

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

CTL T0h vs CTL T12h

<i>Peak id</i>	<i>Metabolite</i>	<i>Log FC</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T0h</i>	<i>Peak intensity CTL T12h</i>	<i>Identification</i>
68	N-a-Acetyl-L-arginine	-0.85	0.000	0.000	728514	404396	annotated
114	N-Acetyl-L-glutamate 5-semialdehyde	-8.32	0.000	0.000	23794150	74340	annotated
119	Methyl hippurate	-2.30	0.000	0.000	393243	79663	annotated
149	Tromethamine	1.99	0.000	0.000	1081619	4288271	annotated+fragment
165	Hydroxypropyl-Proline	1.60	0.000	0.000	2596837	7885719	annotated
256	Ergothioneine	-0.66	0.000	0.000	1580055	998266	annotated
338	L-gamma-glutamyl-L-leucine	-4.66	0.000	0.000	1162247	46018	annotated
391	Glutaryl-glycine	-10.28	0.000	0.000	4777769	3849	annotated
449	Glycylpropylhydroxyproline	3.11	0.000	0.000	245591	2125192	annotated
479	N-acetyl-L-glutamate	-0.86	0.000	0.000	186614	102546	identified
520	Vinylacetyl-glycine	-2.37	0.000	0.000	2495988	483159	annotated
523	3,5,7-Octatriyn-1-ol	0.77	0.000	0.000	1128722	1920364	annotated
524	Aloesol	1.16	0.000	0.000	204044	456915	annotated
635	Didodecyl thiobispropanoate	0.74	0.000	0.000	833391	1388376	annotated
638	Alpha-CEHC	-0.87	0.000	0.000	1525175	832395	annotated
696	Alanyl-Proline	3.17	0.000	0.000	114924	1036815	annotated
848	L-cis-Cyclo(aspartylphenylalanyl)	-4.51	0.000	0.000	701805	30857	annotated
888	3-Hydroxymelatonin	-3.14	0.000	0.000	90848	10332	annotated
930	(3S)-3-Hydroxy-L-enduracididine	-1.35	0.000	0.000	612598	240798	annotated
932	Trigoforin	1.84	0.000	0.000	20481	73207	annotated
1004	N-Acetyl-L-tyrosine	-2.44	0.000	0.000	178185	32927	annotated

1022	2,3-Dehydrosalvipisone	1.08	0.000	0.000	174020	367036	annotated
1065	Methyl thiophene-2-carboxylate	0.65	0.000	0.000	236966	372278	annotated
1176	Alanyl-Arginine	-1.88	0.000	0.000	343777	93467	annotated
1389	L-Coprine	1.32	0.000	0.000	65093	162904	annotated
1672	delta-1-Pyrroline-5-carboxylate	-0.81	0.000	0.000	121739	69247	annotated
2399	L-Tyrosine	-0.83	0.000	0.000	5570370	3128212	annotated+fragment
2411	hexyl propionate	1.40	0.000	0.000	1370702	3619541	annotated
2417	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	1.86	0.000	0.000	872506	3177231	annotated
2419	Glycerol tributanoate	0.87	0.000	0.000	35883	65636	annotated
2453	Ethyl (±)-3-methylpentanoate	1.86	0.000	0.000	1013559	3686527	annotated
2454	3R-hydroxy-decanoic acid	1.61	0.000	0.000	40098	122198	annotated
2455	Salicylaldehyde	0.96	0.000	0.000	1842803	3582767	annotated+fragment
2530	2-Oxoglutaramate	-8.91	0.000	0.000	3430538	7151	annotated
2582	D-Glucuronic acid	-0.60	0.000	0.000	2552868	1689535	annotated+fragment
2641	Tiglylglycine	-4.67	0.000	0.000	2000964	78589	annotated
2726	2-Dehydro-D-xylonate	-0.48	0.000	0.000	136778	97828	annotated
2800	Methyl benzoate	0.79	0.000	0.000	390205	672898	annotated
2981	2-Methylpropyl propionate	1.08	0.000	0.000	471805	996276	annotated
3000	11-docosenoic acid	3.71	0.000	0.000	59533	777101	annotated
3002	Nonyl octanoate	-0.68	0.000	0.000	1044340	651215	annotated
3063	N,N-Dihydroxy-L-valine	-0.63	0.000	0.000	254348	164732	annotated
3166	Ipomeatetrahydrofuran	-2.17	0.000	0.000	566077	125885	annotated
3167	Oxprenolol	-5.65	0.000	0.000	126660	2520	annotated
3188	3D,7D,11D-Phytanic acid	-0.69	0.000	0.000	638445	395975	annotated
3536	alpha-Valerenol	-1.41	0.000	0.000	247743	93100	annotated
4003	Undecanedioic acid	1.20	0.000	0.000	30372	69560	annotated
4012	3-(2-Hydroxy-4-methylphenyl)-2-butanone	-0.90	0.000	0.000	95075	51064	annotated
167	L-Tyrosine	-0.84	0.000	0.000	13761065	7678238	identified+fragment
200	L-Theanine	-0.62	0.000	0.000	11627115	7568514	annotated
1005	Hydroxypropyl-Serine	-0.97	0.000	0.000	634849	323357	annotated

1353	L-Rhamnose	-1.43	0.000	0.000	124530	46060	annotated
1476	Gamma-Glutamyltyrosine	-0.96	0.000	0.000	167443	86243	annotated
1501	Dambonitol	-1.19	0.000	0.000	114872	50208	annotated
1532	Isoetharine	0.92	0.000	0.000	62488	117985	annotated
3764	1-Naphthalenesulfonic acid	-1.24	0.000	0.000	121979	51773	annotated
753	Homoarecoline	1.13	0.000	0.000	308032	674579	annotated
1320	Piperidine	0.83	0.000	0.000	110538	195838	annotated+fragment
2184	N-Acetyl-L-aspartic acid	-0.71	0.000	0.000	573804	350659	annotated
4146	Sulfolithocholylglycine	2.84	0.000	0.000	7394	52993	annotated
663	1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione	-0.73	0.000	0.001	1536712	923783	annotated
1246	apo-[3-methylcrotonoyl-CoA:carbon-dioxide ligase (ADP-forming)]	0.68	0.000	0.001	192423	308870	annotated
1354	Aspartyl-Glutamine	-0.83	0.000	0.001	236047	132665	annotated
2463	Phenylacetic acid	1.13	0.000	0.001	293119	640011	annotated
66	L-homoserine	-0.47	0.000	0.001	51918117	37569749	identified+fragment
202	3-Ureidopropionate	-0.57	0.000	0.001	12660841	8502293	annotated+fragment
414	Carboxy-ibuprofen	0.56	0.000	0.001	2238386	3298710	annotated
525	3,4-Dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-carboxylic acid	0.82	0.000	0.001	145224	255950	annotated
1288	Aprobarbital	0.90	0.000	0.001	104388	195467	annotated
3752	N-Formyl-L-methionine	-0.57	0.000	0.001	156615	105317	annotated
343	Pirbuterol	0.34	0.000	0.002	836879	1056829	annotated
404	Hydroxypropyl-Arginine	-0.63	0.000	0.002	253814	164287	annotated
4032	PG(18:1(9Z)/18:1(11Z))	3.30	0.000	0.002	8305	81815	annotated
1429	2,3-Butanediol glucoside	-0.77	0.000	0.002	44270	25900	annotated
3521	L-Citrulline	-0.61	0.000	0.002	240291	157353	identified
4001	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/P-18:0)	0.74	0.000	0.002	53645	89589	annotated
187	5-Methylthio-D-ribose	-0.52	0.000	0.003	3911727	2736090	annotated
825	Sakacin P	-1.07	0.000	0.003	612426	291043	annotated

561	Hexaethylene glycol	-0.91	0.000	0.003	246442	131147	annotated
3559	6-Deoxy-D-galactose	0.47	0.000	0.003	190744	264669	annotated
1810	Lysyl-Alanine	0.97	0.000	0.003	31971	62718	annotated
2416	4-Dodecylbenzenesulfonic Acid	-1.13	0.000	0.003	4024210	1835868	annotated
191	1,2-Dihydroxy-5-(methylthio)pent-1-en-3-one	-0.56	0.000	0.003	606653	412062	annotated
44	PE-NMe(18:1(9Z)/18:1(9Z))	0.31	0.000	0.004	44425799	55243014	annotated
1231	S-Propyl-L-cysteine	-0.93	0.000	0.004	335530	176582	annotated+fragment
3577	7-oxo-8-amino-nonanoic acid	1.08	0.001	0.005	71507	151049	annotated
1129	Ethosuximide	0.64	0.001	0.006	173249	269925	annotated
1566	N-gamma-L-Glutamyl-L-methionine	-0.60	0.001	0.006	160507	105621	annotated
1646	Isoleucyl-Threonine	0.46	0.001	0.006	79102	108698	annotated
2456	Menthyl ethylene glycol carbonate	1.02	0.001	0.007	334928	677303	annotated
3005	Acetoxyacetone	-0.54	0.001	0.008	626775	432501	annotated
83	Homoarginine	1.95	0.001	0.008	2495789	9622112	annotated+fragment
3927	(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	0.78	0.001	0.008	60166	103077	annotated
1040	Isopropyl beta-D-glucoside	-4.92	0.001	0.009	231731	7643	annotated
311	L-Glutamate	-0.46	0.001	0.009	7673971	5597139	identified
1108	Dinex	-1.22	0.001	0.009	410798	176845	annotated
1302	6-Acetamido-2-oxohexanoate	-0.50	0.001	0.009	242010	171342	annotated
1480	7-Hydroxyaustrobailignan 5	-0.78	0.001	0.009	155804	90634	annotated
3647	(R)-2,3-Dihydroxypropane-1-sulfonate	-0.77	0.001	0.009	183919	107622	annotated
3029	Aminoadipic acid	-0.47	0.002	0.014	819358	592860	annotated
2198	Sinalexin	-0.40	0.002	0.014	87902	66841	annotated
1784	(R)-3-hydroxybutyrylcarnitine	0.72	0.002	0.016	46752	77099	annotated
71	(5-L-Glutamyl)-L-glutamine	-0.55	0.002	0.017	2088783	1424404	annotated
1	Betaine	-0.46	0.002	0.017	254670809	184957033	identified+fragment
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1505	Cysteineglutathione disulfide	-0.44	0.002	0.018	160907	118792	annotated
3842	Furmecyclox	-0.86	0.002	0.018	89686	49321	annotated
2613	Pyruvic acid	-0.32	0.002	0.019	2277300	1818044	annotated

98	L-Valine	-0.42	0.002	0.019	30523754	22760132	identified+fragment
3165	thymine	2.43	0.002	0.019	81685	440065	identified
1251	5-Methylcytidine	-0.41	0.002	0.020	281081	211473	annotated+fragment
3088	cholesterol sulfate	0.34	0.002	0.020	519569	657105	annotated
1014	Diethanolamine	0.59	0.002	0.020	361474	545713	annotated+fragment
2940	Isosorbide mononitrate	-0.47	0.002	0.021	25906	18722	annotated
1093	Thiacremonone	0.83	0.003	0.022	228784	406670	annotated
2312	3-keto-n-caproic acid	-0.37	0.003	0.024	9076017	7013233	annotated
476	Alanyl-Threonine	-0.34	0.003	0.025	510079	404352	annotated
3933	2-Phenylethyl beta-D-glucopyranoside	-0.54	0.003	0.026	73985	50797	annotated
184	S-2,5-Dimethyl-3-furanyl 3-methylbutanethioate	-0.36	0.003	0.026	173720	135328	annotated
99	Thiabendazole	-0.50	0.003	0.027	121759	86173	annotated
2037	Cyclodopa glucoside	-0.61	0.004	0.029	33484	21923	annotated
1145	L-N2-(2-Carboxyethyl)arginine	-0.64	0.004	0.029	445452	285609	annotated
280	Anandamide (20:2, n-6)	1.79	0.004	0.030	2095232	7232728	annotated
3563	L-trans-alpha-Amino-2-carboxycyclopropaneacetic acid	-0.77	0.004	0.032	207180	121675	annotated
859	N-Formyl-4-amino-5-aminomethyl-2-methylpyrimidine	-0.49	0.004	0.033	923648	658561	annotated
1444	Glycyl-Arginine	-0.89	0.005	0.034	129940	69912	annotated
3994	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	0.84	0.005	0.038	45175	80883	annotated
1073	2-Aminoheptanedioic acid	-0.53	0.006	0.041	417315	288571	annotated
3681	2E-Lauroleic acid	0.78	0.006	0.041	49577	85371	annotated
3715	Orotate	-0.71	0.006	0.041	183524	112161	identified
548	Guanidinoacetate	-1.00	0.006	0.042	1750297	877189	annotated+fragment
1937	3-Amino-1-hydroxy-5,7-dimethyl-adamantane	0.31	0.006	0.043	47131	58626	annotated

CTL T0h vs CTL T24h

<i>Peak id</i>	<i>Metabolite</i>	<i>Log FC</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T0h</i>	<i>Peak intensity CTL T24h</i>	<i>Identification</i>
1	Betaine	-1.01	0.000	0.000	2546708096	1264838080	identified+fragment
37	L-Acetopine	-5.03	0.000	0.000	84710226	2587816	annotated
68	N-a-Acetyl-L-arginine	-0.93	0.000	0.000	728514	382904	annotated
71	(5-L-Glutamyl)-L-glutamine	-1.15	0.000	0.000	2088783	939486	annotated
72	PC(18:1(9Z)/18:1(9Z))	-0.49	0.000	0.000	37387312	26700039	annotated
105	PC(16:0/0:0)	-1.42	0.000	0.000	17170700	6412097	annotated
114	N-Acetyl-L-glutamate 5-semialdehyde	-5.34	0.000	0.000	23794150	587078	annotated
119	Methyl hippurate	-2.02	0.000	0.000	393243	97074	annotated
149	Tromethamine	2.15	0.000	0.000	1081619	4792060	annotated+fragment
156	Alanyl-Aspartate	-5.72	0.000	0.000	16143067	307270	annotated
157	Isoleucyl-Serine	-4.69	0.000	0.000	2571459	99424	annotated
165	Hydroxypropyl-Proline	2.11	0.000	0.000	2596837	11246995	annotated
202	3-Ureidopropionate	-1.10	0.000	0.000	12660841	5889615	annotated+fragment
211	Descarboxyl-lacosamide	-0.68	0.000	0.000	31921	19895	annotated
10	L-Glutamine	-0.53	0.000	0.000	488861984	337516832	identified+fragment
338	L-gamma-glutamyl-L-leucine	-4.58	0.000	0.000	1162247	48665	annotated
391	Glutaryl-glycine	-4.74	0.000	0.000	4777769	179226	annotated
392	Lysyl-Asparagine	//	0.000	0.000	750761	//	annotated
449	Glycylprolylhydroxyproline	3.54	0.000	0.000	245591	2852752	annotated
473	L-isoleucyl-L-proline	0.86	0.000	0.000	1188032	2151267	annotated
25	L-Arginine	-0.45	0.000	0.002	113309352	82720822	identified+fragment
506	N6-Acetyl-5S-hydroxy-L-lysine	-3.47	0.000	0.000	2936840	264942	annotated
520	Vinylacetyl-glycine	-2.72	0.000	0.000	2495988	378122	annotated
637	alpha-linolenic acid	-1.25	0.000	0.000	1371789	578717	annotated

682	Glycyl-Aspartate	-5.55	0.000	0.000	1700329	36386	annotated
688	Butalbital	-1.00	0.000	0.000	1561956	778761	annotated
693	5-Hydroxymethyl-2-furaldehyde	-1.50	0.000	0.000	1142461	403295	annotated
694	Metharbital	-0.67	0.000	0.000	126840	79539	annotated
696	Alanyl-Proline	3.46	0.000	0.000	114924	1262291	annotated
848	L-cis-Cyclo(aspartylphenylalanyl)	-4.41	0.000	0.000	701805	33112	annotated
859	N-Formyl-4-amino-5-aminomethyl-2-methylpyrimidine	-1.02	0.000	0.000	923648	454580	annotated
888	3-Hydroxymelatonin	-2.42	0.000	0.000	90848	17015	annotated
1004	N-Acetyl-L-tyrosine	-1.54	0.000	0.000	178185	61131	annotated
1005	Hydroxypropyl-Serine	-1.45	0.000	0.000	634849	232517	annotated
1074	Homocysteine	-1.11	0.000	0.000	465661	215844	annotated
1122	S-4-Hydroxymephenytoin	-4.65	0.000	0.000	248706	9880	annotated
1163	Glycerophosphocholine	-1.83	0.000	0.000	242818	68130	annotated
1183	Fenpiclonil	-0.80	0.000	0.000	282094	162337	annotated
1288	Aprobarbital	1.14	0.000	0.000	104388	230188	annotated
1304	2-amino-muconic acid	-1.34	0.000	0.000	224873	88990	annotated
1354	Aspartyl-Glutamine	-1.59	0.000	0.000	236047	78337	annotated
1389	L-Coprine	1.90	0.000	0.000	65093	242510	annotated
1476	Gamma-Glutamyltyrosine	-0.95	0.000	0.000	167443	86479	annotated
1672	delta-1-Pyrroline-5-carboxylate	-0.73	0.000	0.000	121739	73341	annotated
2152	L-Homocysteic acid	-4.35	0.000	0.000	10340243	508550	annotated
2382	D-Glucosamine	-1.02	0.000	0.000	1295509	637093	annotated
2385	Nitazoxanide	-1.04	0.000	0.000	74344	36083	annotated
2404	5-Hydroxyindoleacetate	-4.57	0.000	0.000	5762024	242614	annotated
2530	2-Oxoglutaramate	-4.93	0.000	0.000	3430538	112260	annotated
2565	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	-5.33	0.000	0.000	2837522	70573	annotated
2622	2-Oxosuccinamate	-5.00	0.000	0.000	2417151	75478	annotated
2641	Tiglylglycine	-4.43	0.000	0.000	2000964	92831	annotated
2642	2-Methylmaleate	-0.95	0.000	0.000	2058405	1064936	annotated
2646	S-Sulfo-L-cysteine	-1.31	0.000	0.000	1475470	595357	annotated+fragment

2726	2-Dehydro-D-xylonate	-0.59	0.000	0.000	136778	91106	annotated
2832	5-Hydroxy-7-tetracosanone	-1.13	0.000	0.000	107074	49051	annotated
3029	Aminoadipic acid	-0.81	0.000	0.000	819358	468768	annotated
3212	3,6,8-Trimethylallantoin	-5.20	0.000	0.000	562858	15269	annotated
3214	4-Oxononanal	-0.93	0.000	0.000	474121	249505	annotated
3215	15,16-DiHODE	-1.22	0.000	0.000	428613	184000	annotated
3231	4,5-Dihydroorotic acid	-8.04	0.000	0.000	592140	2242	annotated
3350	(-)-Quebrachitol	-0.94	0.000	0.000	432084	225768	annotated
3398	LPA(0:0/16:0)	-1.19	0.000	0.000	269972	118212	annotated
3433	PS(15:0/22:2(13Z,16Z))	-5.14	0.000	0.000	344927	9752	annotated
66	L-homoserine	-0.53	0.000	0.000	51918117	36005647	identified+fragment
3914	(10S)-Juvenile hormone III diol	-1.64	0.000	0.000	84827	27200	annotated
4	Pterolactam	-0.63	0.000	0.000	554959904	359044224	annotated
70	beta-Alanine	-0.96	0.000	0.000	34363884	17638463	identified+fragment
76	L-Methionine	-0.86	0.000	0.000	45433854	25067849	identified+fragment
107	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	-1.21	0.000	0.000	238454	102979	annotated
205	Aspartyl-Threonine	-0.85	0.000	0.000	640580	355433	annotated
528	Methionine sulfoxide	-0.92	0.000	0.000	1970600	1043542	annotated
930	(3S)-3-Hydroxy-L-enduracididine	-1.09	0.000	0.000	612598	287837	annotated
1095	Daidzein 4'-O-glucuronide	-1.15	0.000	0.000	211294	95489	annotated
1104	(2R,2'S)-Isobuteine	-1.13	0.000	0.000	372253	170249	annotated
85	L-Lysine	1.01	0.000	0.001	12259060	24746948	identified+fragment
98	L-Valine	-0.43	0.001	0.006	30523754	22589188	identified+fragment
2680	Mevalonic acid	-0.67	0.000	0.000	282012	177088	annotated
3000	11-docosenoic acid	1.69	0.000	0.000	59533	192155	annotated
3024	Quinic acid	-0.86	0.000	0.000	860147	475264	annotated
3563	L-trans-alpha-Amino-2-carboxycyclopropaneacetic acid	-1.29	0.000	0.000	207180	84881	annotated
3738	Cer(d18:0/16:0)	-1.53	0.000	0.000	106876	37132	annotated
4009	Ovalitenin A	-0.89	0.000	0.000	88239	47602	annotated

8	Gingerenone C	-1.15	0.000	0.000	382859	172520	annotated
167	L-Tyrosine	-0.65	0.000	0.001	13761065	8750022	identified+fragment
268	L-Cystine	-0.51	0.000	0.001	1039434	729986	identified+fragment
86	Nalbuphine	1.64	0.000	0.000	326883	1019066	annotated
476	Alanyl-Threonine	-0.52	0.000	0.000	510079	355757	annotated
1068	delta-Guanidinovaleric acid	-1.27	0.000	0.000	515039	214296	annotated
1210	Prolyl-Valine	-0.71	0.000	0.000	241358	147367	annotated
1734	5-Acetyl-2,4-dimethyloxazole	-0.95	0.000	0.000	88934	46139	annotated
1757	Histidinal	-1.01	0.000	0.000	82112	40843	annotated
2802	Uracil	1.13	0.000	0.000	564693	1237038	annotated
2803	Pseudouridine	1.18	0.000	0.000	528202	1198730	annotated
3030	D-Glycerate	-0.51	0.000	0.000	928978	654123	annotated
3063	N,N-Dihydroxy-L-valine	-0.39	0.000	0.000	254348	193511	annotated
3136	9-hydroxy-hexadecan-1,16-dioic acid	-1.32	0.000	0.000	63961	25670	annotated
3167	Oxprenolol	-1.07	0.000	0.000	126660	60518	annotated
3440	Aldoxycarb	-0.73	0.000	0.000	296592	178378	annotated
1071	1-[(5-Amino-5-carboxypentyl)amino]-1-deoxyfructose	-0.91	0.000	0.000	486351	258169	annotated
2383	N-Ethylammelide	-1.00	0.000	0.000	225206	112831	annotated
3190	Metsulfovax	-0.68	0.000	0.000	496053	309315	annotated
359	8-Hydroxyalanylclavam	-0.70	0.000	0.000	52694	32535	annotated
1464	8-Oxodeoxycoformycin	-1.10	0.000	0.000	159469	74518	annotated
1968	Pyridoxamine	-0.42	0.000	0.000	45238	33739	annotated
2582	D-Glucuronic acid	-0.48	0.000	0.000	2552868	1832544	annotated+fragment
3432	Azelaic acid	-0.89	0.000	0.000	305060	164730	annotated
2090	3-Hydroxypropanoate	-0.55	0.000	0.001	60350562	41150424	annotated
3015	Erythrityl Tetranitrate	-0.70	0.000	0.001	37594	23204	annotated
90	Cilastatin	1.73	0.000	0.001	34787	115421	annotated
109	PC(20:2(11Z,14Z)/16:1(9Z))	-0.39	0.000	0.001	11343538	8646181	annotated
311	L-Glutamate	-0.74	0.000	0.000	7673971	4586754	identified
844	N2-Fructopyranosylarginine	-1.71	0.000	0.001	814480	249614	annotated

2399	L-Tyrosine	-0.62	0.000	0.001	5570370	3613489	annotated+fragment
3407	Sebacic acid	-0.90	0.000	0.001	337676	180894	annotated
4017	Oxoadipic acid	-0.86	0.000	0.001	84022	46189	annotated
11	N-Nitrosoguvacoline	-0.47	0.000	0.001	15148988	10953028	annotated
347	Adenine	-0.55	0.002	0.009	330205	225657	identified+fragment
479	N-acetyl-L-glutamate	-0.86	0.000	0.000	186614	102782	identified
3078	3-hydroxy-tetradecanedioic acid	-1.12	0.000	0.001	587093	269929	annotated
3606	Cer(d18:1/23:0)	-0.75	0.000	0.001	136509	81236	annotated
15	Miraxanthin-I	-1.05	0.000	0.001	480954	231738	annotated
819	Cytidine	0.82	0.000	0.001	535484	944130	identified+fragment
695	2,4-Diamino-6-nitrotoluene	-0.56	0.000	0.001	43368	29455	annotated
1145	L-N2-(2-Carboxyethyl)arginine	-0.85	0.000	0.001	445452	247125	annotated
1505	Cysteineglutathione disulfide	-0.57	0.000	0.001	160907	108375	annotated
3352	(2R)-1-O-beta-D-Galactopyranosylglycerol	-1.04	0.000	0.001	63545	30956	annotated
21	L-Alpha-aminobutyric acid	-0.67	0.000	0.001	146669766	92016572	annotated+fragment
362	L-Acetylcarnitine	-0.84	0.000	0.001	5537363	3092390	annotated
1162	N-acetyl-L-2-aminoadipate(2-)	-1.27	0.000	0.001	362137	149721	annotated
1378	2-Acetyloxazole	-1.29	0.000	0.001	220265	89952	annotated
3223	D-Ribonate	-0.58	0.000	0.001	501915	336282	annotated
3605	DG(15:0/18:4(6Z,9Z,12Z,15Z)/0:0)	-1.55	0.000	0.001	120995	41422	annotated
3818	(3S,5S)-Carbapenam-3-carboxylic acid	-0.82	0.000	0.001	127861	72581	annotated
1075	Tris(2-chloroethyl)phosphate	-0.89	0.000	0.001	390865	211129	annotated+fragment
446	L-Pipecolate	-0.53	0.000	0.001	2798546	1937512	annotated
1566	N-gamma-L-Glutamyl-L-methionine	-1.84	0.000	0.001	160507	44980	annotated
3674	HBOA	-1.02	0.000	0.001	187408	92648	annotated
1108	Dinex	-1.23	0.000	0.001	410798	175490	annotated
2110	Malate	-0.70	0.000	0.001	33639641	20645189	annotated+fragment
2638	PI(18:1(9Z)/18:1(11Z))	-0.47	0.000	0.001	1812696	1312995	annotated
3134	Ethyl 2-hydroxyisovalerate	-0.94	0.000	0.001	492310	256751	annotated
3733	(Z)-2-Methylperoxyaminoacrylate	-0.71	0.000	0.001	148008	90365	annotated

3734	Acetylglycine	-0.71	0.000	0.001	148008	90365	annotated
992	Threoninyl-Phenylalanine	-1.19	0.000	0.001	461860	202128	annotated
4198	Dihydrocaffeic acid 3-O-glucuronide	-1.24	0.000	0.001	42580	18078	annotated
353	Isoleucyl-Aspartate	-0.54	0.000	0.001	106860	73724	annotated
1129	Ethosuximide	0.71	0.000	0.001	173249	283074	annotated
2965	(±)-2-Hydroxy-4-(methylthio)butanoic acid	-1.32	0.000	0.001	573953	229627	annotated
1703	L-Kynurenine	-0.76	0.003	0.014	103970	61395	identified
200	L-Theanine	-0.48	0.000	0.002	11627115	8356023	annotated
419	Midodrine	-0.71	0.000	0.002	4541209	2766580	annotated
735	N-Acetylhistidine	-0.80	0.000	0.002	344117	198326	annotated+fragment
1402	Asparaginyl-Valine	1.29	0.000	0.002	54844	134231	annotated
2478	trans-Aconitate	-0.55	0.000	0.002	4130264	2817939	annotated
3654	Thymidine	0.73	0.000	0.002	115898	192783	annotated
558	L-Homocitrulline	1.06	0.000	0.002	537922	1121777	annotated
2669	L-Arabinose	-0.93	0.000	0.002	1412973	741530	annotated
3166	Ipomeatetrahydrofuran	-0.60	0.000	0.002	566077	373706	annotated
3188	3D,7D,11D-Phytanic acid	-0.40	0.000	0.002	638445	484839	annotated
4356	Glycogen	-1.41	0.000	0.002	28054	10589	annotated
923	3-Keto-scylo-inosamine	-1.24	0.000	0.002	537481	227479	annotated
112	Trigonelline	-0.91	0.000	0.002	23500834	12502392	annotated+fragment
29	Northienamycin	-0.75	0.000	0.003	173875	103236	annotated
1166	Allocystathionine	-0.66	0.000	0.003	357445	225889	annotated+fragment
3980	Desethylchloroquine	-1.03	0.000	0.003	85548	41765	annotated
3079	Hydroiodic acid	-0.64	0.000	0.003	683639	437608	annotated
3141	beta-L-Arabinofuranose	-0.83	0.000	0.003	525020	296124	annotated
79	L-Alloisoleucine	-0.54	0.000	0.003	37091570	25462822	annotated+fragment
1932	6-Imino-5-oxocyclohexa-1,3-dienecarboxylate	-1.08	0.000	0.003	51926	24637	annotated
2592	Ferulic acid 4-sulfate	-0.88	0.000	0.003	171706	93592	annotated
1429	2,3-Butanediol glucoside	-0.67	0.001	0.003	44270	27805	annotated
2413	1-Acetylcyclohexyl acetate	-0.53	0.001	0.003	91883	63428	annotated

2108	citrate	-0.65	0.000	0.000	44782416	28614479	identified+fragment
35	6-Chlorocatechin	-0.71	0.001	0.003	80012	48892	annotated
91	6-Methoxy-9H-carbazole-3-carboxaldehyde	1.00	0.001	0.004	44970	90034	annotated
4146	Sulfolithocholylglycine	2.38	0.001	0.004	7394	38613	annotated
2111	Gentianose	-1.42	0.001	0.004	39735	14849	annotated
2037	Cyclodopa glucoside	-0.69	0.001	0.004	33484	20723	annotated
3752	N-Formyl-L-methionine	-0.46	0.001	0.004	156615	113876	annotated
3690	Dimorphecolic acid	-1.14	0.001	0.004	137319	62492	annotated
472	Pymetrozine	0.59	0.001	0.004	206279	310736	annotated
4007	Auxin b	-0.88	0.001	0.004	76932	41748	annotated
1546	Epidermin	-0.63	0.001	0.005	158246	102552	annotated
3891	Vanillic acid 4-sulfate	-1.12	0.001	0.005	70465	32414	annotated
1188	Triethanolamine	-1.61	0.001	0.005	224903	73564	annotated+fragment
1266	5,6-Dihydrouracil	0.60	0.001	0.005	191748	289722	annotated
3041	Malonic acid	-0.53	0.001	0.005	834089	576851	annotated
3002	Nonyl octanoate	-0.39	0.001	0.005	1044340	796553	annotated
3626	3-keto palmitic acid	-0.63	0.001	0.005	176371	113858	annotated
2219	L-Serine	-0.56	0.000	0.000	13248853	8955985	identified+fragment
1600	3R-aminononanoic acid	-0.43	0.001	0.006	115205	85428	annotated
2133	6-Methoxy-3-(2-thiazolyl)-1H-indole	-0.52	0.001	0.006	93118	64904	annotated
3756	N-Nitrosoproline	-0.74	0.001	0.006	140505	83955	annotated
2513	D-glucose	-0.17	0.002	0.012	4074804	3611206	identified
3460	Phaseolic acid	-0.59	0.001	0.007	147778	98276	annotated
2800	Methyl benzoate	-0.44	0.001	0.007	390205	288588	annotated
2631	3-Furoic acid	-0.95	0.001	0.007	1659639	859578	annotated
60	N-Methylcalystegine C1	-0.53	0.001	0.007	176773	122736	annotated
4026	Diisopropyl sulfate	-1.54	0.001	0.007	68276	23405	annotated
1501	Dambonitol	-0.77	0.001	0.008	114872	67312	annotated
1096	L-Noradrenaline	-0.66	0.002	0.009	172622	109228	annotated
4012	3-(2-Hydroxy-4-methylphenyl)-2-butanone	-0.39	0.002	0.009	95075	72431	annotated

47	3beta,6beta-Dihydroxynortropane	-0.43	0.002	0.009	42931027	31763970	annotated
2623	L-Aspartate	-1.39	0.003	0.014	815828	312041	identified
100	Ectoine	-0.49	0.002	0.010	27534441	19651792	annotated+fragment
1353	L-Rhamnose	-0.89	0.002	0.010	124530	67026	annotated
1730	Estragole	-0.63	0.002	0.010	80792	52294	annotated
3124	Patulin	-0.61	0.002	0.010	480786	314747	annotated+fragment
1664	Hydroxymethyl indol-3-yl ketone	-0.69	0.002	0.010	99987	61774	annotated
3921	Eugenitin	0.93	0.002	0.010	44637	84805	annotated
2587	Quinolinic acid	-1.26	0.002	0.011	262438	109545	annotated
1845	2-hydroxyacetaminophen sulfate	-0.72	0.002	0.011	58643	35537	annotated
2068	2-C-Methyl-D-erythritol 4-phosphate	-0.18	0.002	0.011	96165524	84941682	annotated
3590	Suberic acid	-0.52	0.002	0.011	115834	80625	annotated
3226	4-beta-Hydroxymethyl-4-alpha-methyl-5-alpha-cholest-7-en-3-beta-ol	-0.44	0.002	0.011	426622	314434	annotated+fragment
2872	Galactaric acid	-0.45	0.002	0.011	169774	124144	annotated
3611	3-oxo capric acid	-0.70	0.002	0.011	175105	107968	annotated
3765	4-Aminocatechol	-0.48	0.002	0.012	138971	99784	annotated
1961	7-Nonene-3,5-diyn-1-ol	-0.71	0.002	0.012	44053	26982	annotated
3937	Vulgarole	-0.61	0.002	0.012	101781	66477	annotated
3715	Orotate	-1.57	0.000	0.000	183524	62002	identified
2866	2-Methylcitric acid	-0.52	0.002	0.012	236835	165201	annotated
184	S-2,5-Dimethyl-3-furanyl 3-methylbutanethioate	-0.37	0.002	0.012	173720	134015	annotated
2838	D-Glucono-1,5-lactone	-0.36	0.003	0.013	191735	148988	annotated
2681	2'-Hydroxy-4',6'-dimethoxy-3'-methylacetophenone	-1.25	0.003	0.014	59739	25153	annotated
3994	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	0.90	0.003	0.014	45175	84012	annotated
638	Alpha-CEHC	-0.51	0.003	0.014	1525175	1069045	annotated
2405	Threonic acid	-0.23	0.003	0.014	5769232	4923944	annotated
272	Dihydroferulic acid 4-sulfate	-0.61	0.003	0.014	126782	83143	annotated
497	Choline sulfate	-0.64	0.003	0.014	2059879	1323235	annotated
3736	allantoin	-0.71	0.001	0.006	125139	76700	identified

3902	2-Oxoglutarate	-0.66	0.001	0.003	87056	55145	identified
2543	Taurodeoxycholic acid	-0.67	0.003	0.015	2252154	1417725	annotated
2184	N-Acetyl-L-aspartic acid	-0.44	0.003	0.015	573804	423231	annotated
3764	1-Naphthalenesulfonic acid	-0.79	0.003	0.016	121979	70622	annotated
3745	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	-0.60	0.003	0.016	144590	95226	annotated
1588	Geranyl acetoacetate	-0.64	0.003	0.016	119317	76712	annotated
1232	5,6-Dihydrothymine	-1.07	0.003	0.016	236056	112249	annotated
1544	2-Octenoylcarnitine	0.89	0.003	0.016	61243	113133	annotated
1040	Isopropyl beta-D-glucoside	-1.46	0.003	0.017	231731	84506	annotated
1554	Polyethylene, oxidized	-0.69	0.003	0.017	134564	83203	annotated
2806	Ezetimibe	0.86	0.004	0.017	43457	78706	annotated
3365	Apigenin 7-sulfate	-0.67	0.004	0.017	341123	214331	annotated
256	Ergothioneine	-0.34	0.004	0.020	1580055	1249424	annotated
1719	Heptyl p-hydroxybenzoate	-0.65	0.004	0.020	88596	56303	annotated
1007	N-Lignoceroylsphingosine	-2.17	0.004	0.020	345535	76549	annotated
4011	Isoambergoin	-0.87	0.004	0.020	63760	34961	annotated
3584	Methyl (indol-3-yl)acetate	-0.95	0.005	0.021	170278	87964	annotated
2071	Trehalose	-2.09	0.005	0.022	243664	57105	annotated
835	4-Guanidinobutanoate	-1.04	0.005	0.023	689018	335039	annotated
2657	1,5-Dibutyl methyl hydroxycitrate	-0.55	0.005	0.024	58810	40183	annotated
4080	4-Coumarate	-0.64	0.005	0.024	75412	48309	identified
910	N-Formimino-L-glutamate	-0.49	0.006	0.025	562978	400210	annotated
1384	L-alpha-glutamyl-L-hydroxyproline	0.61	0.006	0.025	149744	228274	annotated
3428	3,4-Methylenesebacic acid	-0.79	0.006	0.026	277348	160328	annotated
94	Caryoptosidic acid	1.33	0.006	0.027	18876	47467	annotated
2198	Sinalexin	-0.34	0.006	0.028	87902	69223	annotated
3462	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	-0.39	0.007	0.029	140637	107537	annotated
1176	Alanyl-Arginine	-0.88	0.007	0.029	343777	186350	annotated
562	L-glycyl-L-hydroxyproline	-0.53	0.007	0.030	1714733	1189113	annotated
2653	trans-p-Menthane-1,7,8-triol 8-glucoside	-0.46	0.007	0.031	59470	43308	annotated

1218	Talbutal	-0.37	0.008	0.033	310443	239727	annotated
1620	L-alpha-Amino-1H-pyrrole-1-hexanoic acid	-0.55	0.008	0.034	104518	71330	annotated
1711	2-Acetylpyrrole	-0.63	0.008	0.036	81526	52805	annotated
944	Norepinephrine sulfate	-0.45	0.009	0.037	138877	101496	annotated
2652	7(14)-Bisabolene-2,3,10,11-tetrol	-0.54	0.009	0.037	42174	28974	annotated
3058	Ethyl hydrogen sulfate	0.53	0.009	0.038	422076	608081	annotated+fragment
730	Valerylglycine	-0.36	0.009	0.038	407236	316865	annotated
3125	Methyl 3-(2,3-dihydroxy-3-methylbutyl)-4-hydroxybenzoate	-0.81	0.009	0.038	66025	37731	annotated
1749	Ligustilide	-0.62	0.009	0.038	60729	39488	annotated
622	L-Histidine trimethylbetaine	-0.49	0.009	0.039	1593855	1131307	annotated
2416	4-Dodecylbenzenesulfonic Acid	-0.81	0.009	0.040	4024210	2290919	annotated
1253	1-(2,3-Dihydro-1H-pyrrolizin-5-yl)-2-propen-1-one	0.68	0.010	0.040	157536	252685	annotated
83	Homoarginine	1.45	0.010	0.040	2495789	6834937	annotated+fragment
791	D-1-Amino-2-pyrrolidinecarboxylic acid	-0.43	0.010	0.042	28114	20855	annotated
2415	Catechol sulfate	-0.77	0.010	0.043	4022731	2358427	annotated
3508	Hexadecanedioate	-0.49	0.010	0.043	281126	200729	annotated
3933	2-Phenylethyl beta-D-glucopyranoside	-0.47	0.010	0.043	73985	53242	annotated
3536	alpha-Valerenol	-0.32	0.011	0.044	247743	197883	annotated
1423	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	-0.83	0.011	0.044	138888	78128	annotated
825	Sakacin P	-0.76	0.011	0.044	612426	362821	annotated
2251	(1R,2R)-3-[(1,2-Dihydro-2-hydroxy-1-naphthalenyl)thio]-2-oxopropanoic acid	0.41	0.011	0.045	28998	38570	annotated
2007	cis-alpha-octenoic acid	-0.31	0.011	0.046	34214	27626	annotated
561	Hexaethylene glycol	-0.62	0.011	0.046	246442	160727	annotated
3866	4-Hydroxycyclohexylcarboxylic acid	-0.30	0.011	0.046	102624	83114	annotated
343	Pirbuterol	0.21	0.012	0.047	836879	968031	annotated
1829	Isoquinoline	-0.66	0.012	0.048	64567	40827	annotated
3904	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	-0.55	0.012	0.048	69070	47022	annotated
3713	2-(1-Ethoxyethoxy)propanoic acid	-0.62	0.012	0.049	83535	54185	annotated

CTL T0h vs CTL T48h

<i>Peak id</i>	<i>Metabolite</i>	<i>Log FC</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T0h</i>	<i>Peak intensity CTL T48h</i>	<i>Identification</i>
114	N-Acetyl-L-glutamate 5-semialdehyde	-8.30	0.000	0.000	23794150	75398	annotated
119	Methyl hippurate	-2.05	0.000	0.000	393243	94873	annotated
149	Tromethamine	3.82	0.000	0.000	1081619	15299739	annotated+fragment
156	Alanyl-Aspartate	-12.75	0.000	0.000	16143067	2348	annotated
165	Hydroxypropyl-Proline	1.53	0.000	0.000	2596837	7485302	annotated
338	L-gamma-glutamyl-L-leucine	-4.54	0.000	0.000	1162247	50029	annotated
391	Glutaryl-glycine	-9.28	0.000	0.000	4777769	7684	annotated
414	Carboxy-ibuprofen	0.93	0.000	0.000	2238386	4259777	annotated
449	Glycylprolylhydroxyproline	3.16	0.000	0.000	245591	2192204	annotated
479	N-acetyl-L-glutamate	-0.78	0.000	0.000	186614	108953	identified
520	Vinylacetyl-glycine	-2.45	0.000	0.000	2495988	457480	annotated
523	3,5,7-Octatriyn-1-ol	1.08	0.000	0.000	1128722	2386638	annotated
524	Aloesol	1.53	0.000	0.000	204044	590288	annotated
525	3,4-Dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-carboxylic acid	1.23	0.000	0.000	145224	341003	annotated
635	Didodecyl thiobispropanoate	1.20	0.000	0.000	833391	1908947	annotated
696	Alanyl-Proline	3.01	0.000	0.000	114924	925766	annotated
848	L-cis-Cyclo(aspartylphenylalanyl)	-4.53	0.000	0.000	701805	30320	annotated
932	Trigoforin	2.25	0.000	0.000	20481	97515	annotated
1004	N-Acetyl-L-tyrosine	-1.94	0.000	0.000	178185	46299	annotated
1022	2,3-Dehydrosalvipisono	1.47	0.000	0.000	174020	483698	annotated
1064	Adenosine	-1.83	0.000	0.000	393389	110772	identified+fragment
1065	Methyl thiophene-2-carboxylate	1.10	0.000	0.000	236966	506379	annotated
1320	Piperidine	1.04	0.000	0.000	110538	226597	annotated+fragment

1532	Isoetharine	1.41	0.000	0.000	62488	166215	annotated
2312	3-keto-n-caproic acid	-0.71	0.000	0.000	9076017	5538908	annotated
2411	hexyl propionate	1.41	0.000	0.000	1370702	3636744	annotated
2417	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	2.53	0.000	0.000	872506	5026923	annotated
2419	Glycerol tributanoate	1.31	0.000	0.000	35883	89227	annotated
2453	Ethyl (±)-3-methylpentanoate	1.49	0.000	0.000	1013559	2841454	annotated
2455	Salicylaldehyde	1.06	0.000	0.000	1842803	3841396	annotated+fragment
2463	Phenylacetic acid	3.36	0.000	0.000	293119	3002442	annotated
2530	2-Oxoglutaramate	-9.36	0.000	0.000	3430538	5222	annotated
2641	Tiglylglycine	-4.70	0.000	0.000	2000964	76737	annotated
2800	Methyl benzoate	1.82	0.000	0.000	390205	1380027	annotated
3000	11-docosenoic acid	3.57	0.000	0.000	59533	707524	annotated
3166	Ipomeatetrahydrofuran	-1.48	0.000	0.000	566077	202371	annotated
3536	alpha-Valerenol	-1.45	0.000	0.000	247743	90428	annotated
3752	N-Formyl-L-methionine	-0.75	0.000	0.000	156615	93081	annotated
3764	1-Naphthalenesulfonic acid	-1.84	0.000	0.000	121979	34012	annotated
3933	2-Phenylethyl beta-D-glucopyranoside	-1.05	0.000	0.000	73985	35731	annotated
4003	Undecanedioic acid	1.08	0.000	0.000	30372	64078	annotated
4012	3-(2-Hydroxy-4-methylphenyl)-2-butanone	-0.99	0.000	0.000	95075	47735	annotated
404	Hydroxypropyl-Arginine	-0.79	0.000	0.000	253814	146808	annotated
1176	Alanyl-Arginine	-1.67	0.000	0.000	343777	107984	annotated
1288	Aprobarbital	1.10	0.000	0.000	104388	223947	annotated
2513	D-glucose	-0.29	0.000	0.000	4074804	3337556	identified
3063	N,N-Dihydroxy-L-valine	-0.42	0.000	0.000	254348	189554	annotated
3652	Tetradecanedioic acid	0.97	0.000	0.000	91839	180343	annotated
3784	Ferulate	2.37	0.000	0.000	19161	99342	annotated
4379	3-Furanmethanol glucoside	1.01	0.000	0.000	12942	26022	annotated
200	L-Theanine	-0.62	0.000	0.000	11627115	7586102	annotated
1389	L-Coprine	1.21	0.000	0.000	65093	150976	annotated
2981	2-Methylpropyl propionate	0.78	0.000	0.000	471805	808767	annotated

1646	Isoleucyl-Threonine	0.57	0.000	0.000	79102	117585	annotated
561	Hexaethylene glycol	-1.04	0.000	0.001	246442	119819	annotated
1810	Lysyl-Alanine	1.14	0.000	0.001	31971	70502	annotated
2726	2-Dehydro-D-xylonate	-0.35	0.000	0.001	136778	107143	annotated
663	1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione	-0.75	0.000	0.001	1536712	912030	annotated
3521	L-Citrulline	-0.70	0.000	0.001	240291	148084	identified
1380	Deoxyguanidinoproclavaminic acid	-2.62	0.000	0.001	216816	35374	annotated
1672	delta-1-Pyrroline-5-carboxylate	-0.52	0.000	0.001	121739	84955	annotated
68	N-a-Acetyl-L-arginine	-0.58	0.000	0.001	728514	488265	annotated
1083	Thiomorpholine 3-carboxylate	1.03	0.000	0.001	197207	402720	annotated
2454	3R-hydroxy-decanoic acid	1.19	0.000	0.001	40098	91707	annotated
1353	L-Rhamnose	-1.11	0.000	0.002	124530	57739	annotated
2582	D-Glucuronic acid	-0.42	0.000	0.003	2552868	1902116	annotated+fragment
930	(3S)-3-Hydroxy-L-enduracididine	-0.84	0.000	0.003	612598	343323	annotated
3088	cholesterol sulfate	0.42	0.000	0.003	519569	694920	annotated
825	Sakacin P	-1.06	0.000	0.003	612426	292792	annotated
1251	5-Methylcytidine	-0.50	0.000	0.003	281081	198561	annotated+fragment
2416	4-Dodecylbenzenesulfonic Acid	-1.19	0.000	0.004	4024210	1759812	annotated
3896	Salicyluric acid	-1.40	0.000	0.004	86753	32900	annotated
2198	Sinalexin	-0.47	0.000	0.004	87902	63605	annotated
288	Secobarbital	0.29	0.000	0.005	6134948	7490395	annotated
187	5-Methylthio-D-ribose	-0.48	0.001	0.005	3911727	2798193	annotated
342	1-Pyrroline-5-carboxylic acid	-0.49	0.001	0.005	5685504	4045824	annotated
1129	Ethosuximide	0.65	0.001	0.005	173249	271679	annotated
41	Fluocinolone	0.53	0.001	0.006	602468	869531	annotated
1908	Heterophyllin	-1.33	0.001	0.006	51306	20411	annotated
2218	3-methylmalate(2-)	-0.44	0.001	0.006	13278944	9777932	annotated+fragment
2456	Menthyl ethylene glycol carbonate	1.03	0.001	0.006	334928	683332	annotated
202	3-Ureidopropionate	-0.48	0.001	0.008	12660841	9072486	annotated+fragment

2457	Ethyl tiglate	0.53	0.001	0.008	147492	212879	annotated
1255	1,6,7-Trimethylnaphthalene	0.79	0.001	0.009	142117	245959	annotated
3587	3,3'-Thiobispropanoic acid	-0.40	0.001	0.011	183125	138352	annotated
476	Alanyl-Threonine	-0.37	0.001	0.011	510079	393910	annotated
256	Ergothioneine	-0.39	0.001	0.012	1580055	1204225	annotated
473	L-isoleucyl-L-proline	0.52	0.001	0.012	1188032	1700099	annotated
268	L-Cystine	0.39	0.001	0.012	1039434	1360700	identified+fragment
184	S-2,5-Dimethyl-3-furanyl 3-methylbutanethioate	-0.39	0.001	0.012	173720	132305	annotated
1068	delta-Guanidinovaleric acid	-0.77	0.001	0.012	515039	301866	annotated
1266	5,6-Dihydrouracil	-0.64	0.001	0.012	191748	123439	annotated
1163	Glycerophosphocholine	0.72	0.001	0.013	242818	398726	annotated
4014	PI(18:2(9Z,12Z)/22:3(10Z,13Z,16Z))	1.09	0.001	0.013	35443	75287	annotated
1444	Glycyl-Arginine	-1.02	0.001	0.014	129940	64191	annotated
3459	Trifluoroacetic acid	-0.34	0.002	0.015	315253	248894	annotated
753	Homoarecoline	0.76	0.002	0.017	308032	521915	annotated
4001	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/P-18:0)	0.60	0.002	0.019	53645	81367	annotated
3540	Methylphosphate	0.78	0.002	0.020	134148	229998	annotated
1109	Choline phosphate	1.31	0.002	0.020	125032	310486	identified
785	4-Aminosalicylate	-0.62	0.002	0.021	60772	39415	annotated
621	Terbutaline	1.14	0.003	0.024	64954	142925	annotated
1501	Dambonitol	-0.73	0.003	0.025	114872	69089	annotated
1246	apo-[3-methylcrotonoyl-CoA:carbon-dioxide ligase (ADP-forming)]	0.47	0.003	0.028	192423	266703	annotated
2095	ethyl tetradecanoate	0.41	0.003	0.029	38859485	51482368	annotated
66	L-homoserine	-0.33	0.004	0.035	51918117	41164654	identified+fragment
3737	Norambrereinolide	0.92	0.004	0.037	82411	156408	annotated
1302	6-Acetamido-2-oxohexanoate	-0.42	0.005	0.038	242010	180656	annotated
3681	2E-Lauroleic acid	0.77	0.005	0.038	49577	84274	annotated
1544	2-Octenoylcarnitine	0.96	0.005	0.039	61243	119233	annotated
3994	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	0.85	0.005	0.041	45175	81473	annotated

3966	Caproate (6:0)	2.46	0.005	0.041	10981	60557	annotated
1566	N-gamma-L-Glutamyl-L-methionine	-0.45	0.006	0.045	160507	117778	annotated
1696	Metaldehyde	-0.74	0.006	0.045	90061	53884	annotated
1684	3-Amino-2-piperidone	-0.57	0.006	0.045	94437	63497	annotated
1108	Dinex	-0.91	0.006	0.045	410798	218592	annotated
2541	Caproic acid	-0.42	0.006	0.048	2055274	1532859	annotated
320	PC(20:4(5Z,8Z,11Z,14Z)/16:1(9Z))	-0.31	0.006	0.048	2094776	1694167	annotated
3627	Acetoacetic acid	-0.42	0.006	0.049	168362	125477	annotated
3930	Phenylpyruvate	-0.87	0.007	0.050	72225	39391	identified

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

CTL T0h vs CTS T0h

<i>Peak Id</i>	<i>Metabolite</i>	<i>Log FC</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T0</i>	<i>Peak intensity CTS T0</i>	<i>Identification</i>
37	L-Acetopine	-2.36	0.000	0.000	84710226	16496722	annotated
114	N-Acetyl-L-glutamate 5-semialdehyde	-2.21	0.000	0.000	23794150	5159202	annotated
116	L-cis-Cyclo(aspartylphenylalanyl)	-2.24	0.000	0.000	636727	135191	annotated
119	Methyl hippurate	-1.31	0.000	0.000	393243	158684	annotated
149	Tromethamine	1.25	0.000	0.000	1081619	2567848	annotated+fragment
156	Alanyl-Aspartate	-2.35	0.000	0.000	16143067	3165593	annotated
157	Isoleucyl-Serine	-2.44	0.000	0.000	2571459	473803	annotated
160	Histidiny-Aspartate	-2.12	0.000	0.000	124296	28676	annotated
161	Thionazin	-2.15	0.000	0.000	105269	23685	annotated
165	Hydroxypropyl-Proline	1.33	0.000	0.000	2596837	6515856	annotated
338	L-gamma-glutamyl-L-leucine	-2.14	0.000	0.000	1162247	262942	annotated
391	Glutaryl-glycine	-2.19	0.000	0.000	4777769	1044222	annotated
392	Lysyl-Asparagine	-2.32	0.000	0.000	750761	149884	annotated
395	Mimosine	-3.39	0.000	0.000	88656	8447	annotated
414	Carboxy-ibuprofen	-0.78	0.000	0.000	2238386	1300758	annotated
449	Glycylprolylhydroxyproline	2.43	0.000	0.000	245591	1322838	annotated
458	L-1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	-2.45	0.000	0.000	140195	25610	annotated
506	N6-Acetyl-5S-hydroxy-L-lysine	-0.98	0.000	0.000	1412613	714404	annotated
520	Vinylacetyl-glycine	-2.39	0.000	0.000	2936840	559310	annotated
524	Didodecyl thiobispropanoate	-0.60	0.000	0.000	1128722	742727	annotated
638	Alpha-CEHC	-0.73	0.000	0.000	833391	503884	annotated
682	Glycyl-Aspartate	-1.05	0.000	0.000	1525175	736913	annotated
696	Alanyl-Proline	-2.72	0.000	0.000	1700329	258735	annotated
932	Methyl benzoate	-1.21	0.000	0.000	90848	39344	annotated
1075	Tris(2-chloroethyl)phosphate	-0.44	0.000	0.000	236966	175269	annotated+fragment
1077	alpha, alpha'-Trehalose 6-mycolate	-1.40	0.000	0.000	390865	148056	annotated
1122	S-4-Hydroxymephenytoin	-2.22	0.000	0.000	494738	106515	annotated
1123	Ornaline	-2.22	0.000	0.000	494738	106515	annotated
1839	2-aminomuconic acid semialdehyde	0.97	0.000	0.000	65093	127379	annotated
1842	N-(1-Deoxy-1-fructosyl)histidine	-0.54	0.000	0.000	121739	83864	annotated

2152	L-Homocysteic acid	-2.58	0.000	0.000	68290	11413	annotated
2404	5-Hydroxyindoleacetate	-0.54	0.000	0.000	38859485	26717955	annotated
2416	4-Dodecylbenzenesulfonic Acid	-1.55	0.000	0.000	10340243	3519879	annotated
2530	2-Oxoglutaramate	-0.72	0.000	0.000	872506	530457	annotated
2565	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	-0.98	0.000	0.000	293119	148219	annotated
2622	2-Oxosuccinamate	-2.36	0.000	0.000	3430538	667574	annotated
2636	4-(2-Aminophenyl)-2,4-dioxobutanoate	-2.18	0.000	0.000	2837522	627166	annotated
2641	Tiglylglycine	-2.30	0.000	0.000	2417151	491347	annotated
3002	Nonyl octanoate	-0.28	0.000	0.000	136778	112709	annotated
3166	Ipomeatetrahydrofuran	-0.26	0.000	0.000	254348	212651	annotated
3167	Oxprenolol	-1.22	0.000	0.000	566077	242828	annotated
3188	3D,7D,11D-Phytanic acid	-1.27	0.000	0.000	126660	52584	annotated
3212	3,6,8-Trimethylallantoin	-0.78	0.000	0.000	638445	371717	annotated
3231	4,5-Dihydroorotic acid	-2.37	0.000	0.000	562858	109003	annotated
3433	PS(15:0/22:2(13Z,16Z))	-2.48	0.000	0.000	592140	106248	annotated
3536	alpha-Valerenol	-2.24	0.000	0.000	344927	72787	annotated
3585	Aspartyl-Proline	-0.77	0.000	0.000	247743	145594	annotated
3599	Hydroxypropyl-Hydroxyproline	-3.36	0.000	0.000	137205	13340	annotated
3653	1-Pyrenylsulfate	-1.75	0.000	0.000	175597	52297	annotated
4212	Neodunol	-0.61	0.000	0.000	95075	62129	annotated
3764	1-Naphthalenesulfonic acid	-0.44	0.000	0.000	128528	94643	annotated
4012	3-(2-Hydroxy-4-methylphenyl)-2-butanone	-1.34	0.000	0.000	121979	48197	annotated
2417	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	-2.30	0.000	0.000	5762024	1170746	annotated
1004	N-Acetyl-L-tyrosine	-0.82	0.000	0.000	20481	11597	annotated
1672	delta-1-Pyrroline-5-carboxylate	0.96	0.000	0.000	135747	263841	annotated
1064	Adenosine	-1.29	0.000	0.001	178185	72761	identified+fragment
547	(E)-Urocanic acid	-0.59	0.000	0.001	145224	96316	annotated+fragment
888	3-Hydroxymelatonin	2.44	0.000	0.002	114924	624884	annotated
3035	Isogingerenone B	-0.45	0.000	0.002	788323	577302	annotated
523	3,5,7-Octatriyn-1-ol	-1.82	0.000	0.002	2495988	706037	annotated
3034	3',4',5'-Trimethoxycinnamyl alcohol acetate	-0.79	0.000	0.003	1044340	604551	annotated
502	Hyperforin	-0.98	0.000	0.004	1412613	714404	annotated
2095	ethyl tetradecanoate	-1.88	0.000	0.004	78461	21320	annotated
1319	Valyl-Valine	0.80	0.000	0.004	104388	182303	annotated
1288	Aprobarbital	-1.46	0.000	0.006	248706	90196	annotated
2463	Phenylacetic acid	-1.69	0.001	0.007	4024210	1245107	annotated
1065	Methyl thiophene-2-carboxylate	-1.22	0.001	0.009	393389	169016	annotated
1389	L-Coprine	-0.48	0.001	0.009	242010	173299	annotated
2726	2-Dehydro-D-xylonate	-2.87	0.001	0.009	397881	54507	annotated

635	Aloesol	-1.25	0.001	0.012	1466920	614880	annotated
525	3,4-Dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-carboxylic acid	-0.65	0.001	0.017	204044	129991	annotated
2800	Trigoforin	-2.26	0.002	0.031	2000964	418304	annotated
3680	Undecylic acid	-1.99	0.003	0.042	194202	48850	annotated
3063	N,N-Dihydroxy-L-valine	-0.54	0.003	0.044	662084	453796	annotated

CTL T12h vs CTS T12h

<i>Peak Id</i>	<i>Metabolite</i>	<i>Log FC</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T12</i>	<i>Peak intensity CTS T12</i>	<i>Identification</i>
37	L-Acetopine	-2.36	0.000	0.000	84710226	16496722	annotated
114	N-Acetyl-L-glutamate 5-semialdehyde	-2.21	0.000	0.000	23794150	5159202	annotated
116	L-cis-Cyclo(aspartylphenylalanyl)	-2.24	0.000	0.000	636727	135191	annotated
119	Methyl hippurate	-1.31	0.000	0.000	393243	158684	annotated
149	Tromethamine	1.25	0.000	0.000	1081619	2567848	annotated+fragment
156	Alanyl-Aspartate	-2.35	0.000	0.000	16143067	3165593	annotated
157	Isoleucyl-Serine	-2.44	0.000	0.000	2571459	473803	annotated
160	Histidiny-Aspartate	-2.12	0.000	0.000	124296	28676	annotated
161	Thionazin	-2.15	0.000	0.000	105269	23685	annotated
165	Hydroxypropyl-Proline	1.33	0.000	0.000	2596837	6515856	annotated
338	L-gamma-glutamyl-L-leucine	-2.14	0.000	0.000	1162247	262942	annotated
391	Glutaryl-glycine	-2.19	0.000	0.000	4777769	1044222	annotated
392	Lysyl-Asparagine	-2.32	0.000	0.000	750761	149884	annotated
395	Mimosine	-3.39	0.000	0.000	88656	8447	annotated
414	Carboxy-ibuprofen	-0.78	0.000	0.000	2238386	1300758	annotated
449	Glycylprolylhydroxyproline	2.43	0.000	0.000	245591	1322838	annotated
458	L-1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	-2.45	0.000	0.000	140195	25610	annotated
506	N6-Acetyl-5S-hydroxy-L-lysine	-0.98	0.000	0.000	1412613	714404	annotated
520	Vinylacetyl-glycine	-2.39	0.000	0.000	2936840	559310	annotated
524	Didodecyl thiobispropanoate	-0.60	0.000	0.000	1128722	742727	annotated
638	Alpha-CEHC	-0.73	0.000	0.000	833391	503884	annotated
682	Glycyl-Aspartate	-1.05	0.000	0.000	1525175	736913	annotated
696	Alanyl-Proline	-2.72	0.000	0.000	1700329	258735	annotated
932	Methyl benzoate	-1.21	0.000	0.000	90848	39344	annotated
1075	Tris(2-chloroethyl)phosphate	-0.44	0.000	0.000	236966	175269	annotated+fragment
1077	alpha,alpha'-Trehalose 6-mycolate	-1.40	0.000	0.000	390865	148056	annotated
1122	S-4-Hydroxymephenytoin	-2.22	0.000	0.000	494738	106515	annotated
1123	Ornaline	-2.22	0.000	0.000	494738	106515	annotated

1839	2-aminomuconic acid semialdehyde	0.97	0.000	0.000	65093	127379	annotated
1842	N-(1-Deoxy-1-fructosyl)histidine	-0.54	0.000	0.000	121739	83864	annotated
2152	L-Homocysteic acid	-2.58	0.000	0.000	68290	11413	annotated
2404	5-Hydroxyindoleacetate	-0.54	0.000	0.000	38859485	26717955	annotated
2416	4-Dodecylbenzenesulfonic Acid	-1.55	0.000	0.000	10340243	3519879	annotated
2530	2-Oxoglutaramate	-0.72	0.000	0.000	872506	530457	annotated
2565	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	-0.98	0.000	0.000	293119	148219	annotated
2622	2-Oxosuccinamate	-2.36	0.000	0.000	3430538	667574	annotated
2636	4-(2-Aminophenyl)-2,4-dioxobutanoate	-2.18	0.000	0.000	2837522	627166	annotated
2641	Tiglylglycine	-2.30	0.000	0.000	2417151	491347	annotated
3002	Nonyl octanoate	-0.28	0.000	0.000	136778	112709	annotated
3166	Ipomeatetrahydrofuran	-0.26	0.000	0.000	254348	212651	annotated
3167	Oxprenolol	-1.22	0.000	0.000	566077	242828	annotated
3188	3D,7D,11D-Phytanic acid	-1.27	0.000	0.000	126660	52584	annotated
3212	3,6,8-Trimethylallantoin	-0.78	0.000	0.000	638445	371717	annotated
3231	4,5-Dihydroorotic acid	-2.37	0.000	0.000	562858	109003	annotated
3433	PS(15:0/22:2(13Z,16Z))	-2.48	0.000	0.000	592140	106248	annotated
3536	alpha-Valerenol	-2.24	0.000	0.000	344927	72787	annotated
3585	Aspartyl-Proline	-0.77	0.000	0.000	247743	145594	annotated
3599	Hydroxyprolyl-Hydroxyproline	-3.36	0.000	0.000	137205	13340	annotated
3653	1-Pyrenylsulfate	-1.75	0.000	0.000	175597	52297	annotated
4212	Neodunol	-0.61	0.000	0.000	95075	62129	annotated
3764	1-Naphthalenesulfonic acid	-0.44	0.000	0.000	128528	94643	annotated
4012	3-(2-Hydroxy-4-methylphenyl)-2-butanone	-1.34	0.000	0.000	121979	48197	annotated
2417	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	-2.30	0.000	0.000	5762024	1170746	annotated
1004	N-Acetyl-L-tyrosine	-0.82	0.000	0.000	20481	11597	annotated
1672	delta-1-Pyrroline-5-carboxylate	0.96	0.000	0.000	135747	263841	annotated
1064	Adenosine	-1.29	0.000	0.001	178185	72761	identified+fragment
547	(E)-Urocanic acid	-0.59	0.000	0.001	145224	96316	annotated+fragment
888	3-Hydroxymelatonin	2.44	0.000	0.002	114924	624884	annotated
3035	Isogingerenone B	-0.45	0.000	0.002	788323	577302	annotated
523	3,5,7-Octatriyn-1-ol	-1.82	0.000	0.002	2495988	706037	annotated
3034	3',4',5'-Trimethoxycinnamyl alcohol acetate	-0.79	0.000	0.003	1044340	604551	annotated

502	Hyperforin	-0.98	0.000	0.004	1412613	714404	annotated
2095	ethyl tetradecanoate	-1.88	0.000	0.004	78461	21320	annotated
1319	Valyl-Valine	0.80	0.000	0.004	104388	182303	annotated
1288	Aprobarbital	-1.46	0.000	0.006	248706	90196	annotated
2463	Phenylacetic acid	-1.69	0.001	0.007	4024210	1245107	annotated
1065	Methyl thiophene-2-carboxylate	-1.22	0.001	0.009	393389	169016	annotated
1389	L-Coprine	-0.48	0.001	0.009	242010	173299	annotated
2726	2-Dehydro-D-xylonate	-2.87	0.001	0.009	397881	54507	annotated
635	Aloesol	-1.25	0.001	0.012	1466920	614880	annotated
525	3,4-Dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran- 2-carboxylic acid	-0.65	0.001	0.017	204044	129991	annotated
2800	Trigoforin	-2.26	0.002	0.031	2000964	418304	annotated
3680	Undecylic acid	-1.99	0.003	0.042	194202	48850	annotated
3063	N,N-Dihydroxy-L-valine	-0.54	0.003	0.044	662084	453796	annotated

CTL T48h vs CTS T48h

Peak Id	Metabolite	Log FC	p	Adjusted p	Peak intensity CTL T48	Peak intensity CTS T48	Identification
41	Fluocinolone	-0.46	0.000	0.000	869531	630175	annotated+fragment
149	Tromethamine	-1.55	0.000	0.000	15299739	5234545	annotated
150	Gibberellin A61	-1.81	0.000	0.000	102702	29358	annotated
156	Alanyl-Aspartate	//	0.000	0.000	2348	//	identified+fragment
213	Isobutyryl-L-carnitine	-1.78	0.000	0.000	156391	45591	annotated
391	Glutaryl-glycine	0.46	0.000	0.000	7684	10605	annotated
414	Carboxy-ibuprofen	-0.54	0.000	0.000	4259777	2923495	annotated+fragment
635	Didodecyl thiobispropanoate	-0.60	0.000	0.000	1908947	1263102	annotated
638	Alpha-CEHC	-0.68	0.000	0.000	1107648	690977	annotated
753	Homoarecoline	-1.08	0.000	0.000	521915	247387	annotated
1064	Adenosine	1.74	0.000	0.000	110772	368969	annotated
1065	Methyl thiophene-2-carboxylate	-0.63	0.000	0.000	506379	328315	annotated
1532	Isoetharine	-0.63	0.000	0.000	166215	107679	annotated
2095	ethyl tetradecanoate	-0.52	0.000	0.000	51482368	35946250	annotated
2312	3-keto-n-caproic acid	0.63	0.000	0.000	5538908	8545676	annotated
2411	hexyl propionate	-1.38	0.000	0.000	3636744	1398427	annotated
2417	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	-0.75	0.000	0.000	5026923	2984306	annotated
2419	Glycerol tributanoate	-0.62	0.000	0.001	89227	58099	annotated
2453	Ethyl (±)-3-methylpentanoate	-1.18	0.000	0.001	2841454	1254823	annotated
2454	3R-hydroxy-decanoic acid	-1.17	0.000	0.001	91707	40895	annotated
2455	Salicylaldehyde	-1.07	0.000	0.001	3841396	1826559	annotated
2456	Menthyl ethylene glycol carbonate	-1.70	0.000	0.001	683332	210867	annotated
2457	Ethyl tiglate	-0.66	0.000	0.001	212879	135109	annotated
2463	Phenylacetic acid	-2.06	0.000	0.001	3002442	718553	annotated
2800	Methyl benzoate	-0.83	0.000	0.002	1380027	774936	annotated

2981	2-Methylpropyl propionate	-0.67	0.000	0.002	808767	506810	annotated
2982	Dodecanedioic acid	-1.23	0.000	0.005	211182	90087	annotated
3000	11-docosenoic acid	-1.96	0.000	0.005	707524	182441	annotated
3002	Nonyl octanoate	-0.55	0.000	0.006	1010969	690001	annotated
3166	Ipomeatetrahydrofuran	-0.73	0.000	0.006	202371	122235	annotated
3188	3D,7D,11D-Phytanic acid	-0.60	0.000	0.006	553537	364446	annotated
3378	Talaromycin A	-1.23	0.000	0.006	162545	69061	annotated
3577	7-oxo-8-amino-nonanoic acid	-1.50	0.000	0.006	121301	42950	annotated
3606	Cer(d18:1/23:0)	0.88	0.000	0.007	121183	223657	annotated
3626	3-keto palmitic acid	-0.60	0.000	0.009	193873	128049	annotated
3652	Tetradecanedioic acid	-0.84	0.000	0.018	180343	100930	annotated
3680	Undecylic acid	-0.94	0.000	0.020	166033	86560	annotated
3681	trans-Dodec-2-enoic acid	-0.94	0.001	0.024	84274	44047	annotated
3737	Norambreinolide	-1.16	0.001	0.037	156408	69966	annotated
3784	Ferulate	-2.42	0.001	0.041	99342	18561	annotated
3966	Caproate (6:0)	-1.69	0.001	0.042	60557	18767	annotated
4003	Undecanedioic acid	-1.29	0.001	0.043	64078	26133	annotated
4257	2-Methyl-4-propyl-1,3-oxathiane	-0.51	0.001	0.044	47650	33523	annotated