	N-Acetyl-L-aspartate	-0.87	0.0000	0.0000	315928	173155	annotated
3654	3R-hydroxy-decanoic acid	1.61	0.0000	0.0000	78521	239725	annotated
3715	4,5-Dihydroorotic acid	-3.42	0.0000	0.0000	405568	37843	annotated
4082	Glycylprolylhydroxyproline	1.76	0.0000	0.0000	30394	102957	annotated
4279	L-gamma-glutamyl-L-leucine	-1.09	0.0000	0.0000	141972	66689	annotated
4393	2-aminomuconic acid semialdehyde	-1.73	0.0000	0.0000	110493	33217	annotated
4468	Ascorbate	-1.30	0.0000	0.0000	56913	23116	annotated
280	L-Theanine	-0.74	0.0000	0.0001	8980666	5358547	annotated
281	Neolinustatin	-0.81	0.0000	0.0001	398256	227230	annotated
1103	N-Jasmonoyltyrosine	0.58	0.0000	0.0001	116434	173715	annotated
1533	Neotussilage	0.59	0.0000	0.0001	45722	68883	annotated
1599	(3S)-3-Hydroxy-L-enduracididine	-1.14	0.0000	0.0001	197370	89832	annotated
1697	Cyclovariegatin	-0.77	0.0000	0.0001	175726	103217	annotated
2191	Bromisovalum	0.08	0.0000	0.0001	140902	148845	annotated
2259	Ethyl (±)-3-methylpentanoate	0.55	0.0000	0.0001	5465330	8002862	annotated
3123	3D,7D,11D-Phytanic acid	-0.69	0.0000	0.0001	724603	450485	annotated
3188	Methyl benzoate	0.88	0.0000	0.0001	147322	271187	annotated
842	Isoleucyl-Aspartate	-0.63	0.0000	0.0002	139345	89866	annotated

1095	Thiomorpholine 3-carboxylate	0.98	0.0000	0.0002	211207	417749	annotated
1107	Gamma-Glutamyl Glutamine	-0.74	0.0000	0.0002	770025	461178	annotated
1967	Hyperforin	0.50	0.0000	0.0002	24034	34084	annotated
4305	Tetradecanedioic acid	0.65	0.0000	0.0002	43522	68341	annotated
1312	1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione	-0.68	0.0000	0.0004	324734	202358	annotated
4056	(R)-3-Hydroxooctanoic acid	0.40	0.0000	0.0004	121004	159859	annotated
1455	PE(22:4(7Z,10Z,13Z,16Z)/P-18:0)	0.54	0.0000	0.0006	145554	212252	annotated
2726	Nonyl octanoate	-0.67	0.0000	0.0006	1266366	794837	annotated+fragment
3522	Indolelactate	0.95	0.0000	0.0006	191423	371021	annotated
1715	PI(18:1(9Z)/16:1(9Z))	1.18	0.0001	0.0008	70477	159144	annotated
696	3-Ureidopropionate	-0.65	0.0001	0.0010	2849243	1819167	annotated+fragment
1050	Sakacin P	-1.12	0.0001	0.0010	249517	114560	annotated
1052	Dinex	-1.30	0.0001	0.0010	345678	140134	annotated
1317	Pirbuterol	0.21	0.0001	0.0011	362749	418340	annotated
1824	Ligustilide	0.41	0.0001	0.0011	64283	85519	annotated
4420	7-oxo-8-amino-nonanoic acid	0.95	0.0001	0.0011	28368	54629	annotated
1074	N2-Acetyl-L-aminoadipate	-0.67	0.0001	0.0012	56961	35845	annotated
1395	PE(22:5(7Z,10Z,13Z,16Z,19Z)/P-18:0)	0.46	0.0001	0.0012	209573	287998	annotated
4216	Oxprenolol	-0.77	0.0001	0.0013	123102	72033	annotated
4645	Acenaphthenequinone	-0.52	0.0001	0.0013	48453	33804	annotated
1	Betaine	-0.54	0.0001	0.0014	1704046315	1175697621	identified+fragment
1935	Butenylcarnitine	0.62	0.0001	0.0014	37329	57323	annotated
51	Miraxanthin-I	-0.72	0.0001	0.0015	1346913	815996	annotated
1096	Cer(d18:1/24:1(15Z))	-0.83	0.0002	0.0020	622358	351224	annotated
47	L-Glutamine	-0.45	0.0002	0.0021	157564731	115120831	identified+fragment
2771	D-Glucosamine	-0.52	0.0002	0.0021	1569767	1095655	annotated
3578	4-Methoxybenzyl formate	0.98	0.0002	0.0025	105542	208143	annotated
1104	Benzenepropanenitrile	0.50	0.0003	0.0027	124949	176742	annotated
982	Homoarecoline	1.23	0.0003	0.0028	337756	789996	annotated
991	Cytidine	-0.68	0.0003	0.0028	625725	390525	identified
3840	2-Amino-1,7,9-trimethylimidazo[4,5-g]quinoxaline	0.18	0.0003	0.0028	126221	142575	annotated
48	N-Nitrosoguvacoline	-0.46	0.0003	0.0030	7777423	5665569	annotated
1058	Ethosuximide	0.29	0.0003	0.0030	182985	223358	annotated
3095	thymine	0.29	0.0003	0.0030	452429	551328	identified
1980	Anhalamine	-0.71	0.0003	0.0031	64827	39766	annotated
1994	Kamahine C	-0.69	0.0003	0.0031	50418	31303	annotated
231	Hypoxanthine	-0.77	0.0003	0.0034	16841451	9850372	identified+fragment
1452	Isolinderanolide	-0.65	0.0003	0.0034	98872	62912	annotated
4485	PG(18:1(9Z)/18:0)	0.44	0.0004	0.0035	44897	60720	annotated

2594	Ovalitenin A	-0.61	0.0004	0.0036	79008	51651	annotated
166	Anandamide (20:2, n-6)	1.37	0.0004	0.0039	3372075	8730494	annotated
3936	7-bromo-5-heptynoic acid	0.16	0.0005	0.0046	206599	230439	annotated
1733	N,N-Dihydroxy-L-valine	-0.47	0.0005	0.0051	178342	128824	annotated
2203	2-Methylcitric acid	-0.54	0.0005	0.0051	56878	39191	annotated
2492	GW 6471	-0.54	0.0005	0.0051	80304	55257	annotated
4562	Homocystine	-0.75	0.0005	0.0051	41814	24783	identified
1007	L-N2-(2-Carboxyethyl)arginine	-1.23	0.0006	0.0052	408866	174399	annotated
724	Didodecyl thiobispropanoate	0.43	0.0006	0.0053	808723	1090896	annotated
234	Dihydrobiopterin	-0.69	0.0006	0.0058	97804	60635	annotated
659	5-Methylthio-D-ribose	-0.58	0.0006	0.0059	2621915	1754330	annotated
1225	5-Methylcytidine	-0.51	0.0006	0.0059	257742	180848	annotated+fragment
1592	11-Aminoundecanoic acid	0.34	0.0007	0.0062	70768	89399	annotated
1048	N-Methylcalystegine B2	-0.56	0.0007	0.0064	376538	255142	annotated
1690	Asparaginyl-Valine	-0.80	0.0007	0.0064	73756	42458	annotated
2130	4-Dodecylbenzenesulfonic Acid	-1.45	0.0007	0.0066	3325987	1219618	annotated+fragment
73	L-Arginine	-0.47	0.0009	0.0076	57344499	41398532	identified+fragment
407	NG,NG-Dimethyl-L-arginine	-0.47	0.0009	0.0080	3751218	2713402	annotated
2586	N-Formimino-L-glutamate	-0.68	0.0010	0.0082	355762	222175	annotated
1393	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/P-18:0)	0.35	0.0011	0.0089	253394	322503	annotated
1846	Hexamethylene bisacetamide	0.87	0.0011	0.0093	30664	56220	annotated
843	L-Ornithine	-0.61	0.0012	0.0100	1649963	1078471	identified+fragment
4182	Hexanoylglycine	-0.96	0.0012	0.0100	92138	47332	annotated
276	PC(O-16:0/18:2(9Z,12Z))	0.24	0.0013	0.0104	258338	304455	annotated
1441	Diethanolamine	0.33	0.0013	0.0105	241478	302645	annotated
928	Guanidinoacetate	-1.39	0.0013	0.0106	740056	283162	annotated
2471	Methionyl-Cysteine	-0.42	0.0014	0.0109	23091	17271	annotated
4769	Benzoylmalic acid	-0.68	0.0014	0.0113	20823	13034	annotated
2464	trans-Grandmarin	-0.40	0.0015	0.0121	47896	36409	annotated
2499	7-Hydroxybutylideneephthalide 7-(6-malonylglucoside)	-0.42	0.0018	0.0139	49219	36735	annotated
1991	Cysteineglutathione disulfide	-0.51	0.0019	0.0145	65142	45656	annotated
4563	Phenindione	-0.52	0.0020	0.0149	59613	41716	annotated
2604	Pseudouridine	-0.63	0.0020	0.0154	1099719	711687	annotated+fragment
1366	Etrimfos	-0.62	0.0021	0.0156	82486	53758	annotated
2754	Alloxanthine	-0.53	0.0021	0.0159	1478996	1024335	annotated+fragment
2236	Chloroform	-0.37	0.0022	0.0164	26285640	20390595	annotated
1407	N-gamma-L-Glutamyl-L-methionine	-0.61	0.0023	0.0169	326596	214331	annotated
1027	PE(20:0/15:0)	0.19	0.0024	0.0177	771517	877957	annotated
1587	Glyburide	-0.68	0.0025	0.0182	83089	52031	annotated

1883	S-Propyl-L-cysteine	-0.65	0.0026	0.0191	74284	47287	annotated
4683	Phenylpyruvate	-0.61	0.0026	0.0192	38658	25313	annotated
3543	7(14)-Bisabolene-2,3,10,11-tetrol	0.28	0.0027	0.0195	23509	28509	annotated
3446	Amino adipic acid	-0.54	0.0027	0.0197	485616	334100	annotated+fragment
1601	(2R,2'S)-Isobuteine	-0.66	0.0028	0.0201	178834	113166	annotated
2535	Cvclocommunin	0.66	0.0028	0.0202	8062	12778	annotated
1591	N-lactoyl-Methionine	-1.34	0.0031	0.0216	40847	16100	annotated
167	L-Valine	-0.45	0.0031	0.0221	23293168	17034966	identified+fragment
88	O-Desmethyicarvedilol	-0.66	0.0032	0.0226	76148	48132	annotated
715	5'-Phosphoribosylglycinamide	0.18	0.0033	0.0233	32557	36956	annotated
3586	3R-hydroxy-hexanoic acid	0.35	0.0034	0.0238	245629	314129	annotated
1977	1,2,3-Trimethylbenzene	0.43	0.0039	0.0264	38786	52171	annotated
4378	3-Sulfinoalanine	-0.67	0.0039	0.0267	72175	45434	annotated
2596	Dienestrol	-0.59	0.0041	0.0279	54656	36210	annotated
1890	Cyclobrassinone	-0.52	0.0043	0.0285	81943	57134	annotated
1032	9-Bromo-16alpha-methyl-pregn-4-ene-3,11,20-trione	0.24	0.0043	0.0286	117917	138906	annotated
3787	3R-hydroxy-octadecanoic acid	-0.48	0.0046	0.0304	210070	150635	annotated
1374	Hydroxypropyl-Threonine	-0.58	0.0049	0.0322	57594	38446	annotated
1853	N-Acetyl-L-methionine	-0.68	0.0049	0.0323	66957	41932	annotated
4045	cis-3-Hexenyl pyruvate	0.15	0.0050	0.0325	97810	108588	annotated
2649	Loteprednol	0.03	0.0050	0.0327	106105	108142	annotated
2707	Tauro-b-muricholic acid	0.85	0.0053	0.0343	869335	1570577	annotated+fragment
3132	cholesterol sulfate	0.18	0.0056	0.0357	577076	654785	annotated
136	PC(16:0/0:0)	0.46	0.0057	0.0365	13097980	18046273	annotated
3616	L-trans-alpha-Amino-2-carboxycyclopropaneacetic acid	-0.67	0.0060	0.0380	307612	193548	annotated
1474	N-Acetylhistidine	-0.82	0.0061	0.0384	198941	112996	annotated
61	(S)-2-Aminobutanoate	-0.38	0.0062	0.0391	131321504	101091921	annotated+fragment
2791	N-Nitrosofolic acid	-0.42	0.0066	0.0408	22757	16962	annotated
170	L-Methionine	-0.46	0.0068	0.0416	27563852	20095208	identified+fragment
1436	N-acetyl-L-2-amino adipate(2-)	-0.80	0.0070	0.0429	243087	139591	annotated
3640	Patulin	0.30	0.0070	0.0429	259748	319111	annotated+fragment
678	Trimethylamine N-oxide	-0.68	0.0071	0.0430	2785145	1734477	annotated
1535	(3S,5S)-Carbapenam-3-carboxylic acid	-0.70	0.0071	0.0431	322983	198415	annotated
1687	3alpha,4,5,7alpha-Tetrahydro-5-hydroxy-1H-isoindole-	-0.49	0.0071	0.0432	142465	101426	annotated+fragment
3544	Ipomeatetrahydrofuran	0.47	0.0071	0.0433	150546	207868	annotated
2105	5-Hexenyl glucosinolate	0.31	0.0072	0.0437	17839	22131	annotated
2517	Dimethylenetriurea	0.22	0.0073	0.0440	178222	207263	annotated
2248	Firocoxib	-0.54	0.0077	0.0459	98034	67360	annotated
831	PE(20:2(11Z,14Z)/16:0)	0.15	0.0083	0.0490	1793132	1985846	annotated

CTL T0h vs CTL T48h

Peak id	Metabolite	Log fc	p	Adjusted p	Peak intensity CTL T0h	Peak intensity CTL T48h	Identification
136	PC(16:0/0:0)	1.12	0.000	0.000	13097980	28491636	annotated
249	PC(18:0/0:0)	0.93	0.000	0.000	6753844	12909960	annotated+fragment
256	N6-Acetyl-5S-hydroxy-L-lysine	-8.94	0.000	0.000	4030878	8213	annotated
263	Hydroxypropyl-Proline	1.51	0.000	0.000	1361485	3886300	annotated
291	(S)-2,3,4,5-Tetrahydropyridine-2-carboxylate	-4.85	0.000	0.000	9054823	312886	annotated
299	Dihydroclavaminic acid	-4.04	0.000	0.000	115922	7039	annotated
302	Pyroglutamylglycine	-7.68	0.000	0.000	113826	555	annotated
308	Succinylproline	-1.98	0.000	0.000	27049	6837	annotated
316	Alanyl-Aspartate	-8.81	0.000	0.000	7612220	16988	annotated
337	gibberellin A2 O-beta-D-glucoside	3.08	0.000	0.000	45789	388118	annotated
534	Tromethamine	4.04	0.000	0.000	244275	4028183	annotated+fragment
724	Didodecyl thiobispropanoate	1.44	0.000	0.000	808723	2186680	annotated
817	Melledonal B	0.51	0.000	0.000	13643	19475	annotated
934	L-cis-Cyclo(aspartylphenylalanyl)	-3.88	0.000	0.000	307593	20898	annotated
969	LysoPC(16:1(9Z))	1.19	0.000	0.000	740361	1686056	annotated
1012	Pantothenic acid	-0.70	0.000	0.000	1054925	647598	annotated+fragment
1050	Sakacin P	-1.41	0.000	0.000	249517	93639	annotated
1063	(S)-Spinacine	-1.19	0.000	0.000	108860	47665	annotated
1064	2,4-Diamino-6-nitrotoluene	-1.19	0.000	0.000	108860	47665	annotated
1069	Haloperidol 1,2,3,6-tetrahydropyridine	-0.91	0.000	0.000	36777	19532	annotated
1074	N2-Acetyl-L-aminoadipate	-0.92	0.000	0.000	56961	30203	annotated
1102	2,3-Dehydrosalvipisone	1.93	0.000	0.000	84055	320993	annotated
1103	N-Jasmonoyltyrosine	1.46	0.000	0.000	116434	319940	annotated
1104	Benzenepropanenitrile	1.37	0.000	0.000	124949	323645	annotated
1203	N,2,3-Trimethyl-2-(1-methylethyl)butanamide	-0.82	0.000	0.000	623391	353128	annotated
1204	Adenosine	-2.13	0.000	0.000	336284	76640	identified+fragment
1218	(S)-11,12,13-Trinor-7-calamenone	2.75	0.000	0.000	93148	625497	annotated
1253	Alanyl-Proline	1.97	0.000	0.000	89889	352173	annotated
1276	Alanyl-Threonine	-0.67	0.000	0.000	513882	322130	annotated
1356	Mammea B/AC cyclo D	1.62	0.000	0.000	127432	392037	annotated
1533	Neotussilagine	0.73	0.000	0.000	45722	75631	annotated
1591	N-lactovl-Methionine	-1.90	0.000	0.000	40847	10962	annotated
1594	Alanyl-Arginine	-1.81	0.000	0.000	195615	55890	annotated

1688	dodecanamide	-0.80	0.000	0.000	155143	88857	annotated
1690	Asparaginy-Valine	-1.43	0.000	0.000	73756	27294	annotated
1763	1-Acetylcyclohexyl acetate	0.65	0.000	0.000	85922	134839	annotated
1807	5-Hydroxytryptophol	-2.21	0.000	0.000	97622	21134	annotated
1824	Ligustilide	1.04	0.000	0.000	64283	132087	annotated
1914	1,2-Dimethoxy-13-methyl-[1,3]benzodioxolo[5,6-	-1.03	0.000	0.000	20522	10031	annotated
1921	Glycyl-Arginine	-1.12	0.000	0.000	58312	26777	annotated
1933	trizma acetate	-1.29	0.000	0.000	42963	17562	annotated
1967	Hyperforin	1.50	0.000	0.000	24034	67870	annotated
2034	Triethylene Glycol Monomethyl Ether	-1.12	0.000	0.000	40014	18408	annotated
2060	(2S,2'S)-Pyrosaccharopine	1.67	0.000	0.000	12009	38163	annotated
2236	Chloroform	-0.50	0.000	0.000	26285640	18613114	annotated
2437	Phenylacetic acid	3.39	0.000	0.000	447073	4675986	annotated
2603	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	1.22	0.000	0.000	1198880	2798537	annotated
2633	Glycylproline	-2.04	0.000	0.000	169620	41128	annotated
2756	2-Oxoglutaramate	-3.19	0.000	0.000	1519381	166829	annotated
2757	Glutaryl-glycine	-6.08	0.000	0.000	1403951	20771	annotated
2760	L-gamma-glutamyl-L-isoleucine	-5.39	0.000	0.000	141972	3382	annotated
2804	PI(18:2(9Z,12Z)/20:1(11Z))	0.47	0.000	0.000	1058482	1470230	annotated
3081	Dodecanedioic acid	3.23	0.000	0.000	54745	514823	annotated
3082	2-Oxosuccinamate	-6.09	0.000	0.000	913517	13409	annotated
3102	Methyl benzoate	1.18	0.000	0.000	300493	681407	annotated
3131	(3xi.6xi)-Cvclo(alanylvalyl)	0.26	0.000	0.000	235994	281798	annotated
3179	Tiglylglycine	-3.89	0.000	0.000	724633	48867	annotated
3185	5,6-Dihydrothymine	-2.67	0.000	0.000	779146	122628	annotated
3188	Methyl benzoate	2.09	0.000	0.000	147322	625348	annotated
3465	Methyl benzoate	1.72	0.000	0.000	233220	767563	annotated
3466	4-Hydroxycyclohexylcarboxylic acid	0.73	0.000	0.000	427237	708348	annotated
3467	Azelaic acid	0.75	0.000	0.000	136194	229593	annotated
3520	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	3.06	0.000	0.000	36062	300226	annotated
3525	2,4,6-Triethyl-1,3,5-trioxane	1.10	0.000	0.000	177546	379666	annotated
3543	7(14)-Bisabolene-2,3,10,11-tetrol	0.86	0.000	0.000	23509	42591	annotated
3544	Ipomeatetrahydrofuran	1.41	0.000	0.000	150546	400445	annotated
3581	Nevirapine	0.61	0.000	0.000	333739	508620	annotated
3654	3R-hydroxy-decanoic acid	1.77	0.000	0.000	78521	268285	annotated
3715	4,5-Dihydroorotic acid	-3.08	0.000	0.000	405568	47952	annotated
3840	2-Amino-1,7,9-trimethylimidazo[4,5-g]quinoxaline	0.44	0.000	0.000	126221	171085	annotated
4049	(2E,4E,6E)-4-Methylocta-2,4,6-trienedial	0.52	0.000	0.000	21460	30801	annotated
4056	(R)-3-Hydroxyoctanoic acid	0.86	0.000	0.000	121004	219564	annotated

4082	Glycylprolylhydroxyproline	1.90	0.000	0.000	30394	113137	annotated
4182	Hexanoylglycine	-2.00	0.000	0.000	92138	23087	annotated
4216	Oxprenolol	-1.65	0.000	0.000	123102	39152	annotated
4279	L-gamma-glutamyl-L-leucine	-0.98	0.000	0.000	141972	71754	annotated
4305	Tetradecanedioic acid	1.11	0.000	0.000	43522	93659	annotated
4393	2-aminomuconic acid semialdehyde	-1.76	0.000	0.000	110493	32570	annotated
4420	7-oxo-8-amino-nonanoic acid	1.44	0.000	0.000	28368	76819	annotated
4468	Ascorbate	-1.44	0.000	0.000	56913	20994	annotated
4473	Glycerol tripropanoate	0.95	0.000	0.000	40122	77281	annotated
4593	xi-3-Methyl-3-cyclohexen-1-ol	0.88	0.000	0.000	28887	53022	annotated
4602	Dicyclohexyl disulfide	0.91	0.000	0.000	27866	52224	annotated
99	PC(18:1(9Z)/18:1(9Z))	0.28	0.000	0.000	44872845	54304628	annotated
280	L-Theanine	-0.60	0.000	0.000	8980666	5916113	annotated
959	15beta-Hydroxy-7alpha-mercapto-pregn-4-ene-3,20-dione	0.64	0.000	0.000	1044487	1623429	annotated
979	hydroxyisovaleroyl carnitine	1.18	0.000	0.000	42296	95795	annotated
1216	PI(18:1(9Z)/18:2(9Z,12Z))	0.52	0.000	0.000	110136	158438	annotated
1312	1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione	-0.67	0.000	0.000	324734	204222	annotated
3539	4-beta-Hydroxymethyl-4-alpha-methyl-5-alpha-cholest-7-	-0.44	0.000	0.000	543493	401897	annotated+fragment
3586	3R-hydroxy-hexanoic acid	0.69	0.000	0.000	245629	397041	annotated
4134	(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	0.92	0.000	0.000	43496	82261	annotated
4431	Phenylpropanoate	0.76	0.000	0.000	29552	50209	annotated
536	Glutamylphenylalanine	-0.56	0.000	0.000	422898	286439	annotated+fragment
1027	PE(20:0/15:0)	-0.45	0.000	0.000	771517	565359	annotated
1452	Isolinderanolide	-0.66	0.000	0.000	98872	62400	annotated
1592	11-Aminoundecanoic acid	0.58	0.000	0.000	70768	105652	annotated
2938	3-Hydroxy-2-methyl-[S-(R,R)]-butanoic acid	-0.49	0.000	0.000	1198803	854599	annotated
807	L-phenylalanyl-L-hydroxyproline	-0.83	0.000	0.000	553165	310685	annotated
1960	Dambonitol	-0.78	0.000	0.000	52150	30359	annotated
2259	Ethyl (±)-3-methylpentanoate	0.61	0.000	0.000	5465330	8347271	annotated
810	(Ac)2-L-Lys-D-Ala	-0.74	0.000	0.000	133498	79678	annotated
1052	Dinex	-1.22	0.000	0.000	345678	148850	annotated
1097	PE(22:5(7Z,10Z,13Z,16Z,19Z)/16:0)	0.35	0.000	0.000	629623	800970	annotated
1483	SM(d18:0/18:1(9Z))	-0.47	0.000	0.000	270930	195290	annotated
999	Mephobarbital	-1.19	0.000	0.001	799140	351250	annotated
1551	Normetanephrene	-0.69	0.000	0.001	234624	145920	annotated
1839	Thymidine	-0.61	0.000	0.001	82530	53978	annotated
4045	cis-3-Hexenyl pyruvate	0.41	0.000	0.001	97810	129725	annotated
1446	3,4-Methyleneazelaic acid	0.77	0.000	0.001	41221	70519	annotated
1830	(4-Hydroxy-3-methoxyphenyl)ethanol	-0.91	0.000	0.001	57645	30727	annotated

3132	cholesterol sulfate	0.45	0.000	0.001	577076	788703	annotated
1826	PI(18:1(9Z)/18:3(6Z,9Z,12Z))	0.40	0.000	0.001	83372	109677	annotated
1604	Cer(d18:1/23:0)	-0.68	0.000	0.001	182507	113659	annotated
1268	N-Lignoceroylsphingosine	-0.67	0.000	0.001	368948	232281	annotated
1370	O-Ureido-L-serine	0.33	0.000	0.001	308340	388618	annotated
1832	apo-[3-methylcrotonoyl-CoA:carbon-dioxide ligase (ADP-	0.54	0.000	0.001	65499	95236	annotated
1936	Geranyl acetoacetate	0.44	0.000	0.001	61204	83239	annotated
3924	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	0.58	0.000	0.001	167448	250919	annotated
4562	Homocystine	-0.69	0.000	0.001	41814	25914	identified
1096	Cer(d18:1/24:1(15Z))	-0.74	0.000	0.001	622358	371385	annotated
1474	N-Acetylhistidine	-0.94	0.000	0.001	198941	103382	annotated
1630	3-hydroxy-dodecanedioic acid	-0.73	0.000	0.001	145410	87369	annotated
3540	3-(2-Hydroxy-4-methylphenyl)-2-butanone	-0.70	0.000	0.001	199014	122756	annotated
2015	Myrtine	0.56	0.000	0.002	42368	62562	annotated
137	PE(20:4(5Z,8Z,11Z,14Z)/0:0)	0.75	0.000	0.002	236263	397511	annotated
251	LysoPE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	0.60	0.000	0.002	104799	159146	annotated
843	L-Ornithine	-0.57	0.000	0.002	1649963	1114771	identified+fragment
1288	2-Dimethylamino-5,6-dimethylpyrimidin-4-ol	0.82	0.000	0.002	169066	299064	annotated
1753	Phenylethyl alcohol	0.59	0.000	0.002	97685	146868	annotated
1364	Daidzein 4'-O-glucuronide	-1.02	0.000	0.002	261165	128992	annotated
4525	2,2-Dichloroacetaldehyde	0.37	0.000	0.002	53494	69056	annotated
250	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	0.65	0.000	0.002	190766	299989	annotated
2436	3-Oxohexanoic acid	0.47	0.000	0.002	2956786	4098778	annotated
1053	N-Butyrylglycine	-0.57	0.000	0.003	365362	245953	annotated
3278	Apigenin 7-sulfate	-0.75	0.000	0.003	422784	250892	annotated
3603	Metaldehyde	0.69	0.000	0.003	111255	179947	annotated
1595	Aprobarbital	0.58	0.000	0.003	104568	156736	annotated
3095	thymine	0.40	0.000	0.003	452429	598945	identified
1273	(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid	-0.35	0.000	0.003	458580	358684	annotated
1660	3alpha,4,7,7alpha-Tetrahydro-1H-isoindole-1,3(2H)-dione	-0.56	0.000	0.003	170646	115359	annotated
1715	PI(18:1(9Z)/16:1(9Z))	1.25	0.000	0.003	70477	167116	annotated
4708	Dihydrolipoamide	-0.66	0.000	0.003	22332	14121	annotated
1468	6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one	-0.29	0.000	0.003	263564	215444	annotated
1779	Peperinic acid	0.42	0.001	0.004	101632	135909	annotated
1932	Heptyl p-hydroxybenzoate	0.50	0.001	0.004	50612	71736	annotated
2114	2-Hydroxynicotinic acid	-0.46	0.001	0.004	19270	13998	annotated
230	PC(P-18:0/0:0)	0.53	0.001	0.004	67679	97409	annotated
1212	Tributyl phosphate	-0.53	0.001	0.005	581258	402037	annotated
1225	5-Methylcytidine	-0.41	0.001	0.005	257742	193921	annotated+fragment

1401	Norambreinolide	0.62	0.001	0.005	149875	230334	annotated
4650	PE(O-18:1(9Z)/0:0)	0.44	0.001	0.006	25771	34884	annotated
662	L-Glutamate	-0.31	0.001	0.006	4080611	3288425	identified+fragment
1537	N-(3-oxo-octanoyl)-homoserine lactone	0.55	0.001	0.006	37226	54613	annotated
1007	L-N2-(2-Carboxyethyl)arginine	-1.08	0.001	0.007	408866	192796	annotated
1357	Isoetharine	1.06	0.001	0.007	92580	192785	annotated
281	Neolinustatin	-0.48	0.001	0.007	398256	286222	annotated
1220	Butalbital	-0.54	0.001	0.007	602682	415079	annotated
108	Methyl N-methylanthranilate	-0.27	0.001	0.008	39907689	33113567	annotated+fragment
1080	4-Aminosalicylate	-0.49	0.001	0.008	25273	17964	annotated
1442	SM(d18:2/18:1)	-0.49	0.001	0.008	252747	179531	annotated
1999	2,6-Dimethoxyphenol	-0.52	0.001	0.008	44508	31023	annotated
696	3-Ureidopropionate	-0.43	0.001	0.008	2849243	2110458	annotated+fragment
1006	7-Methylguanine	-0.44	0.001	0.009	921756	677885	annotated
3536	N-Acetyl-L-aspartate	-0.49	0.001	0.009	315928	225178	annotated
1497	delta-Guanidinovaleric acid	-0.75	0.001	0.009	200482	119076	annotated
2594	Ovalitenin A	-0.44	0.001	0.009	79008	58070	annotated
1048	N-Methylcalystegine B2	-0.42	0.001	0.010	376538	281521	annotated
3640	Patulin	-0.52	0.002	0.011	259748	181083	annotated+fragment
1384	Alanyl-Alanine	-0.45	0.002	0.011	365552	268038	annotated
3509	Furmecyclox	-0.56	0.002	0.011	359772	243241	annotated
1536	Cumene	0.89	0.002	0.012	88986	164486	annotated
166	Anandamide (20:2, n-6)	1.36	0.002	0.012	3372075	8626231	annotated
1728	beta,beta-dimethyl acrylic acid	-0.79	0.002	0.012	121106	70009	annotated
1599	(3S)-3-Hydroxy-L-enduracididine	-0.61	0.002	0.014	197370	129397	annotated
1449	PE(20:2(11Z,14Z)/P-16:0)	-0.40	0.002	0.014	300027	226847	annotated
3331	Acetoxyacetone	-0.31	0.002	0.015	588982	474438	annotated
1762	N-Methylcalystegine C1	-0.37	0.002	0.016	131055	101157	annotated
2271	9-Octadecenoic acid 1-[(phosphonoxy)methyl]-1,2-	0.28	0.002	0.016	114180	138922	annotated
1601	(2R,2'S)-Isobutene	-0.53	0.002	0.016	178834	123599	annotated
170	L-Methionine	-0.38	0.003	0.018	27563852	21183247	identified+fragment
3446	Amino adipic acid	-0.42	0.003	0.018	485616	362384	annotated+fragment
2029	(R,S)-Nicotine	-0.48	0.003	0.018	37814	27117	annotated
1291	Methoxybrassinin	0.19	0.003	0.019	452079	516756	annotated
1402	2-Methyl-1,3-cyclohexadiene	0.58	0.003	0.019	213514	319448	annotated
1635	5-L-Glutamyl-taurine	-0.68	0.003	0.020	138977	86743	annotated
2284	Caproic acid	0.43	0.003	0.021	4240815	5718616	annotated
2754	Alloxanthine	-0.39	0.003	0.021	1478996	1125873	annotated+fragment
1564	3,5-Dimethoxytoluene	-0.56	0.003	0.022	183264	124494	annotated

4450	Barogenin	-0.65	0.004	0.022	62447	39703	annotated
126	PE(22:1(13Z)/15:0)	0.28	0.004	0.023	25252349	30573273	annotated
4666	2-(4-Methyl-5-thiazolyl)ethyl propionate	-2.83	0.004	0.023	25518	3591	annotated
1733	N,N-Dihydroxy-L-valine	-0.29	0.004	0.023	178342	145556	annotated
1683	Tranexamic acid	0.35	0.004	0.025	140457	179618	annotated
234	Dihydrobiopterin	-0.49	0.004	0.026	97804	69800	annotated
109	Phensuximide	-0.30	0.004	0.026	194925	157793	annotated
1264	3'-Amino-3'-deoxythimidine	-0.56	0.004	0.026	457390	310728	annotated
2954	Citramalate	-0.50	0.005	0.031	640205	452599	annotated
2770	2-Hydroxy-2-(2-oxopropyl)butanedioic acid	0.59	0.005	0.031	834404	1253628	annotated
1697	Cyclovariegatin	-0.36	0.006	0.034	175726	136759	annotated
4524	Nifuradene	-0.43	0.006	0.036	44476	33026	annotated
1101	Lentialexin	0.78	0.006	0.036	397506	682057	annotated
231	Hypoxanthine	-0.50	0.006	0.037	16841451	11892666	identified+fragment
3610	3-hydroxy-tetradecanedioic acid	0.59	0.006	0.038	281163	421896	annotated
1077	Porphobilinogen	-0.31	0.007	0.041	47121	37943	annotated
1535	(3S,5S)-Carbapenam-3-carboxylic acid	-0.58	0.007	0.041	322983	216519	annotated
1624	LysoPC(22:5(4Z,7Z,10Z,13Z,16Z))	0.39	0.007	0.042	139789	183529	annotated
407	NG,NG-Dimethyl-L-arginine	-0.28	0.008	0.044	3751218	3094704	annotated
842	Isoleucyl-Aspartate	-0.30	0.008	0.044	139345	112799	annotated
4040	5-Hydroxypyrazinamide	0.26	0.008	0.045	176975	211251	annotated
1038	PE(20:2(11Z,14Z)/14:0)	-0.40	0.009	0.049	744250	563796	annotated
2685	Glycyl-Threonine	-0.37	0.009	0.049	16125	12472	annotated

Dietary effect- complete study plasma (identified and annotated metabolites)

CTL T0h vs CTS T0h

Peak id	Metabolite	Log fc	p	Adjusted p	Peak intensity CTL T0h	Peak intensity CTS T0h	Identification
106	L-Acetopine	-2.74	0.000	0.000	46033555	6902232	annotated
256	N6-Acetyl-5S-hydroxy-L-lysine	-2.62	0.000	0.000	4030878	655222	annotated
263	Hydroxypropyl-Proline	1.30	0.000	0.000	1361485	3350537	annotated
291	(S)-2,3,4,5-Tetrahydropyridine-2-carboxylate	-2.20	0.000	0.000	9054823	1977365	annotated
295	L-alpha-glutamyl-L-hydroxyproline	-3.43	0.000	0.000	170964	15851	annotated
299	Dihydroclavaminc acid	-2.02	0.000	0.000	115922	28630	annotated
301	Seriny-Tyrosine	-1.57	0.000	0.000	105472	35418	annotated
302	Pyroglutamylglycine	-2.18	0.000	0.000	113826	25094	annotated
308	Succinylproline	-1.46	0.000	0.000	27049	9806	annotated
316	Alanyl-Aspartate	-2.47	0.000	0.000	7612220	1369807	annotated
320	Thionazin	-2.05	0.000	0.000	387545	93748	annotated
324	Histidiny-Aspartate	-2.18	0.000	0.000	68927	15192	annotated
327	Diazinon	-1.70	0.000	0.000	55110	16961	annotated
330	Bicozamycin	-1.25	0.000	0.000	40020	16777	annotated
337	gibberellin A2 O-beta-D-glucoside	2.40	0.000	0.000	45789	242243	annotated
368	Zizybeoside II	-3.49	0.000	0.000	170929	15203	annotated
534	Tromethamine	1.62	0.000	0.000	244275	752145	annotated+fragment
751	Isoleucyl-Serine	-2.56	0.000	0.000	2266946	383521	annotated
817	Melledonal B	0.32	0.000	0.000	13643	17037	annotated
932	Hydroxypropyl-Hydroxyproline	-1.56	0.000	0.000	1524416	517055	annotated
933	Hypoglycin B	-2.57	0.000	0.000	953523	161129	annotated
934	L-cis-Cyclo(aspartylphenylalanyl)	-2.31	0.000	0.000	307593	61936	annotated
935	Etoazole	-3.06	0.000	0.000	188279	22554	annotated

1063	(S)-Spinacine	-1.40	0.000	0.000	108860	41234	annotated
1064	2,4-Diamino-6-nitrotoluene	-1.40	0.000	0.000	108860	41234	annotated
1204	Adenosine	-1.60	0.000	0.000	336284	111231	identified+fragment
1253	Alanyl-Proline	1.49	0.000	0.000	89889	251888	annotated
1269	Glycyl-Aspartate	-2.64	0.000	0.000	536466	85974	annotated
1270	Lysyl-Asparagine	-2.42	0.000	0.000	336963	63125	annotated
1807	5-Hydroxytryptophol	-2.13	0.000	0.000	97622	22345	annotated
2010	N-(1-Deoxy-1-fructosyl)histidine	-2.19	0.000	0.000	59419	13022	annotated
2179	L-Homocysteic acid	-1.66	0.000	0.000	16524138	5213751	annotated
2477	5-Hydroxyindoleacetic acid	-2.50	0.000	0.000	3119805	551004	annotated
2633	Glycylproline	-1.80	0.000	0.000	169620	48658	annotated
2730	N-Acetyl-L-glutamate 5-semialdehyde	-2.35	0.000	0.000	1758411	344767	annotated
2756	2-Oxoglutamamate	-2.49	0.000	0.000	1519381	271323	annotated
2757	Glutaryl-glycine	-2.22	0.000	0.000	1403951	301121	annotated
2760	L-gamma-glutamyl-L-isoleucine	-1.99	0.000	0.000	141972	35692	annotated
3082	2-Oxosuccinamate	-2.32	0.000	0.000	913517	183509	annotated
3179	Tiglylglycine	-2.31	0.000	0.000	724633	146404	annotated
3185	5,6-Dihydrothymine	-1.92	0.000	0.000	779146	206440	annotated
3715	4,5-Dihydroorotic acid	-2.57	0.000	0.000	405568	68499	annotated
3757	3,6,8-Trimethylallantoin	-2.53	0.000	0.000	373951	64546	annotated
3759	N-Desmethylidiltiazem	-4.59	0.000	0.000	38406	1590	annotated
3772	1-Pyrenylsulfate	-2.16	0.000	0.000	350986	78402	annotated
4082	Glycylprolylhydroxyproline	1.13	0.000	0.000	30394	66293	annotated
4111	Adefovir	-2.11	0.000	0.000	27493	6351	annotated
4393	2-aminomuconic acid semialdehyde	-1.38	0.000	0.000	110493	42439	annotated
4441	Margrapine B	-2.14	0.000	0.000	45270	10246	annotated
1690	Asparaginy-Valine	-1.07	0.000	0.001	73756	35252	annotated
1097	PE(22:5(7Z,10Z,13Z,16Z,19Z)/16:0)	0.21	0.000	0.001	629623	729455	annotated
4279	L-gamma-glutamyl-L-leucine	-0.71	0.000	0.002	141972	86728	annotated
1921	Glycyl-Arginine	-0.87	0.000	0.005	58312	31796	annotated

1983	3-Hydroxymelatonin	-1.10	0.001	0.010	55209	25772	annotated
1074	N2-Acetyl-L-aminoadipate	-0.59	0.001	0.015	56961	37739	annotated
1853	N-Acetyl-L-methionine	-0.81	0.001	0.021	66957	38083	annotated
1632	6-Hydroxy-9,9-dimethyl-5-(3-methyl-1-oxobutyl)-1-propyl-3H,9H-[1,2]-dioxolo[3',4':4,5]furo[2,3-f][1]benzopyran-3-one	-0.44	0.001	0.022	151010	111108	annotated
969	LysoPC(16:1(9Z))	0.64	0.001	0.023	740361	1154325	annotated
1452	Isolinderanolide	-0.59	0.002	0.035	98872	65665	annotated
724	Didodecyl thiobispropanoate	-0.51	0.002	0.036	808723	568453	annotated
2804	PI(18:2(9Z,12Z)/20:1(11Z))	0.15	0.002	0.039	1058482	1171429	annotated
1048	N-Methylcalystegine B2	-0.53	0.002	0.043	376538	260764	annotated

CTL T12h vs CTS T12h

Peak id	Metabolite	Log fc	<i>p</i>	Adjusted <i>p</i>	Peak intensity CTL T12h	Peak intensity CTS T12h	Identification
106	L-Acetopine	-0.08	0.000	0.000	5298638	5025848	annotated
256	N6-Acetyl-5S-hydroxy-L-lysine	0.02	0.000	0.000	1810013	1835337	annotated
291	(S)-2,3,4,5-Tetrahydropyridine-2-carboxylate	0.51	0.000	0.000	1040978	1487016	annotated
301	Seriny-Tyrosine	1.30	0.000	0.000	20132	49677	annotated
316	Alanyl-Aspartate	0.36	0.000	0.000	645907	829943	annotated
320	Thionazin	0.52	0.000	0.000	42987	61520	annotated
324	Histidiny-Aspartate	1.90	0.000	0.000	3999	14958	annotated
327	Diazinon	1.94	0.000	0.000	3665	14102	annotated
724	Didodecyl thiobispropanoate	-0.84	0.000	0.000	914583	512605	annotated
751	Isoleucyl-Serine	0.38	0.000	0.000	271174	352597	annotated
932	Hydroxyprolyl-Hydroxyproline	1.14	0.000	0.000	250935	552913	annotated
935	Etoxazole	1.79	0.000	0.000	9859	34119	annotated
2179	L-Homocysteic acid	0.38	0.000	0.000	4323385	5624747	annotated
2477	5-Hydroxyindoleacetic acid	-0.07	0.000	0.000	607914	580224	annotated
2730	N-Acetyl-L-glutamate 5-semialdehyde	0.01	0.000	0.000	213624	215018	annotated
2757	Glutaryl-glycine	0.59	0.000	0.000	184451	277648	annotated
2760	L-gamma-glutamyl-L-isoleucine	1.02	0.000	0.000	13546	27410	annotated
3082	2-Oxosuccinamate	0.12	0.000	0.000	147119	159598	annotated
3772	1-Pyrenylsulfate	0.39	0.000	0.000	35408	46542	annotated
4111	Adefovir	1.17	0.000	0.000	5159	11603	annotated
4441	Margrapine B	1.32	0.000	0.000	2900	7263	annotated
330	Bicozamycin	2.46	0.000	0.000	3778	20776	annotated
934	L-cis-Cyclo(aspartylphenylalanyl)	-0.08	0.000	0.000	68665	64785	annotated

2437	Phenylacetic acid	-0.84	0.000	0.000	514394	286480	annotated
1097	PE(22:5(7Z,10Z,13Z,16Z,19Z)/16:0)	0.38	0.000	0.000	707576	918042	annotated
337	gibberellin A2 O-beta-D-glucoside	-0.71	0.000	0.001	504605	308569	annotated
3179	Tiglylglycine	-0.16	0.000	0.001	139983	125688	annotated
1102	2,3-Dehydrosalvipisone	-0.69	0.000	0.001	81914	50782	annotated
3581	Nevirapine	-0.38	0.000	0.001	371370	285988	annotated
969	LysoPC(16:1(9Z))	0.77	0.000	0.001	306936	524198	annotated
3757	3,6,8-Trimethylallantoin	-0.01	0.000	0.001	45695	45333	annotated
1356	Mammea B/AC cyclo D	-0.53	0.000	0.002	130457	90454	annotated
368	Zizybeoside II	1.75	0.000	0.002	9182	30820	annotated
4516	Ascorbalamic acid	-0.82	0.000	0.002	31816	18028	annotated
1967	Hyperforin	-0.52	0.000	0.003	26262	18278	annotated
2685	Glycyl-Threonine	-0.57	0.000	0.003	19294	12995	annotated
3787	3R-hydroxy-octadecanoic acid	-0.52	0.000	0.004	207375	144505	annotated
302	Pyroglutamylglycine	0.32	0.000	0.005	14963	18639	annotated
1933	trizma acetate	1.00	0.000	0.006	22930	45857	annotated
88	O-Desmethylcarvedilol	-0.68	0.000	0.006	40538	25372	annotated
1218	(S)-11,12,13-Trinor-7-calamenone	-0.50	0.000	0.007	108405	76729	annotated
1103	N-Jasmonoyltyrosine	-0.40	0.001	0.018	104814	79519	annotated
1204	Adenosine	-1.08	0.001	0.026	243495	115317	identified+fragment
299	Dihydroclavaminic acid	0.20	0.001	0.027	26469	30482	annotated
1096	Cer(d18:1/24:1(15Z))	0.55	0.001	0.027	528012	773715	annotated
1921	Glycyl-Arginine	-0.71	0.001	0.030	39740	24215	annotated
534	Tromethamine	-0.90	0.001	0.036	1153678	619229	annotated+fragment
2710	Thiosulfuric acid	0.70	0.002	0.045	746247	1215492	annotated
3465	Methyl benzoate	-0.52	0.002	0.046	252505	176127	annotated
136	PC(16:0/0:0)	0.47	0.002	0.048	6706384	9315886	annotated

CTL T48h vs CTS T48h

Peak id	Metabolite	Log fc	<i>p</i>	Adjusted <i>p</i>	Peak intensity CTL T48h	Peak intensity CTS T48h	Identification
534	Tromethamine	-1.57	0.000	0.000	4028183	1359450	annotated+fragment
979	hydroxyisovaleroyl carnitine	-1.42	0.000	0.000	95795	35889	annotated
1012	Pantothenic acid	0.53	0.000	0.000	647598	936607	annotated+fragment
1027	PE(20:0/15:0)	0.61	0.000	0.000	565359	861575	annotated
1204	Adenosine	2.03	0.000	0.000	76640	313766	identified+fragment
1268	N-Lignoceroylsphingosine	0.96	0.000	0.000	232281	452704	annotated
1483	SM(d18:0/18:1(9Z))	0.57	0.000	0.000	195290	289505	annotated
1537	N-(3-oxo-octanoyl)-homoserine lactone	-0.85	0.000	0.000	54613	30345	annotated
1753	Phenylethyl alcohol	-0.83	0.000	0.000	146868	82829	annotated
1763	1-Acetylcyclohexyl acetate	-0.62	0.000	0.000	134839	87847	annotated
1994	Kamahine C	-0.89	0.000	0.000	61159	33044	annotated
2060	(2S,2'S)-Pyrosaccharopine	-1.25	0.000	0.000	38163	16025	annotated
2437	Phenylacetic acid	-1.56	0.000	0.000	4675986	1583508	annotated
2938	3-Hydroxy-2-methyl-[S-(R,R)]-butanoic acid	0.64	0.000	0.000	854599	1327537	annotated
3081	Dodecanedioic acid	-3.17	0.000	0.000	514823	57300	annotated
3467	Azelaic acid	-0.68	0.000	0.000	229593	143225	annotated
3520	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	-2.32	0.000	0.000	300226	60240	annotated
3539	4-beta-Hydroxymethyl-4-alpha-methyl-5-alpha-cholest-7-en-3-beta-ol	0.54	0.000	0.000	401897	585724	annotated+fragment
3654	3R-hydroxy-decanoic acid	-1.47	0.000	0.000	268285	96595	annotated
4056	(R)-3-Hydroxyoctanoic acid	-0.74	0.000	0.000	219564	131177	annotated
4134	(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	-1.12	0.000	0.000	82261	37892	annotated
4182	Hexanoylglycine	1.36	0.000	0.000	23087	59111	annotated
4305	Tetradecanedioic acid	-1.11	0.000	0.000	93659	43460	annotated

4420	7-oxo-8-amino-nonanoic acid	-1.38	0.000	0.000	76819	29528	annotated
4473	Glycerol tripropanoate	-0.94	0.000	0.000	77281	40167	annotated
4602	Dicyclohexyl disulfide	-0.87	0.000	0.000	52224	28668	annotated
1536	Cumene	-1.45	0.000	0.000	164486	60244	annotated
1982	Hydroxypropionylcarnitine	-0.93	0.000	0.000	35527	18675	annotated
3525	2,4,6-Triethyl-1,3,5-trioxane	-1.12	0.000	0.000	379666	174770	annotated
1932	Heptyl p-hydroxybenzoate	-0.74	0.000	0.000	71736	42874	annotated
3466	4-Hydroxycyclohexylcarboxylic acid	-0.67	0.000	0.000	708348	444275	annotated
1936	Geranyl acetoacetate	-0.54	0.000	0.000	83239	57078	annotated
1604	Cer(d18:1/23:0)	0.83	0.000	0.000	113659	202168	annotated
2034	Triethylene Glycol Monomethyl Ether	1.00	0.000	0.000	18408	36742	annotated
1781	Polyethylene, oxidized	-0.76	0.000	0.001	103723	61354	annotated
1533	Neotussilagine	-0.65	0.000	0.001	75631	48358	annotated
1446	3,4-Methyleneazelaic acid	-0.88	0.000	0.001	70519	38237	annotated
2015	Myrtine	-0.64	0.000	0.001	62562	40231	annotated
2514	N-Nonanoylglycine	-1.93	0.000	0.002	1243688	326281	annotated
1095	Thiomorpholine 3-carboxylate	0.95	0.000	0.002	323222	624226	annotated
1357	Isoetharine	-1.52	0.000	0.002	192785	67128	annotated
2236	Chloroform	0.31	0.000	0.002	18613114	23125906	annotated
3586	3R-hydroxy-hexanoic acid	-0.64	0.000	0.003	397041	254243	annotated
4151	Diethyl sulfate	-1.34	0.000	0.003	94555	37436	annotated
1999	2,6-Dimethoxyphenol	0.65	0.000	0.003	31023	48531	annotated
1551	Normetanephine	0.67	0.000	0.003	145920	231379	annotated
1096	Cer(d18:1/24:1(15Z))	0.79	0.000	0.003	371385	640952	annotated
1102	2,3-Dehydrosalvipisone	-0.78	0.000	0.004	320993	187471	annotated
3543	7(14)-Bisabolene-2,3,10,11-tetrol	-0.53	0.000	0.004	42591	29570	annotated
2436	3-Oxohexanoic acid	-0.50	0.000	0.005	4098778	2897709	annotated
1614	S-Allylcysteine	1.00	0.000	0.006	81074	162605	annotated
1402	2-Methyl-1,3-cyclohexadiene	-0.72	0.000	0.006	319448	193631	annotated

4045	cis-3-Hexenyl pyruvate	-0.38	0.000	0.006	129725	99509	annotated
3640	Patulin	0.58	0.000	0.007	181083	271299	annotated+fragment
1967	Hyperforin	-0.55	0.000	0.007	67870	46376	annotated
1356	Mammea B/AC cyclo D	-0.65	0.000	0.007	392037	249555	annotated
2726	Nonyl octanoate	-0.45	0.000	0.008	1213666	886120	annotated+fragment
1103	N-Jasmonoyltyrosine	-0.58	0.000	0.010	319940	213773	annotated
3581	Nevirapine	-0.39	0.000	0.010	508620	387293	annotated
3603	Metaldehyde	-0.70	0.000	0.010	179947	110502	annotated
3605	Indoxyl sulfate	-1.46	0.000	0.010	216670	78539	annotated
3924	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	-0.55	0.000	0.010	250919	171475	annotated
1104	Benzenepropanenitrile	-0.67	0.000	0.010	323645	203421	annotated
1779	Peperinic acid	-0.44	0.000	0.011	135909	100489	annotated
1218	(S)-11,12,13-Trinor-7-calamenone	-0.50	0.000	0.013	625497	442148	annotated
3792	Ethyl 1-(ethylthio)propyl disulfide	0.97	0.001	0.015	114267	224207	annotated
1914	1,2-Dimethoxy-13-methyl-[1,3]benzodioxolo[5,6-c]phenanthridine	0.70	0.001	0.015	10031	16351	annotated
4216	Oxprenolol	0.56	0.001	0.016	39152	57691	annotated
1283	N-Palmitoylsphingosine	0.45	0.001	0.017	348210	474075	annotated
1311	3-hydroxyhexanoyl carnitine	-1.59	0.001	0.022	143635	47578	annotated
2259	Ethyl (±)-3-methylpentanoate	-0.49	0.001	0.023	8347271	5931388	annotated
724	Didodecyl thiobispropanoate	-0.55	0.001	0.024	2186680	1492087	annotated
1921	Glycyl-Arginine	0.64	0.001	0.024	26777	41709	annotated
4593	xi-3-Methyl-3-cyclohexen-1-ol	-0.51	0.001	0.024	53022	37151	annotated
1069	Haloperidol 1,2,3,6-tetrahydropyridine	0.62	0.001	0.026	19532	30047	annotated
4477	4-Oxononanal	0.23	0.001	0.027	77873	91619	annotated
1830	(4-Hydroxy-3-methoxyphenyl)ethanol	0.77	0.001	0.027	30727	52568	annotated
1824	Ligustilide	-0.46	0.001	0.028	132087	95907	annotated
3331	Acetoxyacetone	0.33	0.001	0.028	474438	596951	annotated
1440	QH(2)	-0.63	0.001	0.029	55709	35981	annotated
1001	3-Deoxyvitamin D3	-0.44	0.001	0.031	224129	165100	annotated

1203	N,2,3-Trimethyl-2-(1-methylethyl)butanamide	0.41	0.001	0.032	353128	468210	annotated
3123	3D,7D,11D-Phytanic acid	-0.38	0.001	0.032	721768	554276	annotated
4431	Phenylpropanoate	-0.51	0.001	0.032	50209	35317	annotated
546	Isovalerylcarnitine	-0.96	0.001	0.033	113909	58623	annotated
3978	alpha-15,16-DiHODE	-0.48	0.002	0.042	246155	176947	annotated
1588	Valerylglycine	-0.44	0.002	0.043	152252	111956	annotated
3188	Methyl benzoate	-0.63	0.002	0.048	625348	403437	annotated
166	Anandamide (20:2, n-6)	-1.27	0.002	0.050	8626231	3583511	annotated
3433	4-Sulfobenzoate	-0.25	0.002	0.050	18769	15828	annotated
4039	Sebacic acid	-0.44	0.002	0.050	145457	107421	annotated