

Table S1. Heat map of statistically significant biochemicals profiled in this study. **Red** and **green** shaded cells indicate p<0.05 (**red** indicates that the mean values are significantly higher for that comparison; **green** values significantly lower). **Light red** and **light green** shaded cells indicate 0.05<p<0.10 (**light red** indicates that the mean values trend higher for that comparison; **light green** values trend lower).

Sub Pathway	Biochemical Name	Platform	Comp ID	KEGG	HMDB	PUBCHEM
Glycine, Serine and Threonine Metabolism	glycine	LC/MS pos early	58	C00037	HMDB0000123	750
	dimethylglycine	LC/MS pos early	5086	C03626	HMDB0000092	673
	betaine	LC/MS pos early	3141	C00719	HMDB0000043	247
	serine	LC/MS pos early	1648	C00065	HMDB0000187	5951
	N-acetyls erine	LC/MS pos early	37076		HMDB0002931	65249
	threonine	LC/MS pos early	1284	C00188	HMDB0000167	6288
	N-acetylthreonine	LC/MS polar	33939		HMDB0062557	152204
Alanine and Aspartate Metabolism	alanine	LC/MS pos early	1126	C00041	HMDB0000161	5950
	N-acetylanaline	LC/MS neg	1585	C02847	HMDB0000766	88064
	aspartate	LC/MS pos early	443	C00049	HMDB0000191	5960
	N-acetylaspartate (NAA)	LC/MS polar	22185	C01042	HMDB0000812	65065
	asparagine	LC/MS pos early	512	C00152	HMDB0000168	6267
	N-acetylasparagine	LC/MS pos early	33942		HMDB0006028	99715
	glutamate	LC/MS pos early	57	C00025 C00217	HMDB0000148	33032
Glutamate Metabolism	glutamine	LC/MS neg	53	C00064	HMDB0000641	5961
	N-acetylglutamate	LC/MS pos early	15720	C00624	HMDB0001138	70914
	N-acetylglutamine	LC/MS pos early	33943	C02716	HMDB0006029	182230
	glutamate, gamma-methyl ester	LC/MS pos early	33487		HMDB0061715	68662
	histidine	LC/MS neg	59	C00135	HMDB0000177	6274
Histidine Metabolism	1-methylhistidine	LC/MS pos early	30460	C01152	HMDB0000001	92105
	trans-urocanate	LC/MS polar	607	C00785	HMDB0000301	736715
	carosine	LC/MS pos early	1768	C00386	HMDB0000033	439224
	4-imidazoleacetate	LC/MS pos early	32349	C02835	HMDB0002024	96215
	lysine	LC/MS polar	1301	C00047 C00739	HMDB0003405	5962
Lysine Metabolism	N6-methyllysine	LC/MS pos early	62860	C02728	HMDB0002038	164795
	N6,N6-trimethyllysine	LC/MS pos early	1498	C03793	HMDB0001325	440120
	N,N,N-trimethyl-5-aminovaleate	LC/MS pos early	57687			14274897
	phenylalanine	LC/MS pos early	64	C00079	HMDB0000159	6140
Phenylalanine Metabolism	tyrosine	LC/MS pos early	1299	C00082	HMDB0000158	6057
	4-hydroxyphenylpyruvate	LC/MS neg	1669	C01179	HMDB0000707	979
	3-(4-hydroxyphenyl)lactate	LC/MS neg	32197	C03672	HMDB0000755	9378
Tyrosine Metabolism	tryptophan	LC/MS pos early	54	C00078	HMDB0000929	6305
	kynurenine	LC/MS pos early	15140	C00328	HMDB0000684	161166
	serotonin	LC/MS pos early	2342	C00780	HMDB0000259	5202
	indolactate	LC/MS neg	18349	C02043	HMDB0000671	92904
Leucine, Isoleucine and Valine Metabolism	leucine	LC/MS pos early	60	C00123	HMDB0000687	6106
	4-methyl-2-oxopentanoate	LC/MS neg	22116	C00233	HMDB0000695	70
	beta-hydroxyisovalerylcarbitine	LC/MS pos early	35433			
	3-methylglutaconate	LC/MS polar	57747		HMDB0000522	1551553
	isoleucine	LC/MS pos early	1125	C16424 C00407 C06418	HMDB0000172	6306
	3-methyl-2-oxovalerate	LC/MS neg	15676	C00671 C06008 C03465	HMDB0000491	440877,439286
	2-methylbutyrylcarnitine (C5)	LC/MS pos early	45095		HMDB0000378	6426901
	ethylmalonate	LC/MS polar	15765		HMDB0000622	11756
	methylsuccinate	LC/MS polar	15745		HMDB0001844	10349
	valine	LC/MS pos early	1649	C00183	HMDB0000883	6287
Methionine, Cysteine, SAM and Taurine	methionine	LC/MS polar	1302	C00073	HMDB0000696	6137
	N-acetylmethionine	LC/MS neg	1589	C02712	HMDB0011745	448580
	N-formylmethionine	LC/MS neg	2829	C03145	HMDB0001015	439750
	methionine sulfone	LC/MS pos early	44878		HMDB0062174	69961
	methionine sulfoxide	LC/MS pos early	18374	C02989	HMDB0002005	158980
	S-adenosylmethionine (SAM)	LC/MS pos early	15915	C00019	HMDB0001185	34755
	S-adenosylhomocysteine (SAH)	LC/MS neg	42382	C00021	HMDB000939	439155
	homocysteine	LC/MS pos early	15128	C00155	HMDB0000742	778
	cysteine	LC/MS pos early	1868	C00097	HMDB0000574	5862
	N-acetylcysteine	LC/MS neg	1586	C06809	HMDB0001890	12035
	hypotaurine	LC/MS pos early	590	C00519	HMDB0000965	107812
	taurine	LC/MS neg	2125	C00245	HMDB0000251	1123
	N-acetyltaurine	LC/MS polar	48187		HMDB0240253	159864
	3-sulfo-L-alanine	LC/MS polar	47069	C00506	HMDB0002757	72886

Fold of Change	Statistical Values	
Welch's t-Test	Welch's t-Test	
KO T- cells WT T- cells	KO T- cells WT T- cells	
	p-value	q-value
1.08	0.4854	0.9839
1.02	0.9367	0.9839
1.18	0.1879	0.8181
1.12	0.3168	0.9577
1.07	0.5316	0.9839
1.06	0.5434	0.9839
1.04	0.6466	0.9839
1.12	0.2743	0.9238
0.92	0.6176	0.9839
1.03	0.6805	0.9839
1.04	0.6510	0.9839
1.12	0.3780	0.9839
1.00	0.9101	0.9839
1.06	0.5594	0.9839
1.36	0.0268	0.4501
1.75	0.0001	0.0096
1.04	0.6384	0.9839
1.45	0.4104	0.9839
0.84	0.2758	0.9238
1.17	0.6963	0.9839
0.56	0.8791	0.9839
0.89	0.4171	0.9839
0.72	0.1678	0.7798
1.01	0.8846	0.9839
0.97	0.7626	0.9839
0.99	0.8693	0.9839
1.65	0.0005	0.0364
1.00	0.8767	0.9839
1.00	0.9687	0.9846
0.71	0.3043	0.9370
0.77	0.0678	0.6199
0.97	0.9229	0.9839
1.09	0.5030	0.9839
0.73	0.0556	0.6094
0.71	0.0605	0.6094
0.92	0.6367	0.9839
0.96	0.9153	0.9839
0.97	0.9870	0.9971
0.76	0.1403	0.7748
0.86	0.2771	0.9238
0.67	0.2924	0.9370
0.93	0.9068	0.9839
0.95	0.9399	0.9839
0.94	0.8682	0.9839
0.92	0.5729	0.9839
0.99	0.9434	0.9839
1.28	0.0696	0.6199
0.83	0.1656	0.7798
0.93	0.6638	0.9839
0.89	0.4462	0.9839
1.15	0.1996	0.8265
1.12	0.3748	0.9839
1.08	0.8831	0.9839
1.00	0.8696	0.9839
0.63	0.0432	0.5700
1.29	0.0562	0.6094
1.19	0.1597	0.7798
0.82	0.1642	0.7798
1.06	0.9616	0.9839

Chemical ID	CAS	RI	Mass
340	56-40-6	1375	76.03931
806	1118-68-9	1104	104.07061
799	107-43-7	1064	118.08626
503	56-45-1	1239	106.04987
100001851	97-14-3	800	148.06044
564	72-19-5	1514	120.06552
100001274	17093-74-2	1700	160.06153
811	56-41-7	1700	90.05496
1110	97-69-8	861	130.05096
234	56-84-8	1165	134.04479
100000787	997-55-7,997-55-7	3143	174.04079
917	70-47-3	1225	133.06077
100001257	4033-40-3	785	175.07134
561	56-86-0	1500	148.06044
563	56-85-9	692	145.06186
100000282	83717	1050	190.071
100001253	2490-97-3	845	189.08699
100001103	1499-55-4,1499-55-4	2170	162.07609
355	5934-29-2	755.9	154.0622
100001051	332-80-9	2755	170.09241
537	104-98-3	1882.5	137.03565
249	305-84-0	2942	227.11387
100001207	645-65-8	2055	127.05021
407	56-87-1	5431.1	145.09825
100003415	1188-07-4	2831	161.12846
189	23284-33-5	2825	189.15976
100015962		2186	160.13321
460	63-91-2	2878	166.08626
815	60-18-4	2430	182.08117
1141	156-39-8	1690	179.03498
240	6482-98-0	1379	181.05063
565	73-22-3	2996	205.09716
100000265	2922-83-0	2739	209.09207
504	153-98-0	2550	177.10224
100000463	832-97-3	2286	204.06661
397	61-90-5	2864	132.10191
100000551	816-66-0	2170	129.05571
100001594	99159-87-2	2584	262.1649
100002458	5746-90-7	2700	99.04518
376	73-32-5	2800	132.10191
100000036	1460-34-0,51829-07-3	2064.2	129.05572
100001509	31023-25-3	3050	246.16999
2054	601-75-2	2785	131.03498
2051	498-21-5	2800	131.03498
566	72-18-4	2479	118.08626
415	63-68-3	1871.8	148.04377
1083	65-82-7	1787	190.05434
194	4289-98-9	1543.8	176.03869
100004635	820-10-0	1250	182.04816
100000039	3226-65-1	1272	166.05325
1263	24346-00-7,86867-01-8,86867-01-8	3002	399.14452
197	979-92-0	1832.4	383.11431
311	454-29-5	2155	136.04268
800	52-90-4,56-89-3	1475	122.02703
1107	616-91-1	1108	162.02304
358	300-84-5	724	110.02703
512	107-35-7	690	124.00739
100005466		1249	166.01795
382	498-40-8	2890	167.96722

Urea cycle; Arginine and Proline Metab	arginine	LC/MS pos early	1638	C00062	HMD80000517	6322	0.97	0.7888	0.9839	231	1119-34-2	2825	175.11896	
	argininosuccinate	LC/MS pos early	1547	C03406	HMD80000052	60150382	1.21	0.2832	0.9272	232	156637-58-0	2745	291.12992	
	ornithine	LC/MS pos early	1493	C00077	HMD80000214	6282	1.27	0.0751	0.6315	444	3184-13-2	2800	133.09716	
	2-oxoarginine*	LC/MS pos early	55072	C03773	HMD80004225	558	0.60	0.0107	0.3044	100002784	104175	1780	174.08732	
	citrulline	LC/MS pos early	2132	C00327	HMD80000904	9750	1.15	0.7397	0.9839	391	372-75-8	1520	176.10297	
	homocystine	LC/MS pos early	22137	C01924	HMD80000670	9085	0.91	0.5501	0.9839	100000961	156-86-5	2882	189.13461	
	proline	LC/MS pos early	1998	C00148 C000763	MDB0000162 HMD8000034	145742;614;8989	1.21	0.1529	0.7748	490	147-85-3	1603	116.07061	
	dimethylarginine (SDMA + ADMA)	LC/MS pos early	36808	C21189 C03626	MDB0003334 HMD8000019	123831;169148	1.44	0.0189	0.3594	100001810	102783-24-4	2850	203.15026	
	N-acetylarginine	LC/MS pos early	33953	C02562	HMD80004620	67427	1.05	0.6529	0.9839	100001266	155-84-0	2245	217.12952	
	N-delta-acetylornithine	LC/MS neg	43249	C00437	HMD80003357	9620500	0.79	0.0901	0.6802	100004523		858	173.09316	
	trans-4-hydroxyproline	LC/MS pos early	32306	C01157	HMD80000725	5810	1.09	0.4416	0.9839	1001	51-35-4	1064	132.06552	
	pro-hydroxy-pro	LC/MS pos early	35127		HMD80005695	11902893	0.82	0.4355	0.9839	100001167	18884-24-7	2128	229.11829	
	N-methylproline	LC/MS pos early	37431		HMD80094696	643474	0.92	0.6818	0.9839	100001956	475-11-6	1335	130.08626	
	N,N,N-trimethyl-L-arginine betaine (TMAP)	LC/MS pos early	62947		HMD80240365		1.58	0.1373	0.7898	100020217		2470	229.15467	
Creatine Metabolism	guanidinoacetate	LC/MS pos early	43802	C00581	HMD80000128	763	4.29	0.0000	0.0053	344	352-97-6	1937	118.06111	
	creatine	LC/MS pos early	27718	C00300	HMD80000064	586	1.12	0.3352	0.9779	1221	57-00-1	1947	132.07676	
	creatinine	LC/MS pos early	513	C00791	HMD80000562	598	0.92	0.8065	0.9839	275	60-27-5	2055	114.06919	
	creatine phosphate	LC/MS polar	33951	C02305	HMD80001511	587;9548602	0.71	0.0749	0.6315	100000112	922-32-7	3831	210.02853	
	putrescine	LC/MS pos early	1408	C00134	HMD80001414	1045	1.19	0.3864	0.9839	49	110-60-1	3027	89.10733	
Polyamine Metabolism	spermidine	LC/MS pos early	485	C00315	HMD80001257	1102	0.87	0.4922	0.9839	50	124-20-9	3355	146.16518	
	(N(1) + N(8))-acetylspermidine	LC/MS pos early	57814	C00612 C01029	MDB0001276 HMD8000021	123889;496	1.03	0.9020	0.9839	100016038		3080	188.17574	
	spermine	LC/MS pos late	603	C00750	HMD80001256	1103	1.20	0.8006	0.9839	507	71-44-3	758	203.22303	
	5-methylthioadenosine (MTA)	LC/MS pos early	1419	C00170	HMD80001173	439176	0.95	0.7465	0.9839	212	2457-80-9	2752	298.09884	
	4-guanidinobutanoate	LC/MS pos early	15681	C01035	HMD80003464	500	2.04	0.0001	0.0096	100000096	463-003;463-00-3	2320	146.09241	
Guandinio and Acetamido Metabolism	glutathione, reduced (GSH)	LC/MS neg	2127	D00014 C00051	HMD80000125	124886	1.25	0.2331	0.8713	496	70-18-8	790	306.07653	
	glutathione, oxidized (GSSG)	LC/MS pos early	27727	D00031 C00127	HMD80003337	65359	1.00	0.8638	0.9839	448	103239-24-3	2667	613.15925	
	S-lactylglutathione	LC/MS pos early	19731	C03451	HMD80001066	440018	0.92	0.7786	0.9839	1343	54398-03-7	2124	380.11222	
	cysteinylglycine	LC/MS pos early	35637	C01419	HMD80000078	439498	1.16	0.1517	0.7748	278	19246-18-5	2132	179.0485	
	5-oxoproline	LC/MS neg	1494	C01879 C02237	HMD80000267	439685;7405	0.94	0.6851	0.9839	1021	98-79-3	738.5	128.03531	
	ophthalmate	LC/MS pos early	34592		HMD800005765	7018721	1.38	0.0320	0.4934	100001311	495-27-2	2085	290.13467	
	S-(1,2-dicarboxyethyl)glutathione	LC/MS neg	63009			9802383	1.32	0.1330	0.7898	100020967	1115-52-2	543	422.08748	
	Co-A-glutathione*	LC/MS neg	62804	C00920		46873828	1.03	0.5385	0.9839	289	6477-52-7	1326	535.0944	
Gamma-glutamyl Amino Acid	gamma-glutamylcysteine	LC/MS pos early	1778	C00669	HMD80001049	123938	1.84	0.0025	0.1178	1036	636-58-8	2118	251.06963	
	gamma-glutamylglutamate	LC/MS pos early	36738	C05282	HMD80011737	92865	1.06	0.7298	0.9839	331	1116-22-9	1775	277.10303	
	gamma-glutamylglycine	LC/MS pos early	33949		HMD80011667	100099	0.91	0.6323	0.9839	100001294	1948-29-9	1535	205.0819	
Acetylated Peptides	phenylacetyl-glycine	LC/MS neg	33945	C05598	HMD80000821	68144	0.90	0.3542	0.9779	100001275	500-98-1	2375	192.06661	
	Modified Peptides	LC/MS pos early	64571				0.98	0.9438	0.9839	100022041		2500	241.15467	
Glycolysis, Gluconogenesis, and Pyru	glucose	LC/MS polar	20468	C00031	HMD80000122	5793	0.90	0.8817	0.9839	572	50-99-7	2342	179.05511	
	fructose 1,6-diphosphate/glucose 1,6-diphosph	LC/MS neg	46896	C05378 C00354 C01231	MDB0003514 HMD8000010	588350;124383956;445374	0.55	0.0013	0.0699	100002180		551	338.98897	
	dihydroxyacetone phosphate (DHAP)	LC/MS neg	15522	C00111	HMD800001473	668	0.83	0.0982	0.7154	309	102783-56-2	603	168.99075	
	3-phosphoglycerate	LC/MS neg	1414	C00597	HMD80000807	724	0.69	0.1294	0.7898	132	80731-10-8	583	184.98566	
	phosphoenolpyruvate (PEP)	LC/MS neg	597	C00074	HMD80000263	1005	0.98	0.0838	0.6684	463	10526-80-4	587.3	166.97511	
	pyruvate	LC/MS polar	48990	C00022	HMD80000243	1080	1.11	0.4357	0.9839	823	127-17-3	1083	87.00877	
	lactate	LC/MS polar	527	C00186	HMD80000190	612	1.00	0.8470	0.9839	482	79-33-4	1469	89.02442	
	glycerate	LC/MS polar	1572	C00258	MDB0006372 HMD8000001	752;439194	0.92	0.5093	0.9839	1052	600-19-1	2070.4	105.01933	
	Pentose Phosphate Pathway	6-phosphogluconate	LC/MS neg	15442	C00345	HMD80001316	91493	0.66	0.0704	0.6199	100000341	921-62-0;53411-70-4	583.9	275.01735
		sedoheptulose-7-phosphate	LC/MS pos early	35649	C05382	HMD80001068	616	1.97	0.0206	0.3638	100001628	2846-35-7	540	273.037
ribose		LC/MS polar	1471	C00121	HMD80000283	5779	1.64	0.0111	0.3044	914	50-69-1	1508.2	195.05103	
Pentose Metabolism	ribitol	LC/MS polar	15772	8532 C01904 C00474 C000	MDB0000508 HMD8000018	6912	0.97	0.9147	0.9839	100000406	488-81-3	1789.6	151.06119	
	ribonate	LC/MS polar	27731	C01685	HMD80000867	5460677	0.98	0.7538	0.9839	100001007	8/3/36	2425	165.04046	
	arabitol/xylitol	LC/MS polar	48885	C00542 C01904 C00379	2917 HMD80001851 HMD	6912;94154	0.88	0.1606	0.7798	100006430		1932.4	151.0612	
	arabonate/xylonate	LC/MS polar	48255	C00502 C05411	HMD80000539	122045;6602431	0.98	0.8299	0.9839	100006115		2700	165.04046	
	lyxonate	LC/MS polar	61858				0.88	0.4454	0.9839	100019968		2350	165.04046	
	fructose	LC/MS polar	577	C00095	HMD80000660	2723872	0.81	0.1798	0.7919	878	57-48-7	2065	179.05511	
Fructose, Mannose and Galactose Meta	mannitol/sorbitol	LC/MS polar	46142	C00392 C00794	MDB0000247 HMD8000007	6251;5780	0.96	0.8621	0.9839	100001740		2320	181.07176	
	galactonate	LC/MS polar	27719	C15930 C00880	HMD80000565	12310779;128869	1.28	0.1491	0.7748	100001026	299-28-5	3085	195.05102	
Nucleotide Sugar	UDP-glucose	LC/MS polar	32344	C00029	HMD80000286	8629	0.99	0.9890	0.9971	1096	117756-22-6	3950	565.04775	
	UDP-galactose	LC/MS polar	15860	C00052	HMD80000302	18068	0.95	0.8621	0.9839	100000298	2956-16-3;91183-98-1;137869-52-1	4000	565.04774	
	UDP-gucuronate	LC/MS neg	2763	C00167	HMD80000935	17473	0.93	0.7788	0.9839	1097	28053-08-9;63700-19-6	588	579.02701	
	UDP-N-acetylglucosamine/galactosamine	LC/MS polar	46148	C00203 C00043	MDB0000304 HMD8000002	44576;1167	1.10	0.3458	0.9779	100002957		3665	606.07429	
Aminosugar Metabolism	glucuronate	LC/MS polar	15443	C16245	HMD80000127	94715;23677978;65041;444	0.94	0.7460	0.9839	100000257	207300-70-7	3233.3	193.05337	
	N-acetylneuraminate	LC/MS pos early	32377	C00270	HMD80000230	439197	1.29	0.0578	0.6094	1162	131-48-6	660	310.11326	
	N-acetylglucosaminylasparagine	LC/MS pos early	48149	C04540	HMD80000489	123828	1.17	0.2974	0.9370	1215	2776-93-4	1212	336.14015	
	erythronate*	LC/MS polar	42420		HMD80000613	2781043	0.99	0.9148	0.9839	100001320	88759-55-1	2186	135.02989	
	N-acetylglucosamineN-acetylgalactosamine	LC/MS pos early	46539	C01074	MDB0000212 HMD8000002	84265;439174	1.22	0.1699	0.7798	100006435		715	222.0272	
	N-glycylneuraminate	LC/MS pos early	37123	C03410	HMD80000833	123802	1.00	0.7780	0.9839	100001491	1113-83-3	636	326.10818	
TCA Cycle	citrate	LC/MS neg	1564	C00158	HMD80000094	311	1.05	0.5520	0.9839	1124	77-92-9	582	191.01973	
	aconitate [cis or trans]	LC/MS neg	46173	C02341 C004174	MDB0000589 HMD8000000	643757;444212	1.07	0.5846	0.9839	100001359		580	173.00916	
	alpha-ketoglutarate	LC/MS polar	528	C00026	HMD80000208	51	0.97	0.9510	0.9839	93	305-72-6;328-50-7;22202-68-2	2700	145.01425	
	succinate	LC/MS polar	1437	C00042	HMD80000254	1110	0.71	0.0392	0.5389	252	110-15-6	3149	117.01933	
	fumarate	LC/MS polar	1643	C00122	HMD80000134	444972	0.93	0.7216	0.9839	330	100-17-8	3084	115.03688	
	malate	LC/MS polar	1303	C00497 C00149 C00711	0744 HMD800031518 HMD	525	0.87	0.3275	0.9694	409	6915-15-7	3343.1	133.01425	
	2-methylcitrate/homocitrate	LC/MS neg	52282	C01251	MDB0002518 HMD8000003	515;439459	0.82	0.5225	0.9839	100008929		575	205.03538	
Oxidative Phosphorylation	acetylphosphate	LC/MS polar	15488	C00227	HMD80001494	186	0.96	0.8656	0.9839	1211	94249-01-1	4013.9	138.98018	
	phosphate	LC/MS pos early	42109	C00009	HMD80001429	1061	1.02	0.8130	0.9839	461	7664-38-2	576	98.98418	

Long Chain Saturated Fatty Acid	stearate (18:0)	LC/MS neg	1358	C01530	HMDB0000827	5281	0.95	0.9140	0.9839	439	57-11-4	5872	283.26425	
	arachidate (20:0)	LC/MS neg	1118	C06425	HMDB0002212	10467	1.11	0.4776	0.9839	893	506-30-9	6240	311.29555	
	10-nonadecenoate (19:1n9)	LC/MS neg	33972		HMDB0013622	5312513		0.8149	0.9839	100001277	73033-09-7	5780	295.26425	
Long Chain Monounsaturated Fatty Acid	eicosenoate (20:1)	LC/MS neg	33587	C16526	MDB0002231	HMDB0006242	282769;5282768;94159	0.93	0.9029	0.9839	100001335		5950	309.2799
	erucate (22:1n9)	LC/MS neg	1552	C08316	HMDB0002068	8216;5281116	1.34	0.8893	0.9839	1087	112-86-7	6355.6	337.3112	
Long Chain Polyunsaturated Fatty Acid	tetradecadienoate (14:2)*	LC/MS neg	62850		HMDB0000560	5312409	1.07	0.4542	0.9839	100020343	39039-37-7	5292	223.17035	
	docosapentaenoate (n3 DPA; 22:5n3)	LC/MS neg	32504	C16513	MDB0001976	HMDB000065	6441454	0.88	0.8418	0.9839	100001181	2234-74-4	5571	329.2486
	docosahexaenoate (DHA; 22:6n3)	LC/MS neg	44675	C06429	HMDB0002183	445580	0.78	0.7978	0.9839	100000665	6217-54-5	5525	327.23295	
	dihomo-linoleate (20:2n6)	LC/MS neg	17805	C16525	HMDB0005060	6439848	0.87	0.7648	0.9839	1231	2091-39-6	5730	307.26425	
	dihomo-linolenate (20:3n3 or n6)	LC/MS neg	35718	C03242	HMDB0002925	5280581	0.77	0.7370	0.9839	100001739	17046-59-2	5596	305.2486	
	arachidonate (20:4n6)	LC/MS neg	1110	C00219	HMDB0001043	444899	0.73	0.6587	0.9839	229	506-32-1	5535	303.23295	
	docosapentaenoate (n6 DPA; 22:5n6)	LC/MS neg	37478	C16513	HMDB0001976	6441454	0.92	0.9405	0.9839	100001580	25182-74-5	5624.5	329.2486	
	docosadienoate (22:2n6)	LC/MS neg	32415	C16533	HMDB0061714	5282807	0.90	0.9115	0.9839	100001182	7370-49-2	6034	335.29555	
Fatty Acid, Dicarboxylate	glutarate (C5-DC)	LC/MS polar	396	C00489	HMDB0000661	743;4418048	0.90	0.6758	0.9839	339	110-94-1	2900	131.03498	
	2-hydroxyglutarate	LC/MS pos early	52294	C02630	HMDB0059655	43	1.04	0.6528	0.9839	100002070	40951-21-1	958	166.071	
	adipate (C6-DC)	LC/MS polar	21134	C06104	HMDB0000448	196	1.00	0.8806	0.9839	100000863	124-04-9	3000	145.05063	
Fatty Acid Metabolism (also BCAA Metabolism)	butyrylcarnitine (C4)	LC/MS pos early	32412	C02862	HMDB0002013	439829	0.41	0.0002	0.0206	100001054	25576-40-3	2860	232.15434	
	propionylcarnitine (C3)	LC/MS pos early	32452	C03017	HMDB0000824	107738	0.74	0.0680	0.6199	100001162	17298-37-2	2590	218.13869	
Fatty Acid Metabolism (Acyl Carnitine)	acetyl carnitine (C2)	LC/MS pos early	32198	C02571	HMDB0000201	7045767	1.02	0.8110	0.9839	100000802	5080-50-2	2282	204.12304	
Fatty Acid Metabolism (Acyl Carnitine)	hexanoylcarnitine (C6)	LC/MS pos early	32328		HMDB0000756	6426853	0.62	0.3184	0.9577	100000781	6920-35-0	3358	260.18564	
Carnitine Metabolism	deoxycarnitine	LC/MS pos early	36747	C01181	HMDB0001161	22620	1.04	0.6374	0.9839	100001662	6249-56-5	2052	146.11756	
	carnitine	LC/MS pos early	15500	C00487	C00308	HMDB0000062	288	1.15	0.2556	0.9008	100000007	461-05-2	1978	162.11247
Fatty Acid, Dihydroxy	2S,3R-dihydroxybutyrate	LC/MS polar	62950		HMDB0002453	10964471	1.16	0.4208	0.9839	100002284	5057-93-2	1660	119.03498	
	2R,3R-dihydroxybutyrate	LC/MS polar	63109		HMDB0000498	13120901	0.92	0.9946	0.9973	100002367	759-06-8	1543	119.03498	
Endocannabinoid	stearoyl ethanolamide	LC/MS pos late	38625		HMDB0013078	27902	0.91	0.9507	0.9839	100002254	111-57-9	1787	328.32101	
Inositol Metabolism	myo-inositol	LC/MS polar	1124	C00137	HMDB0000211	892	0.97	0.9832	0.9967	363	87-89-8	3506.3	225.06159	
	choline	LC/MS pos early	15506	C00114	HMDB0000097	305	0.78	0.0863	0.6684	1256	67-48-1	1961	104.10699	
Phospholipid Metabolism	choline phosphate	LC/MS pos early	34396	C00588	HMDB0001565	1014	1.25	0.0796	0.6544	267	72556-74-2	700	184.07332	
	cytidine 5'-diphosphocholine	LC/MS pos early	34418	C00307	HMDB0001413	13804	1.26	0.1005	0.7154	1220	33818-15-4	725	489.11461	
	glycerophosphorylcholine (GPC)	LC/MS pos early	15990	C00670	HMDB0000086	71920	0.84	0.2126	0.8265	100000269	28319-77-9	672	258.1101	
	phosphoethanolamine	LC/MS neg	1600	C00346	HMDB0000224	1015	1.14	0.2460	0.8924	1026	1071-23-4	638	140.01182	
	cytidine-5'-diphosphoethanolamine	LC/MS polar	34410	C00570	HMDB0001564	123727	1.36	0.0168	0.3458	100001407	72842-05-8	4210	445.0531	
	glycerophosphoethanolamine	LC/MS polar	37455	C01233	HMDB0000014	123874	1.21	0.0867	0.6684	100001620	33049-08-0	3075	214.04859	
	glycerophosphoserine*	LC/MS polar	57404			3081457	1.67	0.0086	0.3044	100015666		3541	258.03842	
	glycerophosphoinositol*	LC/MS pos early	52307			167572	1.27	0.1002	0.7154	100001621	16824-65-0	516	335.07378	
Monoacylglycerol	1-palmitoylglycerol (16:0)	LC/MS neg	21127		HMDB0011564	14900	1.63	0.2730	0.9238	100000827	542-44-9	6550	255.23293	
	1-oleoylglycerol (18:1)	LC/MS neg	21184		HMDB0011567	5283468	1.31	0.7638	0.9839	100000824	111-03-5	6650	281.24858	
	1-linoleoylglycerol (18:2)	LC/MS neg	27447		HMDB0011568	5283469	0.94	0.8984	0.9839	100001040	2277-28-3	6477	279.23293	
	1-dihomo-lindelylglycerol (20:3)	LC/MS neg	48341				2.07	0.6125	0.9839	100006121		6400	305.24858	
	1-arachidonoylglycerol (20:4)	LC/MS neg	34397	C13857	HMDB11578	16019980;5282281	0.68	0.4561	0.9839	100001433	35474-99-8	6250	303.23293	
	1-docosahexaenoylglycerol (22:6)	LC/MS neg	35153		HMDB0011587	53480995	0.79	0.6397	0.9839	100001481		6150	309.22236	
	2-linoleoylglycerol (18:2)	LC/MS neg	32506		HMDB0011538	5365676	0.85	0.7909	0.9839	100000987	3443-82-1	6250	279.23293	
	2-arachidonoylglycerol (20:4)	LC/MS neg	19266	C13856	HMDB0004666	5282280	0.83	0.6102	0.9839	100000584	53847-30-6	6170	303.23293	
Diacylglycerol	palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]	LC/MS pos late	54958		HMDB0007112	9543736	0.66	0.4997	0.9839	100010925		3015	634.54051	
	stearoyl-arachidonoyl-glycerol (18:0/20:4) [1]	LC/MS pos late	57450	C00165	HMDB0007170	6438587	0.63	0.5504	0.9839	100010949		3404	662.57181	
	stearoyl-arachidonoyl-glycerol (18:0/20:4) [2]	LC/MS pos late	57449		HMDB0007170	6438587	0.71	0.6911	0.9839	100010950		3522	662.57181	
	oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]	LC/MS pos late	54961		HMDB0007228	9543786	0.66	0.4200	0.9839	100010937		2990	660.55616	
Sphingolipid Synthesis	sphinganine	LC/MS pos late	17769	C00836	HMDB0000269	3126	0.72	0.4214	0.9839	313	3102-56-5	1413	302.30536	
Dihydroceramides	N-palmitoyl-sphinganine (d18:0/16:0)	LC/MS pos late	52604		HMDB11760	5283572	0.91	0.8516	0.9839	100009028	5966-29-0	3090	540.53503	
	N-palmitoyl-sphingosine (d18:1/16:0)	LC/MS pos late	44877		HMDB0004949	5283564	1.00	0.8852	0.9839	1518	24696-26-2	2893	538.51937	
Ceramides	N-stearoyl-sphingosine (d18:1/18:0)*	LC/MS pos late	54979		HMDB0004950	5283565	1.02	0.7871	0.9839	1547	10404-17-3	3392	566.55067	
	N-palmitoyl-sphingadinenine (d18:2/16:0)*	LC/MS pos late	57416				1.05	0.7627	0.9839	100015609		2490	536.50372	
	ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)*	LC/MS pos late	57440				1.00	0.8732	0.9839	100015755		3920	594.58199	
	ceramide (d16:1/24:1, d18:1/22:1)*	LC/MS pos late	57437				1.13	0.6186	0.9839	100015727		3850	620.59763	
	ceramide (d18:2/24:1, d18:1/24:2)*	LC/MS pos late	57443				1.07	0.7208	0.9839	100015744		3858	646.6133	
	glycosyl-N-stearoyl-sphinganine (d18:0/18:0)*	LC/MS pos late	57418			6321364	0.76	0.6474	0.9839	100015694		3134	730.61915	
Hexosylceramides (HCER)	glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	LC/MS pos late	53013				0.93	0.9599	0.9839	100009272		2623	700.5722	
	glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	LC/MS pos late	52234				0.94	0.9589	0.9839	100001882		3063	728.6035	
	glycosyl-N-arachidoyl-sphingosine (d18:1/20:0)	LC/MS pos late	57423		HMDB0004973	6321358	0.90	0.9524	0.9839	100015714		3432	756.6348	
	glycosyl-N-behenoyl-sphingosine (d18:1/22:0)*	LC/MS pos late	57371				0.84	0.8423	0.9839	100015622		4058	784.6661	
	glycosyl-N-nervonoyl-sphingosine (d18:1/24:1)	LC/MS pos late	57369		HMDB0010712	HMDB000049	53480656;20057357	0.91	0.9385	0.9839	100001878		3990	810.68175
	glycosyl ceramide (d16:1/24:1, d18:1/22:1)*	LC/MS pos late	57457				0.93	0.9024	0.9839	100015730		3373	782.65045	
	glycosyl ceramide (d18:2/24:1, d18:1/24:2)*	LC/MS pos late	57453				0.92	0.9380	0.9839	100015745		3380	808.66809	
	palmitoyl dihydrospingomyelin (d18:0/16:0)*	LC/MS pos late	52434		HMDB0010168	9939965	0.49	0.2049	0.8265	100008954		2290	705.5905	
Dihydrospingomyelins	behenoyl dihydrospingomyelin (d18:0/22:0)*	LC/MS pos late	57331		HMDB0012091	44260132	0.48	0.1290	0.7698	100009026		3300	789.68441	
	sphingomyelin (d18:0/18:0, d19:0/17:0)*	LC/MS pos late	57473		HMDB0012087	44260130	0.45	0.2523	0.8977	100009027		2500	733.6218	
	sphingomyelin (d18:0/20:0, d16:0/22:0)*	LC/MS pos late	57476				0.46	0.1246	0.7698	100015786		2850	761.65311	

Sphingomyelins	palmitoyl sphingomyelin (d18:1/16:0)	LC/MS pos late	37506		HMDB0010169	9939941	0.65	0.4536	0.9839	100002107	6254-89-3	2168	703.57485
	stearoyl sphingomyelin (d18:1/18:0)	LC/MS pos late	19503	C00550	HMDB0001348	6453725	0.67	0.4474	0.9839	1538	85187-10-6,85187-10-6	2450	731.60615
	behencyl sphingomyelin (d18:1/22:0)*	LC/MS pos late	48492		HMDB0012103	44260125	0.62	0.3915	0.9839	100006294		3250	787.66876
	tricosanoyl sphingomyelin (d18:1/23:0)*	LC/MS pos late	52436		HMDB0012105		0.68	0.5909	0.9839	100008955		3350	801.68441
	lignoceroyl sphingomyelin (d18:1/24:0)	LC/MS pos late	57330				0.65	0.4318	0.9839	100006298	60037-60-7	3437	815.70006
	sphingomyelin (d18:2/23:1)*	LC/MS pos late	57482				0.70	0.5632	0.9839	100015791		2500	797.65308
	sphingomyelin (d18:2/24:2)*	LC/MS pos late	57479				0.73	0.5174	0.9839	100015789		2400	809.65308
	sphingomyelin (d18:1/14:0, d16:1/16:0)*	LC/MS pos late	42463		HMDB0012097	11433862	0.68	0.5888	0.9839	100004328		1998	675.54355
	sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)	LC/MS pos late	52433				0.68	0.5015	0.9839	100006314	121999-58-4	2082	689.5592
	sphingomyelin (d18:2/16:0, d18:1/16:1)*	LC/MS pos late	42459				0.72	0.5939	0.9839	100004329		2002	701.5592
	sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	LC/MS pos late	52615			46891763	0.61	0.4368	0.9839	100008920	121999-64-2	2350	717.5905
	sphingomyelin (d18:1/18:1, d18:2/18:0)	LC/MS pos late	37529		HMDB0012101	6443882	0.66	0.4664	0.9839	100002106	108392-10-5	2167	729.5905
	sphingomyelin (d18:1/19:0, d19:1/18:0)*	LC/MS pos late	57475				0.57	0.3981	0.9839	100015787		2550	745.62178
	sphingomyelin (d18:1/20:0, d16:1/22:0)*	LC/MS pos late	48490		HMDB0012102	44260124	0.62	0.4225	0.9839	100006290		2800	759.6375
	sphingomyelin (d18:1/20:1, d18:2/20:0)*	LC/MS pos late	48491				0.58	0.3049	0.9370	100006292	222403-67-0	2450	757.6218
	sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)	LC/MS pos late	52495				0.63	0.4026	0.9839	100009025		3000	773.65311
	sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:0)	LC/MS pos late	48493		HMDB0012104		0.65	0.5126	0.9839	100006295		2775	785.65311
	sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:0)	LC/MS pos late	57477				0.62	0.3890	0.9839	100006296		2350	783.63746
	sphingomyelin (d18:1/24:1, d18:2/24:0)*	LC/MS pos late	47153		HMDB0012107	44260126	0.73	0.6062	0.9839	100005986	94359-13-4	3200	813.68441
	sphingomyelin (d18:2/24:1, d18:1/24:2)*	LC/MS pos late	52437			85336023	0.70	0.5587	0.9839	100008957		2750	811.66868
Sphingosines	sphingosine	LC/MS pos late	17747	C00319	HMDB0000252	5280335	0.78	0.6494	0.9839	297	123-78-4	1393	300.28971
Mevalonate Metabolism	3-hydroxy-3-methylglutarate	LC/MS polar	531	C03761	HMDB0000355	1662:545993	0.94	0.7088	0.9839	112	503-49-1	2850	161.04555
Sterol	cholesterol	LC/MS pos late	63	C00187	HMDB0000067	9432584;11025495;5997	0.81	0.7784	0.9839	266	57-88-5	2707	369.35159
	cholesterol sulfate	LC/MS polar	35324	C18043	HMDB006653	65076	0.79	0.6632	0.9839	100001806	2864-50-8	681	465.30434
	4-cholesten-3-one	LC/MS pos late	38125	C00599	HMDB0000921	91477	1.06	0.6112	0.9839	100002227	601-57-0	2520	385.3465
	campesterol	LC/MS pos late	33997	C01789	HMDB0002869	173183	1.08	0.8485	0.9839	100001269	474-62-4	2873	383.36724
	7-hydroxycholesterol (alpha or beta)	LC/MS pos late	47890	C15610	HMDB0006149	15571093	0.80	0.5971	0.9839	100005999		1930	367.33594
Primary Bile Acid Metabolism	taurochenodeoxycholate	LC/MS neg	18494	C05465	HMDB0000951	387316	0.99	0.9459	0.9839	1629	6009-98-9	5250	498.28948
Purine Metabolism, (Hypo)Xanthine/nucleosides	inosine 5'-monophosphate (IMP)	LC/MS pos early	2133	C00130	HMDB0000175	8582	1.58	0.0115	0.3044	362	4691-65-0	650	349.05438
	inosine	LC/MS neg	1123	C00294	HMDB0000195	6021	1.01	0.6923	0.9839	361	58-63-9	1602.1	267.07349
	hypoxanthine	LC/MS neg	3127	C00262	HMDB0000157	790;135398638	1.16	0.1720	0.7798	171	68-94-0	1291.2	135.03123
	xanthine	LC/MS polar	3147	C00385	HMDB0000292	1188	1.38	0.0194	0.3594	1004	69-89-6	2023	151.02615
	xanthosine	LC/MS neg	15136	C001762	HMDB0000299	64959	0.97	0.9455	0.9839	100000299	146-80-0	1075	283.0684
	urate	LC/MS pos early	1604	C00366	HMDB0000289	1175	0.83	0.2498	0.8972	1134	69-93-2;120K5305	776	169.03562
	allantoin	LC/MS polar	1107	C02350 C02348 C01551	HMDB0000462	204:439714;439713	0.93	0.6990	0.9839	1002	97-59-6	1672	157.03671
Purine Metabolism, Adenine containing	adenosine 5'-monophosphate (AMP)	LC/MS pos early	32342	C00020	HMDB0000045	6083	1.11	0.3775	0.9839	209	149022-20-8	1013	348.07037
	adenosine 3'-monophosphate (3'-AMP)	LC/MS neg	35142	C01267	HMDB0003540	41211	1.02	0.7297	0.9839	100001449	84-21-9	1245	346.0558
	adenosine 2'-monophosphate (2'-AMP)	LC/MS neg	36815	C00946	HMDB0011617	94136	1.61	0.0667	0.6199	100001694	130-49-4	1497.7	346.0558
	adenosine 3',5'-diphosphate	LC/MS neg	15691	C00054	HMDB0000061	159296	1.21	0.2742	0.9238	1214	75431-54-8	575	426.02214
	adenylosuccinate	LC/MS neg	18360	C03794	HMDB0000536	440122	1.06	0.9685	0.9846	1303	19046-78-7	560	230.52974
	adenosine	LC/MS pos early	555	C00212	HMDB0000050	60961	1.25	0.8361	0.9839	798	58-61-7	2169	268.10404
	adenine	LC/MS neg	554	C00147	HMDB0000034	190	1.38	0.0609	0.6094	880	73-24-5	1680	134.04722
Purine Metabolism, Guanine containing	N1-methyladenosine	LC/MS pos early	15650	C02494	HMDB0003331	27476	1.48	0.0462	0.5700	1242	15763-06-1	2120	282.11969
	guanosine 5'-diphosphate (GDP)	LC/MS neg	2848	C00035	HMDB0001201	135398619	0.59	0.0482	0.5751	346	43139-22-6	639	442.01706
	guanosine 5'-monophosphate (5'-GMP)	LC/MS pos early	2849	C00144	HMDB0001397	6804	1.28	0.0368	0.5389	347	12/9/50	800	364.05528
	guanosine	LC/MS neg	1573	C00387	HMDB0000133	6802	1.12	0.4998	0.9839	1099	118-00-3	1662	282.08439
	guanine	LC/MS pos early	32352	C00242	HMDB0000132	135398634	1.23	0.1488	0.7748	172	73-40-5	2032	152.05669
Pyrimidine Metabolism, Orotate containing	N-carbamoylaspartate	LC/MS polar	1594	C00438	HMDB0000828	93072	0.71	0.0139	0.3219	1108	923-37-5	3800	175.03604
	orotate	LC/MS polar	1505	C00295	HMDB0000226	967	0.87	0.3408	0.9779	445	50887-69-9	1638.1	155.00983
	orotidine	LC/MS polar	35172		HMDB0000788	92751	0.80	0.1107	0.7698	100001416	314-50-1	2250	287.05209
Pyrimidine Metabolism, Uracil containing	uridine 5'-triphosphate (UTP)	LC/MS neg	33448	C00075	HMDB0000285	8133	0.38	0.0123	0.3044	871	19817-92-6	572	482.96126
	uridine 5'-diphosphate (UDP)	LC/MS neg	5345	C00015	HMDB0000295	6031	0.66	0.0576	0.6094	870	21931-53-3	599.5	402.99492
	uridine 5'-monophosphate (UMP)	LC/MS polar	2856	C00105	HMDB0000288	6030	1.16	0.2015	0.5150	869	3387-36-8	4150	323.02859
	uridine-2',3'-cyclic monophosphate	LC/MS neg	37137	C02355	HMDB0011640	439715	0.97	0.7002	0.9839	75	40632-52-8	1090	305.01803
	uridine	LC/MS neg	606	C00299	HMDB0000296	6029	1.15	0.2087	0.8265	535	58-96-8	1457.6	243.06226
	uracil	LC/MS polar	605	C00106	HMDB0000300	1174	1.63	0.0012	0.0699	825	66-22-8	1089.7	111.02
	pseudouridine	LC/MS neg	33442	C02067	HMDB0000767	15047	1.14	0.2459	0.8924	821	1445-07-4	1100	243.06226
Pyrimidine Metabolism, Cytidine containing	5,6-dihydrouridine	LC/MS neg	61833		HMDB0000497	94312	0.90	0.5363	0.9839	100001425	5/4/27	1119	245.07791
	cytidine triphosphate	LC/MS neg	2844	C00063	HMDB0000082	6176	0.42	0.0393	0.5389	281	36051-68-0	575	481.97724
	cytidine diphosphate	LC/MS neg	2841	C00112	HMDB0001546	6132	0.76	0.2173	0.8265	280	34393-59-4	580	402.01091
	cytidine 5'-monophosphate (5'-CMP)	LC/MS pos early	2372	C00055	HMDB0000095	6131	1.17	0.1365	0.7698	282	63-37-6	835	324.05914
	cytidine 2',3'-cyclic monophosphate	LC/MS neg	37465	C02354	HMDB0011691	2342172	0.95	0.5554	0.9839	73	15718-51-1	937	304.03401
	cytidine	LC/MS neg	514	C00475	HMDB0000089	6175	1.47	0.0161	0.3458	827	65-46-3	1325	242.07824
	2'-deoxycytidine 5'-monophosphate	LC/MS pos early	533	C00239	HMDB0001202	13945	1.49	0.0099	0.3044	298	1032-65-1	975	308.06422
Pyrimidine Metabolism, Thymine containing	thymidine	LC/MS neg	2183	C00214	HMDB0000273	5789	1.38	0.0462	0.5700	872	50-89-5	1983.7	241.06299
Purine and Pyrimidine Metabolism	methylphosphate	LC/MS pos early	37070		HMDB61711	13130	0.78	0.5521	0.9839	100001805	7023-27-0	544	112.99963

Nicotinate and Nicotinamide Metabolism	nicotinate	LC/MS neg	1504	C00253	HMDB0001488	938	1.17	0.1272	0.7698	567	59-67-6	1180	122.02475
	nicotinamide	LC/MS neg	594	C00153	HMDB0001406	936	1.00	0.8573	0.9839	432	98-92-0	1796.8	121.04073
	nicotinamide riboside	LC/MS pos early	33013	C03150	HMDB0000855	439924	1.19	0.1931	0.8265	100001310	1341-23-7	2040	255.09755
	nicotinamide adenine dinucleotide (NAD+)	LC/MS neg	5278	C00006	HMDB0000217	5892	0.76	0.2748	0.9238	1310	53-84-9	1434	662.10184
	trigonelline (N'-methylnicotinate)	LC/MS pos early	32401	C01004	HMDB0000875	5570	1.18	0.3366	0.9779	100001092	535-83-1	1388	138.05496
	adenosine 5'-diphosphoribose (ADP-ribose)	LC/MS neg	558	C00301	HMDB0001178	192	0.46	0.0116	0.3044	215	68414-18-6	920	558.06439
Riboflavin Metabolism	flavin adenine dinucleotide (FAD)	LC/MS neg	2134	C00016	HMDB0001248	643975	0.85	0.6892	0.9839	327	146-14-5;84366-81-4	2425	784.14985
Pantothenate and CoA Metabolism	pantothenate	LC/MS pos early	1508	C00864	HMDB0000210	6613	1.02	0.8081	0.9839	1024	137-08-6	1667	220.11795
	coenzyme A	LC/MS neg	46322	C00010	HMDB0001423	87642	0.98	0.7694	0.9839	270	85-61-0;18439-24-2	1448	382.55033
Ascorbate and Aldarate Metabolism	2-O-methylascorbic acid	LC/MS polar	63990		HMDB0240294	54726398	0.85	0.3064	0.9370	100003258	17860-87-6	1512	189.04046
	threonate	LC/MS polar	27738	C01620	MDB0000943 HMDB00626	5460407;151152	0.90	0.5188	0.9839	100001022	70753-61-6	2384	135.02989
	gulonate*	LC/MS polar	46957	C00800	HMDB0003290	152304	1.16	0.2874	0.9327	100001586	20246-53-1	2750	195.05102
Tocopherol Metabolism	alpha-tocopherol	LC/MS pos late	1561	C02477	HMDB0001893	86472	0.88	0.9524	0.9839	1105	59-02-9;10191-41-0	2522	430.37818
Pterin Metabolism	pterin	LC/MS neg	43023	C00715	HMDB0000802	135398660	1.06	0.5176	0.9839	100004216	22363-60-4	1370	162.04213
Thiamine Metabolism	thiamin (Vitamin B1)	LC/MS pos early	5341	DG00125 C00378 D08580	HMDB0000235	1130	1.17	0.2189	0.8265	873	59-43-8	3050	265.11176
	thiamin diphosphate	LC/MS neg	35670	C00068	HMDB0001372	1132	0.76	0.3498	0.9779	522	154-87-0	1195.1	423.02986
Vitamin B6 Metabolism	pyridoxine (Vitamin B6)	LC/MS neg	608	D08454	HMDB0000239	1054	0.78	0.1614	0.7798	936	58-56-0	1657	168.06661
	pyridoxate	LC/MS polar	31555	C00847	HMDB0000017	6723	0.81	0.1468	0.7748	100001121	82-82-6	846	182.04588
Benzoate Metabolism	hippurate	LC/MS neg	15753	C01586	HMDB0000714	464	0.83	0.2148	0.8265	100000014	495-69-2	2106.9	178.05096
	benzoate	LC/MS neg	15778	C00180	HMDB0001870	243	0.67	0.2169	0.8265	100000008	65-85-0	1750	121.0295
Food Component/Plant	ergothioneine	LC/MS pos early	37459	C05570	HMDB0003045	5351619	1.46	0.0312	0.4934	100002154	58511-63-0	850	230.09578
	erythritol	LC/MS polar	20699	C00503	HMDB0002994	222285	0.88	0.3577	0.9804	100000846	149-32-6	1491	167.05611
	homostachydrine*	LC/MS pos early	33009	C08283	HMDB0033433	441447	1.09	0.4509	0.9839	100001550	1195-94-4	1750	158.11756
	mannonate*	LC/MS polar	62864			3246006	0.83	0.5080	0.9839	100003695	642-99-9	2736	195.05102
	stachydrine	LC/MS pos early	34384	C10172	HMDB0004827	115244	1.00	0.8985	0.9839	100001296	4136-37-2	1440	144.10191
Drug - Antibiotic	penicillin G	LC/MS pos early	37468	C05551	HMDB0015186	5904	0.77	0.1208	0.7698	100002155	69-57-8	2870	335.10601
Chemical	sulfate*	LC/MS neg	46960	C00059	HMDB01448	5152822	0.85	0.2830	0.9272	100002528	14808-79-8	616	96.9601
	phenol red	LC/MS neg	36817	C12600		4766	0.80	0.1758	0.7839	100001724	143-74-8	3665.9	353.04891
	4-acetamidobenzoate	LC/MS neg	57585	D03836		6918889	0.83	0.1179	0.7698	100009413	556-08-1	1403	178.05096
	thiopropine	LC/MS pos early	53231			93176	0.91	0.8532	0.9839	100009232	34592-47-4	1250	134.02703
Partially Characterized Molecules	glutamine_degradant*	LC/MS pos early	46225				0.88	0.4607	0.9839	100001540	2353-44-8	1900	129.06586