

Markers of PARK2, Human Serum

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).

Pathway Sort Order	Super Pathway	Sub Pathway	Biochemical Name	Platform	Comp ID	KEGG	HMDB	PUBCHEM	FOLD	Welch's Two-Sample t-Test		Average			
									PARK2/CONTROL	PARK2 VS/Control		CONTROL	PARK2	PARKIN HOMOZYGOUS	PARKIN COMPOUND HETEROZYGOUS
										p-value	q-value				
1	Glycine, Serine and Threonine Metabolism	glycine	LC/MS pos early	58	C00037	HMDB00123	750	1.09	0.2101	0.3810	1.0148	1.1016	1.0888	1.0782	
2		N-acetylglycine	LC/MS neg	27710		HMDB00532	10972	1.89	0.0346	0.1682	1.0057	1.8019	1.7693	1.6861	
4		sarcosine	LC/MS pos early	1516	C00213	HMDB00271	1088	1.06	0.4713	0.5067	1.0141	1.0739	1.0362	1.1088	
5		dimethylglycine	LC/MS pos early	5086	C01026	HMDB00092	673	1.20	0.1260	0.3126	0.9950	1.1909	1.1643	1.1540	
6		betaine	LC/MS pos early	3141	C00719	HMDB00043	247	0.95	0.4785	0.5112	1.0023	0.9561	0.9624	0.9606	
9		serine	LC/MS pos early	1648	C00065	HMDB00187	5951	0.99	0.8317	0.6058	1.0174	1.0073	1.0102	1.0275	
10		N-acetylserine	LC/MS polar	37076		HMDB02931	65249	1.06	0.4482	0.5011	1.1016	1.1639	1.1220	1.0965	
16		threonine	LC/MS pos early	1284	C00188	HMDB00167	6288	0.82	0.0032	0.0608	1.1041	0.9104	0.9860	0.9010	
17		N-acetylthreonine	LC/MS neg	33939		HMDB62557	152204	0.99	0.9895	0.6494	1.1259	1.1144	1.0960	0.9868	
22		O-acetylhomoserine	LC/MS polar	31539	C01077		439389	2.95	0.8059	0.5637	1.1383	3.3620	2.9187	5.1537	
28		Alanine and Aspartate Metabolism	alanine	LC/MS pos early	1126	C00041	HMDB00161	5950	0.89	0.0103	0.0987	1.0577	0.9368	0.9431	0.9399
30			N-acetylalanine	LC/MS neg	1585	C02847	HMDB00766	88084	0.99	0.8860	0.6244	1.1131	1.1068	1.0659	0.9996
34			aspartate	LC/MS pos early	443	C00049	HMDB00191	5960	1.08	0.3272	0.4524	1.0078	1.0881	1.0548	1.1524
35			N-acetyl-aspartate (NAA)	LC/MS pos early	22185	C01042	HMDB00812	65085	1.04	0.5417	0.5395	0.9844	1.0286	1.0382	0.9197
38			asparagine	LC/MS pos early	512	C00152	HMDB00168	6267	0.90	0.0008	0.0257	1.0280	0.9203	0.9451	0.8923
39			N-acetyl-asparagine	LC/MS pos early	33942		HMDB06028	99715	1.19	0.2452	0.4129	1.0067	1.1994	1.2091	0.9117
41			glutamate	LC/MS pos early	57	C00025	HMDB00148	611	1.15	0.4638	0.5047	0.9836	1.1297	1.1178	1.1458
42	glutamine	LC/MS pos early	53	C00064	HMDB00641	5961	0.97	0.4581	0.5037	1.0063	0.9785	0.9900	0.9428		
44	Glutamate Metabolism	N-acetylglutamate	LC/MS polar	15720	C00624	HMDB01138	70914	1.03	0.6608	0.5708	1.0860	1.1187	1.0537	1.0532	
45		N-acetylglutamine	LC/MS polar	33943	C02716	HMDB06029	182230	1.12	0.1945	0.3668	0.9901	1.1095	1.0818	1.0845	
47		4-hydroxyglutamate	LC/MS pos early	40499	C03079	HMDB01344	439902	1.38	0.2543	0.4195	0.8581	1.1823	1.1024	1.1961	
51		pyroglutamine*	LC/MS pos early	46225			134508	0.72	0.2143	0.3810	1.6689	1.2059	1.1857	1.3491	
52		N-acetyl-aspartyl-glutamate (NAAG)	LC/MS pos early	36665	C12270	HMDB01067	5255	0.99	0.9834	0.6466	1.0958	1.0823	1.0382	1.0913	
53		beta-citrylglutamate	LC/MS neg	54923	C20775		72715786	1.25	0.0736	0.2516	0.9616	1.1986	1.1534	1.1192	
59		S-1-pyrroline-5-carboxylate	LC/MS pos early	42370	C04322	HMDB01301	1196	0.78	0.1422	0.3340	1.2077	0.9440	0.8935	0.7362	
65	Histidine Metabolism	histidine	LC/MS neg	59	C00135	HMDB00177	6274	0.93	0.1157	0.3004	1.0037	0.9376	0.9555	0.8943	
66		1-methylhistidine	LC/MS pos early	30460	C01152	HMDB00001	92105	0.90	0.4071	0.4827	1.1609	1.0458	1.0252	1.0303	
67		3-methylhistidine	LC/MS neg	15677	C01152	HMDB00479	64989	0.51	0.0289	0.1494	2.0985	1.0681	1.0002	0.8089	
68		N-acetylhistidine	LC/MS neg	33946	C02997	HMDB32055	75619	1.00	0.8021	0.6038	1.0433	1.0476	1.0282	0.8953	
70		N-acetyl-1-methylhistidine*	LC/MS pos early	43255			193270	0.86	0.5030	0.5206	1.2142	1.0424	1.0682	0.7952	
71		hydantoin-5-proprionate	LC/MS polar	40473	C05565	HMDB01212	782	1.00	0.8168	0.6058	1.0317	1.0272	1.0246	1.0275	
72		trans-urocanate	LC/MS pos early	607	C00785	HMDB00301	736715	1.46	0.0287	0.1494	0.9008	1.3158	1.3220	1.2135	
74		imidazole propanoate	LC/MS pos early	40730		HMDB02271	70630	1.72	0.1685	0.3488	1.0718	1.8480	1.7774	2.3763	
76		imidazole lactate	LC/MS pos early	15716	C05568	HMDB02320	440129	1.07	0.7665	0.5982	1.0768	1.1487	1.0945	1.1060	
79		N-acetylcarnosine	LC/MS pos early	43488		HMDB12881	9903482	0.60	0.0253	0.1424	1.6629	0.9971	1.0075	1.0518	
82		1-methylhistamine	LC/MS pos early	43631	C05127	HMDB00898	3614	1.64	0.6760	0.5750	1.1289	1.8556	1.7987	1.4928	
83		1-methyl-4-imidazoleacetate	LC/MS pos early	32350	C05828	HMDB02820	75810	0.80	0.3412	0.4524	1.4795	1.1887	1.1818	1.2662	
86		4-imidazoleacetate	LC/MS pos early	32349	C02835	HMDB02024	96215	1.05	0.6796	0.6207	1.0527	1.1010	1.0981	1.1816	
90		N-acetylhistamine	LC/MS pos early	48679	C05135	HMDB13253	69602	0.56	0.7941	0.6033	1.4657	0.8169	1.1336	1.1029	
93	Lysine Metabolism	lysine	LC/MS pos early	1301	C00047	HMDB00182	5962	0.89	0.0216	0.1290	1.0460	0.9302	0.9693	0.8863	
94		N2-acetyllysine	LC/MS polar	36751	C12989	HMDB00446	92907	0.82	0.6602	0.5708	0.9854	0.8080	0.8484	0.7290	
95		N6-acetyllysine	LC/MS neg	36752	C02727	HMDB00206	92832	0.89	0.2962	0.4397	1.1296	1.0064	0.9904	0.9646	
103		N6,N6,N6-trimethyllysine	LC/MS pos early	1498	C03793	HMDB01325	440120	0.85	0.2583	0.4196	1.1826	1.0039	0.9916	0.9846	
105		5-hydroxylysine	LC/MS pos early	15885	C16741	HMDB00450	1029	0.90	0.7775	0.5998	1.2985	1.1675	1.1445	1.1811	
106		5-(galactosylhydroxy)-L-lysine	LC/MS pos early	43582				0.87	0.6485	0.5690	1.1986	1.0479	1.0246	0.9803	
108		2-aminoadipate	LC/MS polar	6146	C00956	HMDB00510	469	0.97	0.8261	0.6058	1.1304	1.0939	1.0878	1.0472	
112		glutarylcarritine (C5-DC)	LC/MS pos early	44664		HMDB13130	71464488	0.96	0.5513	0.5433	1.0810	1.0328	0.9821	0.8933	

116		ipicolate	LC/MS pos early	1444	C00408	HMDB00070	849	0.75	0.1340	0.3227	1.2388	0.9334	0.9329	1.0091
117		9-oxopiperidine-2-carboxylate	LC/MS neg	43231		HMDB61705	3014237	1.18	0.2067	0.3790	0.9352	1.0991	1.0592	1.0471
119		N-acetyl-cadaverine	LC/MS pos early	43530		HMDB02284	189097	1.75	0.0060	0.0791	1.2355	2.1607	2.3963	2.3255
123		phenylalanine	LC/MS pos early	64	C00079	HMDB00159	6140	0.95	0.2040	0.3788	1.0073	0.9619	0.9668	0.9414
124	Phenylalanine Metabolism	N-acetylphenylalanine	LC/MS neg	33950	C03519	HMDB00512	74839	0.78	0.0435	0.1842	1.1883	0.9287	0.9373	0.8153
128		phenylpyruvate	LC/MS neg	566	C00166	HMDB00205	997	1.08	0.2821	0.4196	0.9906	1.0889	1.0617	1.0682
129		phenyllactate (PLA)	LC/MS neg	22130	C05607	HMDB00779	3848	1.08	0.8349	0.5662	0.9971	1.0801	1.0448	1.0244
134		2-hydroxyphenylacetate	LC/MS polar	1432	C05852	HMDB00669	11970	0.83	0.2646	0.4204	1.1967	0.9981	0.9280	0.8475
140		tyrosine	LC/MS pos early	1299	C00082	HMDB00158	6057	0.97	0.5374	0.5363	1.0389	1.0120	1.0264	0.9692
141		N-acetyltyrosine	LC/MS neg	32390		HMDB00866	68310	0.82	0.1388	0.3283	1.1680	0.9559	0.9871	0.8023
150	4-hydroxyphenylpyruvate	LC/MS neg	1669	C01179	HMDB00707	979	0.76	0.0613	0.2255	1.1634	0.8870	0.9186	0.9575	
153	3-(4-hydroxyphenyl)lactate	LC/MS neg	32197	C03672	HMDB00755	9378	0.95	0.6410	0.5662	1.1113	1.0534	1.0366	0.9989	
157	phenol sulfate	LC/MS neg	32553	C02180	HMDB00015	74426	1.27	0.9902	0.6494	1.3154	1.6677	1.6021	1.7804	
168	vanillylactate	LC/MS neg	54910		HMDB00913	160637	118.98	0.0000	0.0003	0.2790	33.1894	30.2507	32.7776	
169	vanillylmandelate (VMA)	LC/MS neg	1567	C05584	HMDB00291	1245	1.63	0.0133	0.1065	0.8992	1.3733	1.3256	1.1945	
171	3-methoxytyrosine	LC/MS pos early	12017		HMDB01434	1670	115.98	0.0000	0.0003	0.7531	87.3465	85.5326	82.1415	
173	3-methoxytyramine sulfate	LC/MS neg	44618				78.90	0.0000	0.0003	0.0591	4.5448	4.1318	3.6697	
177	homovanillate (HVA)	LC/MS neg	1101	C05582	HMDB00118	1738	11.28	0.0000	0.0006	0.3803	4.2903	4.0394	3.6026	
186	gentisate	LC/MS polar	16280	C00628	HMDB00152	3469	0.83	0.3396	0.4524	1.3690	1.1297	1.1257	1.2234	
188	homovanillate sulfate	LC/MS neg	38349		HMDB11719	2981063	11.70	0.0000	0.0018	0.1070	1.2517	1.1628	0.7991	
190	dopamine 4-sulfate	LC/MS neg	48406	C13691	HMDB04148	123932	42.28	0.0000	0.0016	0.2425	10.2523	11.0740	8.8312	
191	dopamine 3-O-sulfate	LC/MS neg	48407	C13690	HMDB06275	122136	34.41	0.0000	0.0009	0.7231	24.8826	26.3540	20.5519	
192	p-cresol glucuronide*	LC/MS neg	48841		HMDB11686	154035	0.50	0.7043	0.5845	4.4416	2.2379	2.0584	2.2994	
193	tyramine O-sulfate	LC/MS neg	48408		HMDB06409	153005	0.67	0.3237	0.4524	2.3289	1.5513	1.6886	1.5734	
194	N-formylphenylalanine	LC/MS neg	48433			750256	1.10	0.6441	0.5679	1.0223	1.1253	1.0438	1.0042	
198	3,4-dihydroxyphenylacetate sulfate	LC/MS neg	48736			193283	10.88	0.0000	0.0017	0.1834	2.0144	2.3748	1.2295	
209	tyroxine	LC/MS neg	2761	C01829	HMDB01918	5819	1.17	0.1692	0.3488	0.9952	1.1648	1.0920	1.1068	
213	tryptophan	LC/MS pos early	54	C00078	HMDB00929	6305	0.95	0.3655	0.4613	0.9966	0.9442	0.9466	0.9185	
214	N-acetyltryptophan	LC/MS neg	33959	C03137	HMDB13713	700653	0.70	0.0899	0.2674	1.2921	0.9093	0.9358	0.7593	
220	C-glycosyltryptophan	LC/MS pos early	48782			10981970	1.15	0.1300	0.3183	1.0531	1.2058	1.1801	1.1439	
222	tryptophan betaine	LC/MS pos early	37097	C09213	HMDB61115	442106	0.90	0.1622	0.3488	4.2213	3.8126	3.7034	3.2935	
224	kyrurine	LC/MS pos early	15140	C00328	HMDB00684	161166	1.00	0.8749	0.6198	1.0576	1.0623	1.0551	1.0126	
226	N-acetylkyrurine (2)	LC/MS neg	48757				0.51	0.0526	0.2051	1.2680	0.6412	0.6506	0.4933	
228	kyrurate	LC/MS neg	1417	C01717	HMDB00715	3845	0.83	0.1543	0.3451	1.1075	0.9137	0.8905	0.7598	
230	N-formylanthranilic acid	LC/MS polar	43549	C05653	HMDB04089	101399	1.16	0.5575	0.5461	0.9397	1.0917	1.1051	1.2841	
234	xanthurate	LC/MS neg	15679	C02470	HMDB00881	5699	0.78	0.3836	0.4739	1.3123	1.0224	1.0168	0.8750	
236	picolinate	LC/MS pos early	1512	C10164	HMDB02243	1018	1.06	0.8346	0.6058	1.0412	1.0998	1.2227	1.2582	
237	serotonin	LC/MS pos early	2342	C00780	HMDB00259	5202	0.81	0.2619	0.4190	1.1210	0.9085	0.9501	0.9412	
240	5-hydroxyindoleacetate	LC/MS neg	437	C05635	HMDB00763	1826	0.96	0.7754	0.5998	0.9717	0.9374	0.9478	1.0771	
244	indolylactate	LC/MS pos early	18349	C02043	HMDB00671	92904	0.83	0.3907	0.4792	1.2409	1.0315	1.0276	1.0067	
245	indoleacetate	LC/MS pos early	27513	C00954	HMDB00197	802	0.82	0.0258	0.1424	1.3442	1.1068	1.0209	1.4420	
248	indolepropionate	LC/MS pos early	32405		HMDB02302	3744	0.79	0.1670	0.3668	1.3590	1.0786	0.9675	0.9408	
250	indoleacetylglutamine	LC/MS neg	42067		HMDB13240	25200879	0.53	0.0377	0.1721	1.5894	0.8370	0.7650	0.8422	
253	indole-3-carboxylate	LC/MS neg	38116	C19837	HMDB03320	69867	1.01	0.7811	0.5968	1.2288	1.2423	1.1946	1.1999	
258	3-indoxyl sulfate	LC/MS neg	27672		HMDB00682	10256	0.89	0.6655	0.5722	1.1151	0.9932	0.9853	1.0539	
261	5-bromotryptophan	LC/MS neg	53242			96735	0.89	0.1994	0.3735	1.0340	0.9198	0.9359	0.9324	
265	leucine	LC/MS pos early	60	C00123	HMDB00687	6106	0.93	0.3027	0.4444	1.0957	1.0234	1.0383	1.0233	
266	N-acetylleucine	LC/MS neg	1587	C02710	HMDB11756	70912	1.01	0.9707	0.6446	1.0750	1.0895	1.0632	1.0746	
269	4-methyl-2-oxopentanoate	LC/MS neg	22116	C00233	HMDB00695	70	1.16	0.3002	0.4418	1.0093	1.1692	1.1703	1.2447	
272	alpha-hydroxyisocaproate	LC/MS neg	22132	C03264	HMDB00746	83697	1.21	0.1498	0.3419	0.9779	1.1825	1.1866	1.2329	
275	isovalerate (5:0)	LC/MS neg	44656	C08262	HMDB00718	10430	1.36	0.0373	0.1717	0.8840	1.2001	1.1534	1.0073	
276	isovalerylglycine	LC/MS neg	35107		HMDB00678	546304	0.83	0.8316	0.6058	1.2455	1.0398	1.0723	0.8420	
277	isovalerylcarnitine (C5)	LC/MS pos early	34407		HMDB00688	6428851	1.01	0.7862	0.6012	1.0873	1.0930	1.0773	1.1758	
284	beta-hydroxyisovalerate	LC/MS neg	12129		HMDB00754	69362	1.22	0.1170	0.3010	1.0538	1.2843	1.2015	1.4015	

Amino Acid

287		3-methylglutaconate	LC/MS polar	38667		HMDB00522	1551563	0.74	0.3311	0.4524	1.4559	1.0762	1.0469	0.7642
291		3-methylglutaryl carnitine (2)	LC/MS pos early	46548		HMDB00552	128145	0.61	0.4453	0.4999	2.8089	1.7166	1.5664	1.0730
300		isoleucine	LC/MS pos early	1125	C00407	HMDB00172	6306	0.95	0.4510	0.5022	1.1078	1.0564	1.0548	1.0650
302		N-acetyl isoleucine	LC/MS neg	33967		HMDB01684	2802421	0.82	0.2860	0.4347	1.1843	0.9655	0.9438	1.0179
304		3-methyl-2-oxovalerate	LC/MS neg	15676	C00671	HMDB03736	47	1.18	0.2608	0.4196	1.0280	1.2126	1.1843	1.2958
305	Leucine, Isoleucine and Valine Metabolism	alpha-hydroxyisovalerate	LC/MS neg	33937		HMDB00407	99823	1.20	0.1179	0.3018	1.0166	1.2177	1.1524	1.3858
307		2-methylbutyryl carnitine (C5)	LC/MS pos early	45095		HMDB00378	6426901	0.74	0.0568	0.2168	1.3573	1.0110	0.9907	1.0852
310		beta-carnitine (C5-1-DC)	LC/MS pos early	35428		HMDB02366	22833596	0.96	0.5516	0.5433	1.1447	1.0954	1.0849	1.0281
313		3-hydroxy-2-ethylpropionate	LC/MS polar	32387		HMDB00396	188979	1.09	0.5715	0.5478	1.0600	1.1542	1.1133	1.3281
315		ethylmalonate	LC/MS polar	15765		HMDB00622	11756	1.09	0.8218	0.6058	1.0719	1.1652	1.1219	1.3227
316		methylsuccinate	LC/MS polar	15745		HMDB01844	10346	1.07	0.9252	0.6294	0.9946	1.0617	1.0438	1.1407
322		valine	LC/MS pos early	1649	C00183	HMDB00883	6287	0.92	0.2252	0.3941	1.0791	0.9927	1.0015	0.9982
323		N-acetylvaline	LC/MS neg	1591		HMDB11757	66789	1.00	0.8132	0.6056	1.0844	1.0626	1.0542	1.0011
327		3-methyl-2-oxobutyrate	LC/MS neg	44526	C00141	HMDB00019	49	1.23	0.0464	0.1889	0.9959	1.2210	1.1964	1.2966
328		2-hydroxy-3-methylvalerate	LC/MS neg	36746		HMDB00317	164623	1.20	0.2469	0.4130	1.0939	1.3093	1.2418	1.5176
330		isobutyryl carnitine (C4)	LC/MS pos early	33441		HMDB00736	168379	0.85	0.6789	0.5765	1.3086	1.1123	1.1229	1.2104
331		isobutyrylglycine	LC/MS neg	35437		HMDB00730	10855900	1.14	0.3539	0.4591	1.0492	1.1936	1.1728	0.9367
332		3-hydroxyisobutyrate	LC/MS polar	1549	C06001	HMDB00336	87	1.09	0.6213	0.5637	0.9338	1.0201	0.9956	1.1791
333		2,3-dihydroxy-2-methylbutyrate	LC/MS polar	57547		HMDB29576	301941	0.50	0.3708	0.4613	1.1895	0.5939	0.5853	0.6543
336		methionine	LC/MS pos early	1302	C00073	HMDB00696	6137	0.86	0.0217	0.1290	1.0726	0.9251	0.9438	0.8937
337		N-acetylmethionine	LC/MS neg	1589	C02712	HMDB11745	448580	1.04	0.5964	0.5529	1.0059	1.0450	1.0048	0.9503
338		N-formylmethionine	LC/MS neg	2829	C03145	HMDB01015	439750	0.95	0.5779	0.5498	1.0988	1.0406	1.0244	0.8676
339		S-methylmethionine	LC/MS pos early	38127	C05319	HMDB38670	458	1.01	0.3693	0.4613	1.2706	1.2871	1.3211	0.8432
340		methionine sulfone	LC/MS pos early	44878			69961	0.80	0.5114	0.5251	1.3836	1.1107	1.1362	1.0274
341		methionine sulfoxide	LC/MS pos early	18374	C02989	HMDB02005	158980	0.98	0.9075	0.6250	1.1562	1.1273	1.0953	0.9998
347		S-adenosylhomocysteine (SAH)	LC/MS neg	42382	C00021	HMDB00939	439155	1.12	0.4209	0.4904	0.9510	1.0679	0.9842	0.8535
353		cystathionine	LC/MS pos early	15705	C02291	HMDB00099	430258	0.73	0.6405	0.5962	1.5986	1.1635	1.1009	1.0789
355		cysteine	LC/MS pos early	1868	C00097	HMDB00574	5862	0.95	0.8559	0.5708	1.1365	1.0789	1.1048	1.2045
357	Methionine, Cysteine, SAM and Taurine Metabolism	S-methylcysteine	LC/MS neg	36992		HMDB02108	24417	1.23	0.4379	0.4983	1.0179	1.2482	1.2392	1.0406
358		S-methylcysteine sulfoxide	LC/MS pos early	43378		HMDB29432	82142	1.14	0.8777	0.6207	1.1434	1.3016	1.4160	1.0502
360		cysteine s-sulfide	LC/MS pos early	22176	C05824	HMDB00731	115015	0.48	0.3539	0.4591	2.5437	1.2305	1.7309	1.4491
361		cystine	LC/MS pos early	56	C00491	HMDB00192	67678	1.03	0.7655	0.5982	0.9784	1.0073	0.9906	0.9880
364		methionine	LC/MS pos early	42002			98504	1.65	0.6944	0.5831	1.2968	2.1495	1.9399	1.3187
366		cysteine sulfonic acid	LC/MS pos early	37443	C00606	HMDB00996	109	1.18	0.1915	0.3668	0.9796	1.1527	1.1019	1.1297
367		hypotaurine	LC/MS pos early	590	C00519	HMDB00965	107812	1.36	0.0856	0.2638	0.9548	1.3006	1.3176	1.3805
368		taurine	LC/MS neg	2125	C00245	HMDB00251	1123	1.16	0.2010	0.3751	0.9576	1.1106	1.0887	1.1063
369		N-acetyltaurine	LC/MS neg	48187			159864	0.99	0.6501	0.5694	1.1188	1.1056	1.0589	1.0212
370		N-methyltaurine	LC/MS polar	42989			7882	1.15	0.6139	0.5637	1.2774	1.4674	1.2463	1.1513
375		arginine	LC/MS pos early	1638	C00062	HMDB00517	232	0.94	0.1929	0.3668	1.0255	0.9676	0.9756	0.9641
376		argininosuccinate	LC/MS pos early	15497	C03406	HMDB00052	828	1.08	0.9504	0.6381	0.7495	0.8114	0.8769	0.9108
377		urea	LC/MS pos early	1670	C00086	HMDB00294	1176	1.15	0.1303	0.3183	1.0085	1.1648	1.1557	1.1844
379		ornithine	LC/MS pos early	1493	C00077	HMDB03374	6262	1.02	0.6012	0.5629	1.0020	1.0256	1.0269	0.9749
383		2-oxoarginine*	LC/MS pos early	55072	C03771	HMDB04225	568	1.36	0.2663	0.4213	0.7457	1.0116	0.9645	0.7388
384		citrulline	LC/MS pos early	2132	C00327	HMDB00904	9750	0.97	0.6072	0.5637	1.0331	1.0007	1.0212	0.9491
385		homocysteine	LC/MS pos early	22137	C01924	HMDB00670	9085	0.72	0.0033	0.0608	1.1255	0.8114	0.8784	0.7070
386		homocitrulline	LC/MS pos early	22138	C02427	HMDB00679	65072	0.83	0.9275	0.6301	1.4651	1.2108	1.1677	1.2813
387		proline	LC/MS pos early	1898	C00148	HMDB00162	145742	1.18	0.5652	0.5475	1.0182	1.2025	1.1859	1.0126
390	Urea cycle; Arginine and Proline Metabolism	dimethylarginine (SDMA + ADMA)	LC/MS pos early	36908	C03626	HMDB01539	123831	1.00	0.9965	0.6510	1.0584	1.0537	1.0602	1.0133
391		N-acetylarginine	LC/MS pos early	33953	C02562	HMDB04620	67427	1.07	0.3560	0.4591	0.9980	1.0709	1.0917	1.0230
394		N-acetylcitrulline	LC/MS neg	48434	C15532	HMDB00856	656979	0.66	0.3760	0.4656	1.6672	1.0952	1.0985	0.7990
395		N-acetylproline	LC/MS pos early	34387			322640	1.36	0.1136	0.2966	1.1074	1.5048	1.4341	1.5239
396		N-delta-acetylornithine	LC/MS neg	43249			9920500	0.87	0.3416	0.4524	1.2473	1.0835	1.0618	1.0323
397		N-alpha-acetylornithine	LC/MS pos early	32964	C00437	HMDB03357	439232	1.34	0.1543	0.3451	0.9582	1.2807	1.2180	1.0080
401		trans-4-hydroxyproline	LC/MS pos early	32306	C01157	HMDB00725	5910	1.05	0.5203	0.5263	1.0643	1.1173	1.0752	1.0181

403		pro-hydroxy-pro	LC/MS pos early	35127		HMDB06695	11673055	1.10	0.5143	0.5251	1.0948	1.2043	1.1938	1.1922
406		N-methylproline	LC/MS pos early	37431			557	2.37	0.0462	0.1889	1.2524	2.8624	2.5518	1.5070
410		argininate*	LC/MS pos early	57461		HMDB03148	160437	1.04	0.9038	0.6250	1.0533	1.0924	1.0596	0.9737
415		guanidinoacetate	LC/MS pos early	43802	C00581	HMDB00128	763	0.95	0.6689	0.5731	1.0264	0.9797	0.9818	1.0082
416		creatine	LC/MS pos early	27718	C00300	HMDB00064	586	1.09	0.4567	0.5037	0.9703	1.0583	1.0819	1.0009
417		creatinine	LC/MS pos early	513	C00791	HMDB00562	588	0.91	0.0775	0.2550	1.0869	0.9923	0.9861	0.9758
426		spermidine	LC/MS pos early	485	C00315	HMDB01257	1102	1.16	0.7139	0.5865	0.9577	1.1086	1.0889	0.9332
430		acisoga	LC/MS pos early	43268			123997	1.12	0.3687	0.4613	1.1080	1.2458	1.1934	1.3593
434		5-methylthioadenosine (MTA)	LC/MS pos early	1419	C00170	HMDB01173	439176	0.90	0.3662	0.4613	1.0816	0.9707	0.9675	0.8998
435		N-acetylputrescine	LC/MS pos early	37496	C02714	HMDB02064	122356	1.16	0.4002	0.4811	1.0356	1.2053	1.2120	1.1436
439		4-acetamidobutanoate	LC/MS pos early	1558	C02946	HMDB03681	18188	0.95	0.6411	0.5662	1.1521	1.0919	1.0580	0.9540
444		4-guanidinobutanoate	LC/MS pos early	15681	C01035	HMDB03464	500	1.03	0.8661	0.6152	1.2429	1.2852	1.2513	0.9975
445		guanidinoluccinate	LC/MS polar	32446	C03139	HMDB03157	97856	1.36	0.1029	0.2856	1.1794	1.5894	1.5756	1.5951
450		cysteine- glutathione disulfide	LC/MS pos early	35159		HMDB00656	4247235	1.32	0.4841	0.5126	1.0923	1.4449	1.3537	1.1939
453		cysteinylglycine	LC/MS pos early	35637	C01419	HMDB00078	439498	0.72	0.3512	0.4591	1.3892	1.0029	1.0916	1.2114
455		cys-gly, oxidized	LC/MS pos early	18388			333203	0.76	0.1733	0.3533	1.2353	0.9367	0.9672	0.7645
456		5-oxoproline	LC/MS neg	1494	C01879	HMDB00267	7405	1.01	0.7256	0.5855	0.9998	1.0111	1.0089	0.9804
457		2-aminobutyrate	LC/MS pos early	42374	C02261	HMDB00650	439691	0.86	0.0051	0.2333	1.0788	0.9260	0.9690	0.9430
459		2-hydroxybutyrate/2-hydroxyisobutyrate	LC/MS polar	52281				1.18	0.0966	0.2783	0.9912	1.1703	1.1477	1.2528
470		gamma-glutamylalanine	LC/MS pos early	37063		HMDB29142	440103	0.78	0.0102	0.0987	1.1479	0.8941	0.8908	0.8833
472		gamma-glutamylglutamate	LC/MS pos early	36738	C05282	HMDB11737	92865	1.15	0.4302	0.4934	0.9814	1.1281	1.1178	0.9966
473		gamma-glutamylglutamine	LC/MS pos early	2730	C05283	HMDB11738	150914	1.01	0.9114	0.6250	0.9936	1.0054	1.0183	0.9302
474		gamma-glutamylglycine	LC/MS pos early	33949		HMDB11667	165527	1.08	0.7514	0.5938	1.0962	1.1818	1.1455	1.0241
475		gamma-glutamylhistidine	LC/MS pos early	18245			7017195	0.81	0.0159	0.1152	1.1180	0.9040	0.9193	0.8232
476		gamma-glutamylisoleucine*	LC/MS neg	34457		HMDB11170	14253342	0.87	0.3490	0.4588	1.3000	1.1267	1.1020	1.0553
477		gamma-glutamylleucine	LC/MS pos early			HMDB11171	151023	0.82	0.1061	0.2870	1.2071	0.9949	0.9972	0.9297
478		gamma-glutamyl-alpha-lysine	LC/MS pos early	18369			65254	0.82	0.0231	0.1341	1.1397	0.9317	0.9727	0.8519
479		gamma-glutamyl-epsilon-lysine	LC/MS pos early	55015		HMDB03869	7015685	0.85	0.0803	0.2563	1.0643	0.9064	0.9217	0.8127
480		gamma-glutamylmethionine	LC/MS neg	33934		HMDB29155	7005967	0.80	0.0352	0.1684	1.1771	0.9459	0.9495	0.8268
481		gamma-glutamylphenylalanine	LC/MS pos early	44872		HMDB00594	111299	0.78	0.0903	0.2674	1.2496	0.9740	0.9696	0.8857
482		gamma-glutamylthreonine	LC/MS pos early	33422		HMDB29159	76078708	0.88	0.2471	0.4130	1.1495	1.0109	1.1117	0.9369
483		gamma-glutamyltryptophan	LC/MS pos early	33364		HMDB29160	3989307	1.00	0.5186	0.5283	1.1013	1.1039	1.0669	1.0084
484		gamma-glutamyltyrosine	LC/MS neg	33947		HMDB11741	94340	0.90	0.2766	0.4311	1.0950	0.9852	0.9937	0.8184
485		gamma-glutamylvaline	LC/MS pos early	2734		HMDB11172	7015683	0.90	0.3306	0.4524	1.1613	1.0415	1.0447	1.0311
486		gamma-glutamylserine	LC/MS pos early	43829				1.02	0.7932	0.6033	0.9816	1.0010	0.9921	1.0168
488		gamma-glutamyl-2-aminobutyrate	LC/MS pos early	54914				0.65	0.0790	0.2552	0.9814	0.8363	0.6878	0.6716
646	Peptide	glycylvaline	LC/MS pos early	37092		HMDB28854	97417	1.18	0.0569	0.2168	0.8654	1.0169	0.9041	1.1357
651		histidylalanine	LC/MS neg	18357		HMDB28878	351667	0.99	0.8485	0.6084	1.1295	1.1149	1.1241	1.2584
670		isoleucylglycine	LC/MS neg	42027		HMDB28907	342532	1.05	0.4235	0.4921	1.0131	1.0594	1.0533	1.0164
684		leucylalanine	LC/MS pos early	40008		HMDB28922	259321	1.24	0.4210	0.4904	0.9693	1.2053	1.2098	1.3953
689		leucylglycine	LC/MS pos early	40010		HMDB28929	79070	0.99	0.9405	0.6350	0.9783	0.9727	1.0307	1.0089
738		phenylalanylalanine	LC/MS neg	40045			5488196	0.81	0.1262	0.3128	1.0583	0.8527	0.8963	0.8537
742		phenylalanylglycine	LC/MS pos early	41374		HMDB28995	98207	0.95	0.7271	0.5865	1.0799	1.0217	0.9942	0.9164
761		prolylglycine	LC/MS pos early	41370		HMDB11178	6426708	0.79	0.1162	0.3004	1.3883	1.0972	1.0439	1.0565
799		threonylphenylalanine	LC/MS pos early	40703		HMDB29068	4099799	1.15	0.4161	0.4900	1.0567	1.2129	1.1574	1.1095
841		valylglutamine	LC/MS pos early	31530		HMDB29125	5253209	0.99	0.9514	0.6381	1.0508	1.0355	1.0790	1.2172
845		valylleucine	LC/MS pos early	42079		HMDB29131	352039	0.83	0.1550	0.3452	1.0409	0.8598	0.8747	0.8923
855		leucylglutamine*	LC/MS pos early	39994		HMDB28927	4305457	0.84	0.4511	0.5022	1.0835	0.9154	1.0176	1.1229
904		Fibrinopeptide A*	LC/MS pos early	48189			16133137	0.95	0.6203	0.5637	0.8500	0.8050	0.7473	0.8748
912		Fibrinopeptide A, des-ala(1)*	LC/MS neg	33084				1.06	0.6733	0.5745	1.0737	1.1341	1.1036	1.0535
929		phenylacetylcarbamitine	LC/MS pos early	31548			101724840	1.20	0.4423	0.4987	1.6743	2.0054	1.9589	2.7887
931		phenylacetylglutamate	LC/MS neg	48425		HMDB59772	11579826	1.23	0.4046	0.4827	1.1048	1.3548	1.2385	1.6413
932		phenylacetylglutamine	LC/MS neg	52925	C04148	HMDB06344	92258	1.01	0.4972	0.5166	1.5674	1.5824	1.5551	1.7568
934		4-hydroxyphenylacetylglutamine	LC/MS neg	35126				0.94	0.8059	0.6043	1.2865	1.2093	1.1972	0.7389

961			1,5-anhydroglucitol (1,5-AG)	LC/MS neg	55017	C07326	HMDB02712	64990	0.92	0.6512	0.5694	1.0837	1.0006	0.9996	0.8619
964			glucose	LC/MS polar	20675	C00031	HMDB00122	79025	0.96	0.3386	0.4524	1.0468	1.0039	0.9957	0.9917
980		Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	pyruvate	LC/MS polar	48152	C00022	HMDB00243	1090	1.42	0.3000	0.4418	1.0824	1.5354	1.4734	2.0412
981			lactate	LC/MS neg	48990	C00186	HMDB00190	612	1.10	0.3604	0.4613	0.9923	1.0913	1.0729	1.1916
984			glycerate	LC/MS polar	527	C00258	HMDB00139	752	1.15	0.0198	0.1237	0.9746	1.1251	1.1001	1.0573
1002			ribose	LC/MS polar	1572	C00121	HMDB00283	5779	1.29	0.2321	0.3993	0.9839	1.2653	1.1830	1.3311
1003			ribitol	LC/MS polar	1471	C00474	HMDB00508	6912	0.95	0.9250	0.6294	1.0846	1.0348	0.9959	0.9766
1004			ribonate	LC/MS polar	15772	C01685	HMDB00867	5460677	1.18	0.0388	0.1741	0.9473	1.1225	1.0806	1.0572
1008		Pentose Metabolism	xylose	LC/MS polar	27731	C00181	HMDB00098	135191	0.86	0.6800	0.5765	0.9007	0.7780	0.7476	0.5815
1010			arabinose	LC/MS polar	15581	C00216	HMDB00646	66308	1.06	0.3409	0.4524	0.9211	0.9796	0.9333	0.8469
1016			arabitol/xyllitol	LC/MS polar	575	C01904		6912	0.92	0.6148	0.5637	1.2970	1.1914	1.1524	1.2245
1024			arabonate/xyllonate	LC/MS polar	48886				1.08	0.4065	0.4827	1.0376	1.1193	1.0602	0.9976
1027	Carbohydrate		sedoheptulose	LC/MS polar	48255		HMDB03219	5459979	0.55	0.7051	0.5845	2.2030	1.2129	1.1436	0.5722
1037		Glycogen Metabolism	maltose	LC/MS polar	53237	C00208	HMDB00163	10991489	1.00	0.6062	0.5637	1.1946	1.1985	1.0930	1.2619
1059		Disaccharides and Oligosaccharides	sucrose	LC/MS polar	15586	C00089	HMDB00258	5988	2.40	0.0872	0.2642	0.9328	2.2424	1.9357	3.3090
1077			fructose	LC/MS polar	1519	C00095	HMDB00660	5984	0.77	0.0064	0.0791	1.1359	0.8743	0.8890	0.8571
1082		Fructose, Mannose and Galactose Metabolism	mammil/sorbitol	LC/MS polar	48195	C00794	HMDB00247	5780	1.05	0.4561	0.5037	3.9634	4.1493	3.7700	3.0258
1083			mannose	LC/MS polar	46142	C00159	HMDB00169	18950	1.08	0.2098	0.3810	0.9651	1.0430	1.0226	1.0375
1103			galactonate	LC/MS polar	48153	C00880	HMDB00565	128989	0.45	0.3963	0.4798	2.2456	1.0209	0.9496	0.8721
1135			glucuronate	LC/MS polar	27719	C00191	HMDB00127	444791	1.19	0.9105	0.6250	1.1345	1.3539	1.2897	1.0113
1146		Aminosugar Metabolism	N-acetylneuraminic acid	LC/MS polar	15443	C00270	HMDB00230	439197	1.02	0.6663	0.5722	1.0682	1.0911	1.0681	1.0742
1157			N-acetylglucosaminylasparagine	LC/MS pos early	32377	C04540	HMDB00489	123826	1.19	0.4967	0.5051	0.8482	1.0082	0.9670	0.9390
1158			erythronate*	LC/MS polar	48149		HMDB00613	2781043	1.01	0.8333	0.6058	1.0773	1.0850	1.0490	1.0237
1160			N-acetylglucosamineN-acetylgalactosamine	LC/MS pos early	42420		HMDB00215	24139	1.06	0.2803	0.4336	1.0422	1.1075	1.0796	1.0701
1161		Advanced Glycation End-product	NG-carboxymethyllysine	LC/MS pos early	46539			123800	1.16	0.5107	0.5251	1.1580	1.3471	1.3046	1.2208
1165			citrate	LC/MS neg	36713	C00158	HMDB00094	311	1.16	0.1443	0.3340	0.9804	1.1350	1.0879	1.1470
1167			aconitate [cis or trans]	LC/MS neg	1594				1.20	0.1589	0.3488	1.0362	1.2461	1.1836	1.2291
1169			isocitrate	LC/MS pos early	46173	C00311	HMDB00193	1198	0.97	0.7385	0.5903	1.0178	0.9916	0.9959	0.9907
1171			alpha-ketoglutarate	LC/MS polar	12110	C00026	HMDB00208	51	1.11	0.2914	0.4392	1.0667	1.1874	1.1332	1.2906
1173		TCA Cycle	succinylcarnitine (C4-DC)	LC/MS pos early	528		HMDB61717	7146481	1.02	0.7047	0.5845	1.0242	1.0408	1.0310	0.9595
1174			succinate	LC/MS neg	37058	C00042	HMDB00254	1110	1.17	0.1064	0.2870	0.9615	1.1287	1.0847	1.0453
1175			fumarate	LC/MS polar	1437	C00122	HMDB00134	444972	1.00	0.8107	0.6052	1.0158	1.0196	0.9881	1.0335
1177			malate	LC/MS neg	1643	C00149	HMDB00156	525	1.28	0.0104	0.0987	0.9515	1.2151	1.1543	1.1897
1187			2-methylcitrate/homocitrate	LC/MS neg	1303				1.01	0.8062	0.6043	1.0541	1.0617	1.0567	1.0239
1191		Oxidative Phosphorylation	phosphate	LC/MS neg	52282	C00009	HMDB01429	1061	0.95	0.3045	0.4447	0.9964	0.9493	0.9557	0.9895
1193			malonylcarnitine	LC/MS pos early	42109		HMDB02095	22833583	1.01	0.9466	0.6374	1.0571	1.0690	1.0440	1.1091
1194		Fatty Acid Synthesis	malonate	LC/MS polar	37059	C00383	HMDB00691	867	1.39	0.0066	0.0791	0.8812	1.2244	1.1539	1.0766
1195			2-methylmalonylcarnitine (C4-DC)	LC/MS pos early	15872		HMDB13133	53481628	1.08	0.3196	0.4524	0.9901	1.0679	1.0932	0.9823
1211			caprylate (8:0)	LC/MS neg	35482	C06423	HMDB00482	379	1.74	0.0471	0.1894	0.8892	1.5466	1.4035	1.7705
1212			pelargolate (9:0)	LC/MS neg	32492	C01601	HMDB00847	8158	1.03	0.5596	0.5471	1.0984	1.1360	1.0841	1.1112
1213		Medium Chain Fatty Acid	caprate (10:0)	LC/MS neg	12035	C01571	HMDB00511	2969	1.56	0.0157	0.1152	0.9828	1.5319	1.4676	1.9011
1216			10-undecanoate (11:1n1)	LC/MS neg	1642	C13910	HMDB33724	14891	1.61	0.2522	0.4190	0.8697	1.4038	1.3233	1.7886
1217			laurate (12:0)	LC/MS neg	32497	C02679	HMDB00638	3893	1.88	0.0002	0.0078	0.7829	1.5488	1.4656	1.6399
1218			5-dodecanoate (12:1n7)	LC/MS neg	1645		HMDB00529	5312376	2.14	0.0112	0.0967	0.8858	1.8963	1.7508	2.2112
1220			myristate (14:0)	LC/MS neg	33968	C06424	HMDB00806	11005	1.65	0.0119	0.1004	0.8941	1.4761	1.4173	1.7516
1221			myristoleate (14:1n5)	LC/MS neg	1365	C08322	HMDB02000	5281119	1.74	0.0140	0.1092	0.9131	1.5916	1.4879	1.8084
1224			pentadecanoate (15:0)	LC/MS neg	32418	C16537	HMDB00826	13849	1.34	0.0243	0.1386	0.9098	1.2203	1.1925	1.3411
1225			palmitate (16:0)	LC/MS neg	1361	C00249	HMDB00220	985	1.26	0.0282	0.1494	0.8704	1.0925	1.0638	1.1761
1226			palmitoleate (16:1n7)	LC/MS neg	1336	C08362	HMDB03229	445638	1.74	0.0177	0.1198	0.8969	1.5593	1.5130	1.7255
1228			margarate (17:0)	LC/MS neg	33447		HMDB02259	10465	1.48	0.0107	0.0967	0.9350	1.3846	1.3083	1.4570
1229			10-heptadecanoate (17:1n7)	LC/MS neg	1121		HMDB60038	5312435	1.61	0.0215	0.1290	0.8142	1.3136	1.2469	1.4389
1231		Long Chain Fatty Acid	stearate (18:0)	LC/MS neg	33971	C01530	HMDB00827	5281	1.19	0.0294	0.1494	0.9023	1.0733	1.0389	1.1323
1233			decaevaccenate (18:1)	LC/MS neg	1358				1.33	0.0273	0.1494	0.8449	1.1239	1.0793	1.1779
1240			nonadecanoate (19:0)	LC/MS neg	52285	C16535	HMDB00772	12591	1.44	0.0062	0.0791	0.8647	1.2460	1.2052	1.3172

1241		10-nonadecenoate (19:1n6)	LC/MS neg	1356		HMDB13622	5312513	1.66	0.0099	0.0967	0.8408	1.3917	1.2919	1.4493
1244		arachidate (20:0)	LC/MS neg	33972	C06425	HMDB02212	10467	1.30	0.0187	0.1225	0.9789	1.2736	1.2298	1.3696
1247		eicosenoate (20:1)	LC/MS neg	1118	C16526	HMDB02231	5282798	1.74	0.0068	0.0791	0.7917	1.3795	1.3081	1.4054
1252		erucate (22:1n7)	LC/MS neg	33567	C08316	HMDB02068	5281116	2.05	0.0192	0.1226	0.9119	1.8722	1.8711	2.1272
1265		stearidonate (18:4n3)	LC/MS neg	1552	C16300	HMDB06547	5312598	1.84	0.0035	0.0608	0.8280	1.5209	1.5311	1.5856
1266		eicosapentaenoate (EPA; 20:5n3)	LC/MS neg	33969	C06428	HMDB01999	446284	1.14	0.2958	0.4397	1.2882	1.4693	1.7058	1.5374
1267		docosapentaenoate (n3 DPA; 22:5n3)	LC/MS neg	18467	C16513	HMDB06528	6441454	1.16	0.1598	0.3488	0.9370	1.0869	1.0709	1.1092
1268		docosahexaenoate (DHA; 22:6n3)	LC/MS neg	32504	C06429	HMDB02183	445580	1.22	0.1072	0.2870	0.9650	1.1736	1.2224	1.2218
1269		docosatrienoate (22:3n3)	LC/MS neg	44675	C16534	HMDB02823	5312556	1.36	0.2917	0.4362	0.9165	1.2446	1.1220	1.1299
1273		linoleate (18:2n6)	LC/MS neg	32417	C01595	HMDB00673	5280450	1.31	0.0453	0.1889	0.8803	1.1566	1.1118	1.2352
1275		linolenate (alpha or gamma; 18:3n3 or 6)	LC/MS neg	1105	C06426	HMDB03073	5280934	1.43	0.0268	0.1710	1.0035	1.4390	1.4150	1.4698
1277		dhomo-linolenate (20:3n3 or n6)	LC/MS neg	34035	C03242	HMDB02925	5280581	1.22	0.0791	0.2552	0.9354	1.1448	1.0957	1.2116
1278		arachidonate (20:4n6)	LC/MS neg	35718	C00219	HMDB01043	444899	1.08	0.3310	0.4524	0.9507	1.0276	1.0399	1.0324
1279		adrenate (22:4n6)	LC/MS neg	1110	C16527	HMDB02226	5497181	1.20	0.0953	0.2776	0.9524	1.1440	1.1016	1.1681
1280		docosapentaenoate (n6 DPA; 22:5n6)	LC/MS neg	32980	C16513	HMDB01976	6441454	1.24	0.0302	0.1512	0.8718	1.0804	1.0873	1.1431
1281		docosadienoate (22:2n6)	LC/MS neg	37478	C16533	HMDB61714	5282807	1.37	0.0114	0.0987	0.9258	1.2657	1.2055	1.2933
1282		dhomo-linoleate (20:2n6)	LC/MS neg	32415	C16525	HMDB05060	6439848	1.39	0.0179	0.1198	0.9073	1.2633	1.1788	1.2935
1284		mead acid (20:3n7)	LC/MS neg	17805		HMDB10378	5312531	1.40	0.0287	0.1494	1.0021	1.4079	1.3547	1.4246
1285		docosatrienoate (22:3n6)*	LC/MS neg	35174				1.23	0.3090	0.4473	1.1432	1.4091	1.1992	1.1777
1337		(12 or 13)-methylmyristate (a15:0 or 115:0)	LC/MS neg	57467			151014	1.85	0.0432	0.1842	1.0117	1.8680	1.7469	2.5009
1340		(14 or 15)-methylpalmitate (a17:0 or 117:0)	LC/MS neg	38293			17903417	1.51	0.0630	0.2285	0.8919	1.3437	1.2440	1.6210
1344		(16 or 17)-methylstearate (a19:0 or 119:0)	LC/MS neg	38768		HMDB37397	3083779	1.47	0.0156	0.1152	0.8447	1.2399	1.1565	1.3358
1359		glutarate (C5-DC)	LC/MS polar	38296	C00489	HMDB00661	743	0.91	0.2455	0.4129	1.7439	1.5868	1.5017	2.0187
1362		3-methylglutarate/2-methylglutarate	LC/MS polar	396		HMDB00752		1.31	0.7062	0.5845	1.1327	1.4876	1.3866	1.2632
1363		2-hydroxyglutarate	LC/MS polar	54676	C02630	HMDB00606	43	1.17	0.6485	0.5690	1.1419	1.3374	1.2424	1.2289
1365		adipate (C6-DC)	LC/MS polar	37253	C06104	HMDB00448	106	1.50	0.7094	0.5847	0.8928	1.3413	1.2403	1.2346
1367		2-hydroxyadipate	LC/MS polar	21134	C02360	HMDB00321	193593	0.96	0.0463	0.1889	1.3448	0.7499	0.7444	0.6744
1369		3-methyladipate	LC/MS polar	31934		HMDB00555	12392	1.88	0.7356	0.5888	1.1040	2.0791	2.0913	2.6468
1371		malate	LC/MS polar	36749	C01384	HMDB00176	444266	0.92	0.9784	0.6456	1.1766	1.0834	1.0284	1.0909
1372		pinelate (C7-DC)	LC/MS polar	20676	C02656	HMDB00857	385	1.50	0.1679	0.3488	0.8343	1.2553	1.2302	1.2888
1375		suberate (C8-DC)	LC/MS neg	15704	C08278	HMDB00893	10457	1.35	0.1603	0.3488	0.9502	1.2866	1.2240	1.2134
1378		azelate (C9-DC)	LC/MS neg	15730	C08261	HMDB00784	2266	1.34	0.0511	0.2007	0.9023	1.2102	1.1153	1.1365
1380		sebacate (C10-DC)	LC/MS polar	18362	C08277	HMDB00792	5192	1.85	0.1279	0.3153	0.9973	1.8427	1.8465	2.1452
1384		dodecanedioate (C12-DC)	LC/MS neg	32398	C02678	HMDB00623	12736	1.65	0.2650	0.4204	1.0648	1.7541	1.6007	1.6330
1387		tetradecanedioate (C14-DC)	LC/MS neg	32388		HMDB00872	13185	1.62	0.3681	0.4613	1.0977	1.7746	1.6231	1.9347
1388		hexadecanedioate (C16-DC)	LC/MS neg	35699	C19615	HMDB00672	104059	1.79	0.0998	0.2819	1.0036	1.7947	1.6250	1.9331
1391		octadecanedioate (C18-DC)	LC/MS neg	35678		HMDB00782	70095	1.42	0.0837	0.2623	1.1733	1.6611	1.5289	1.7571
1395		eicosanedioate (C20-DC)	LC/MS neg	36754			75502	0.82	0.3396	0.4524	1.1648	0.9578	0.9203	0.8706
1397		docosadioate (C22-DC)	LC/MS neg	39831	C19625		244872	0.71	0.0982	0.2814	1.2391	0.8854	0.8622	0.7589
1398		3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)	LC/MS neg	39837		HMDB61112	123979	0.81	0.2280	0.3948	1.0226	0.8285	0.9967	0.7802
1442		2-aminoheptanoate	LC/MS pos early	31787			227939	1.03	0.8391	0.6058	1.0264	1.0534	1.0257	0.9891
1447		2-aminooctanoate	LC/MS neg	43761		HMDB00991	69522	0.96	0.8572	0.6130	1.0673	1.0236	1.0149	1.0094
1458		butyrylcarnitine (C4)	LC/MS pos early	43343	C02862	HMDB02013	439820	1.16	0.6098	0.5637	1.0315	1.1938	1.1665	1.3106
1461		propionylcarnitine (C3)	LC/MS pos early	32412	C03017	HMDB00824	107738	0.89	0.4581	0.5037	1.1152	0.9931	1.0302	0.9365
1462		propionylglycine	LC/MS neg	32452		HMDB00783	98681	1.33	0.2685	0.4235	1.1115	1.4752	1.4328	1.1265
1464		methylmalonate (MMA)	LC/MS polar	31932	C02170	HMDB00202	487	0.83	0.5759	0.5489	1.5380	1.2713	1.2115	0.8040
1465		hexanoylglycine	LC/MS neg	1496				2.76	0.0487	0.1939	0.8277	2.2867	2.0555	1.6557
1476		hexanoylglycine	LC/MS neg	54907		HMDB00701	99463	3.99	0.0031	0.0608	0.6408	2.5595	2.2546	1.7424
1482		N-palmitoylglycine	LC/MS neg	35436		HMDB13034	151008	1.64	0.0000	0.0018	0.7821	1.2816	1.2157	1.2733
1492		acetyl carnitine (C2)	LC/MS pos early	42092	C02571	HMDB00201	1	1.34	0.1533	0.3451	0.9877	1.3294	1.2688	1.3644
1494		3-hydroxybutyrylcarnitine (1)	LC/MS pos early	32198		HMDB13127	53481617	1.40	0.2572	0.4196	1.0863	1.5161	1.3806	1.6275
1495		3-hydroxybutyrylcarnitine (2)	LC/MS pos early	43264		HMDB13127		1.65	0.1935	0.3668	1.1071	1.8300	1.6604	2.3503
1497		hexanoylcarnitine (C6)	LC/MS pos early	52964		HMDB00705	6428853	1.65	0.1908	0.3668	1.0066	1.6587	1.5379	1.9337
1500		octanoylcarnitine (C8)	LC/MS pos late	32328	C02838	HMDB00791	123701	1.72	0.4468	0.5006	1.0883	1.8674	1.7076	2.3056

1503		decanoylcarnitine (C10)	LC/MS pos late	33936		HMDB00651	10245190	1.59	0.4894	0.5136	1.0618	1.6862	1.5486	2.1138
1506		cis-4-decenoylcarnitine (C10:1)	LC/MS pos late	33941				1.43	0.7452	0.5938	1.1102	1.5827	1.4566	1.9608
1507		laurylcarnitine (C12)	LC/MS pos late	38178		HMDB02250	10427599	1.39	0.6694	0.5731	1.0774	1.4947	1.3907	1.8628
1508		myristoylcarnitine (C14)	LC/MS pos late	34534		HMDB05066	6426854	1.49	0.1920	0.3668	0.9237	1.3724	1.2765	1.5700
1510		palmitoylcarnitine (C16)	LC/MS pos late	33952	C02990	HMDB00222	461	1.18	0.1231	0.3107	0.9353	1.1018	1.0920	1.1459
1511		palmitoleoylcarnitine (C16:1)*	LC/MS pos late	44681			71464547	1.49	0.2261	0.3941	0.9519	1.4204	1.3236	1.4971
1512		stearoylcarnitine (C18)	LC/MS pos late	53223		HMDB00848	6426855	1.30	0.0034	0.0608	0.8964	1.1677	1.1391	1.1354
1513		linoleoylcarnitine (C18:2)*	LC/MS pos late	34409		HMDB06469	6450015	1.06	0.6346	0.5662	1.0712	1.1309	1.0771	1.1608
1514		linolenoylcarnitine (C18:3)*	LC/MS pos late	46223				0.93	0.7851	0.6012	1.1299	1.0538	1.0310	1.0417
1516		oleoylcarnitine (C18:1)	LC/MS pos late	57511		HMDB05065	6441392	1.21	0.2121	0.3810	0.9976	1.2099	1.1568	1.1869
1518		myristoleoylcarnitine (C14:1)*	LC/MS pos late	35160			90659972	1.64	0.4020	0.4811	1.0443	1.7116	1.5513	1.9435
1519	Fatty Acid Metabolism (Acyl Carnitine)	suberoylcarnitine (C8-DC)	LC/MS pos early	48182				1.67	0.7241	0.5855	0.8561	1.4327	1.3067	1.1221
1522		adipoylcarnitine (C6-DC)	LC/MS pos early	52990		HMDB61677	71296139	1.42	0.2408	0.4069	1.0165	1.4457	1.3399	1.3209
1525		pineloylcarnitine/3-methyladipoylcarnitine (C7-DC)	LC/MS pos early	52988				1.00	0.1916	0.3668	1.1244	1.1233	1.4639	1.3040
1529		arachidoylcarnitine (C20)*	LC/MS pos late	53224		HMDB06460		1.40	0.0506	0.2003	0.9374	1.3129	1.2720	1.2018
1530		arachidonoylcarnitine (C20:4)	LC/MS pos late	57513				1.01	0.3444	0.4540	1.1049	1.1152	1.0978	1.0325
1531		adrenoylcarnitine (C22:4)*	LC/MS pos late	57518				1.16	0.0756	0.2548	0.9673	1.1289	1.0880	1.0349
1532		behenoylcarnitine (C22)*	LC/MS pos late	57528				1.81	0.0868	0.2642	0.9680	1.7537	1.6780	1.8914
1534		dhomo-linolenoylcarnitine (C20:3n3 or 6)*	LC/MS pos late	57514				1.18	0.0949	0.2776	1.1045	1.2987	1.2322	1.2346
1535		dhomo-linoleoylcarnitine (C20:2)*	LC/MS pos late	57521				1.29	0.0760	0.2548	0.9689	1.2457	1.1601	1.1244
1536		eicosenoylcarnitine (C20:1)*	LC/MS pos late	57520				1.52	0.0774	0.2550	0.9354	1.4199	1.3419	1.3675
1540		docosapentaenoylcarnitine (C22:5n3)*	LC/MS pos late	57519				1.01	0.6210	0.5637	1.0284	1.0381	1.0305	1.0489
1541		docosahexaenoylcarnitine (C22:6)*	LC/MS pos late	57529				0.96	0.9038	0.6250	1.0929	1.0444	1.0795	1.0801
1543		lignoceroylcarnitine (C24)*	LC/MS pos late	57523				1.40	0.1064	0.2870	0.9667	1.3559	1.3431	1.3809
1544		margaroylcarnitine (C17)*	LC/MS pos late	57515		HMDB06210		1.32	0.0660	0.2333	1.0671	1.4052	1.3531	1.5859
1545		nervonoylcarnitine (C24:1)*	LC/MS pos late	57512				1.48	0.0472	0.1894	0.9449	1.3956	1.3794	1.4399
1546		cerotoylcarnitine (C26)*	LC/MS pos late	57531		HMDB06347		1.08	0.6198	0.5637	1.0623	1.1482	1.1675	1.0810
1547		ximenoylcarnitine (C28:1)*	LC/MS pos late	57516				1.05	0.7780	0.5998	1.0208	1.0742	1.0978	1.0815
1553	Carnitine Metabolism	deoxycarnitine	LC/MS pos early	57517	C01181	HMDB01161	134	0.82	0.0095	0.0987	1.1383	0.9301	0.9288	0.9238
1554		carnitine	LC/MS pos early	36747	C00318	HMDB00062	10917	0.95	0.1655	0.3488	1.0437	0.9873	0.9999	0.9774
1557	Ketone Bodies	acetoacetate	LC/MS pos early	15500	C00164	HMDB00060	96	1.83	0.0714	0.2472	0.8069	1.4769	1.3872	1.5515
1559		3-hydroxybutyrate (BHBA)	LC/MS polar	33963	C01089	HMDB00357	441	2.57	0.0356	0.1684	0.9671	2.4834	2.2747	2.8902
1562		palmitoylcholine	LC/MS pos late	542			151731	0.83	0.3295	0.4524	1.1351	0.9437	1.0112	0.9000
1563		oleoylcholine	LC/MS pos late	52944				0.85	0.4262	0.4933	1.0927	0.9315	0.9890	0.8654
1564		palmitoleoylcholine	LC/MS pos late	53260				0.89	0.5717	0.5478	1.0497	0.9355	1.0442	0.9496
1565		dhomo-linolenoylcholine	LC/MS pos late	53257				0.94	0.5613	0.5473	1.0381	0.9800	0.9848	0.9271
1566	Fatty Acid Metabolism (Acyl Choline)	linoleoylcholine*	LC/MS pos late	53262				0.76	0.1767	0.3574	1.2137	0.9261	0.9639	0.8525
1568		stearoylcholine*	LC/MS pos late	57463				0.79	0.2221	0.3910	1.1037	0.8710	0.9421	0.7914
1569		docosahexaenoylcholine	LC/MS pos late	57464				0.76	0.2870	0.4347	1.1630	0.8860	1.0361	0.8317
1570		arachidonoylcholine	LC/MS pos late	53263				0.82	0.1704	0.3501	1.1455	0.9374	1.0103	0.8682
1571		eicosapentaenoylcholine	LC/MS pos late	53261				0.72	0.1587	0.3488	1.0351	0.7426	0.9988	0.7809
1578		2-hydroxyoctanoate	LC/MS neg	53258		HMDB02264	94180	0.97	0.9659	0.6152	1.1041	1.0678	1.0651	1.0755
1579		2-hydroxydecanoate	LC/MS neg	22036			21488	1.24	0.0603	0.2250	0.9552	1.1847	1.1738	1.3744
1580		2-hydroxydodecanoate	LC/MS neg	42489			97783	0.89	0.3128	0.4516	1.0694	0.9500	0.9559	1.0013
1582		2-hydroxypalmitate	LC/MS neg	52916		HMDB31057	92836	1.18	0.0381	0.1725	0.8736	1.0315	1.0169	1.0938
1584		2-hydroxystearate	LC/MS neg	35675	C03045		69417	1.14	0.0666	0.2842	0.8821	1.0042	0.9892	1.0392
1591		3-hydroxyhexanoate	LC/MS neg	17945			151492	1.41	0.1433	0.3340	0.9669	1.3652	1.2572	1.3555
1592		3-hydroxyoctanoate	LC/MS neg	53230		HMDB01954	26613	1.26	0.4381	0.4963	0.9688	1.2235	1.1278	1.2904
1594	Fatty Acid, Monohydroxy	3-hydroxydecanoate	LC/MS neg	22001		HMDB02203	26612	1.35	0.1450	0.3340	0.8902	1.2022	1.1230	1.3371
1595		3-hydroxydodecanoate	LC/MS neg	22053		HMDB00350	3017884	2.22	0.4200	0.4904	0.7259	1.6118	1.4072	1.4861
1596		3-hydroxydodecanoate	LC/MS neg	31943		HMDB00387	94216	1.34	0.1226	0.3107	1.0061	1.3446	1.2524	1.4423
1604		5-hydroxyhexanoate	LC/MS neg	32457		HMDB00525	170748	0.89	0.9077	0.6250	1.1585	1.0288	1.0070	0.9365
1611		16-hydroxypalmitate	LC/MS neg	31938	C18218	HMDB06294	10466	1.12	0.1071	0.2870	1.0330	1.1541	1.0873	1.0997
1615		13-HODE + 9-HODE	LC/MS neg	39609			43013	1.31	0.0846	0.2632	0.9894	1.2924	1.2891	1.3268

1618		14-HDdHE/17-HDdHE	LC/MS neg	37752				1.64	0.1436	0.3340	1.2005	1.9653	1.8976	1.4837
1630		3-hydroxystearate	LC/MS neg	53034			5282907	1.11	0.1837	0.3646	1.0805	1.1948	1.1687	1.3795
1631		9-hydroxystearate	LC/MS neg	52938		HMDB61661	9570127	1.42	0.0192	0.1226	0.9753	1.3827	1.3738	1.4976
1636	Fatty Acid, Dihydroxy	12,13-DIHOME	LC/MS neg	47120	C14829	HMDB04705	10236635	1.33	0.1741	0.3535	0.8956	1.1879	1.1768	1.3357
1637		9,10-DIHOME	LC/MS neg	38395	C14828	HMDB04704	9966640	1.14	0.9508	0.5433	0.9535	1.0915	1.0491	1.1425
1658		thromboxane B2	LC/MS neg	38399	C05963	HMDB03252	5283137	1.01	0.9117	0.6250	1.6141	1.6249	1.6301	1.8061
1717	Eicosanoid	12-HETE	LC/MS neg	17807		HMDB06111	5312983	1.73	0.3055	0.4447	1.5329	2.6447	2.6735	2.1574
1719		15-HETE	LC/MS neg	37536	C04742	HMDB02110	5280724	1.11	0.5861	0.5529	1.6537	1.8288	1.7788	1.7451
1723		12-HHTrE	LC/MS neg	37538	C20388	HMDB12535	5283141	0.95	0.9392	0.6350	1.8918	1.8040	1.7476	1.8566
1730		oleoyl ethanolamide	LC/MS pos late	57383		HMDB02088	5283454	1.19	0.0742	0.2522	0.9676	1.1474	1.1437	1.1547
1733	Endocannabinoid	palmitoyl ethanolamide	LC/MS neg	38102	C16512	HMDB02100	4671	1.30	0.0057	0.0776	0.9258	1.2045	1.1864	1.1917
1738		arachidonyl ethanolamide	LC/MS pos late	38165	C11695	HMDB04080	5281969	1.20	0.0780	0.2551	0.8998	1.0823	1.0813	1.0207
1742		N-oleoyltaurine	LC/MS neg	32463			6437033	1.67	0.0153	0.1152	0.6575	1.4333	1.3263	1.3559
1743		N-stearoyltaurine	LC/MS neg	39732			168274	1.43	0.0055	0.0771	0.7851	1.1245	1.0681	1.1116
1744		N-palmitoyltaurine	LC/MS neg	39730				1.73	0.0539	0.2083	0.7487	1.2923	1.1433	1.4204
1748		linoleoyl ethanolamide	LC/MS neg	39835		HMDB12252	5283446	1.37	0.0359	0.1684	0.9408	1.2902	1.2329	1.2502
1765			myo-inositol	LC/MS polar	52808	C00137	HMDB00211	892	0.91	0.3707	0.4613	1.1468	1.0487	1.0257
1766	Inositol Metabolism	chiro-inositol	LC/MS polar	1124	C19891	HMDB34220		1.28	0.5498	0.5433	1.3095	1.6724	1.4511	1.3158
1794	Phospholipid Metabolism	choline	LC/MS pos early	37112	C00114	HMDB00097	305	1.03	0.4136	0.4884	1.0127	1.0478	1.0495	1.0088
1795		choline phosphate	LC/MS pos early	15506	C00588	HMDB01565	1014	0.97	0.7257	0.5865	1.1118	1.0803	1.0855	1.0975
1798		glycerophosphorylcholine (GPC)	LC/MS pos early	34396	C00670	HMDB00086	71920	0.81	0.0161	0.1152	1.1075	0.9009	0.9177	0.8696
1800		phosphoethanolamine	LC/MS pos early	15990	C00346	HMDB00224	1015	0.89	0.2702	0.4249	1.2899	1.1498	1.1366	1.3044
1802		glycerophosphoethanolamine	LC/MS pos early	1600	C01233	HMDB00114	123874	0.98	0.7647	0.5962	1.0381	1.0207	1.0212	1.0003
1804		glycerophosphoinositol*	LC/MS neg	37455			167572	0.68	0.0657	0.2333	1.2829	0.8668	0.9351	0.8645
1805			trimethylamine N-oxide	LC/MS pos early	52307	C01104	HMDB00925	1145	1.40	0.6759	0.5750	1.4057	1.9652	1.7648
1839	Phosphatidylcholine (PC)	1,2-dipalmitoyl-GPC (16:0/16:0)	LC/MS pos late	40406		HMDB00564	452110	1.06	0.2818	0.4336	0.9847	1.0428	1.0516	1.0494
1840		1-palmitoyl-2-palmitoleoyl-GPC (16:0/18:1)*	LC/MS pos late	19130		HMDB07969		1.26	0.2931	0.4392	1.1040	1.3922	1.4186	1.5085
1841		1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	LC/MS pos late	52470		HMDB07970		1.03	0.7564	0.5938	1.0596	1.0935	1.1199	1.0606
1843		1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	LC/MS pos late	52616		HMDB07972	6436017	1.08	0.2146	0.3810	0.9690	1.0485	1.0510	1.0472
1846		1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	LC/MS pos late	52461		HMDB07973	5287971	0.99	0.8942	0.6250	1.0077	1.0008	0.9960	1.0104
1848		1-palmitoyl-2-alpha-linolenoyl-GPC (16:0/18:3n3)*	LC/MS pos late	42446		HMDB07975		0.91	0.7081	0.5845	0.9826	0.8956	0.9494	0.9780
1849		1-palmitoyl-2-gamma-linolenoyl-GPC (16:0/18:3n6)*	LC/MS pos late	52694		HMDB07974		1.46	0.0165	0.1152	0.7626	1.1135	1.1579	1.0974
1857		1-palmitoyl-2-arachidonyl-GPC (16:0/20:4n6)	LC/MS pos late	54812		HMDB07982	10747814	1.00	0.8381	0.6058	0.9837	0.9866	0.9922	0.9808
1868		1-palmitoleoyl-2-linoleoyl-GPC (16:1/18:2)*	LC/MS pos late	52462		HMDB08006		0.94	0.5618	0.5473	1.0767	1.0159	0.9823	1.0105
1869		1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)*	LC/MS pos late	52683		HMDB08008		1.01	0.8884	0.6250	1.0867	1.0989	1.1288	1.1540
1879		1-stearoyl-2-oleoyl-GPC (18:0/18:1)	LC/MS pos late	53180		HMDB08038		1.07	0.3418	0.4524	0.9971	1.0711	1.0816	1.0605
1882		1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	LC/MS pos late	52438		HMDB08039		0.98	0.5281	0.5310	1.0213	0.9961	0.9950	0.9718
1890		1-stearoyl-2-arachidonyl-GPC (18:0/20:4)	LC/MS pos late	52452		HMDB08048	16219824	0.96	0.4778	0.5112	1.0203	0.9825	0.9964	0.9533
1915		1,2-dilinoleoyl-GPC (18:2/18:2)	LC/MS pos late	42450		HMDB08138	5288075	1.03	0.9583	0.6388	1.0468	1.0777	1.0430	1.0430
1916		1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*	LC/MS pos late	52693		HMDB08141		0.89	0.3918	0.4792	1.1847	1.0521	1.0647	1.0388
1919		1-linoleoyl-2-arachidonyl-GPC (18:2/20:4n6)*	LC/MS pos late	53176		HMDB08147		1.01	0.7948	0.6033	1.0267	1.0346	1.0121	0.9938
1961		Phosphatidylethanolamine (PE)	1-palmitoyl-2-oleoyl-GPE (16:0/18:1)	LC/MS pos late	52710		HMDB05320	5283496	1.14	0.5671	0.5478	1.1782	1.3409	1.3062
1962	1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)		LC/MS pos late	19263		HMDB05322	9546747	1.17	0.4865	0.5126	1.0010	1.1740	1.1379	1.4100
1965	1-palmitoyl-2-arachidonyl-GPE (16:0/20:4)*		LC/MS pos late	42449		HMDB05323	9546900	1.09	0.3954	0.4591	1.1353	1.2403	1.2204	1.3315
1974	1-stearoyl-2-oleoyl-GPE (18:0/18:1)		LC/MS pos late	52464		HMDB08993		1.10	0.9053	0.6250	1.1595	1.2798	1.2759	1.5423
1977	1-stearoyl-2-linoleoyl-GPE (18:0/18:2)*		LC/MS pos late	42448		HMDB08994	9546749	1.02	0.9599	0.6391	0.9590	0.9710	0.9666	1.0551
1982	1-stearoyl-2-arachidonyl-GPE (18:0/20:4)		LC/MS pos late	52446		HMDB09003	5289133	1.04	0.5957	0.5597	1.0226	1.0607	1.0461	1.0971
2060			1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*	LC/MS polar	52447		HMDB09783		0.98	0.7193	0.5865	1.0453	1.0222	1.0496
2062	Phosphatidylinositol (PI)	1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	LC/MS pos late	52699		HMDB09784		1.24	0.5343	0.5359	1.0417	1.2943	1.2799	1.5943
2064		1-palmitoyl-2-arachidonyl-GPI (16:0/20:4)*	LC/MS pos late	52450		HMDB09789		1.11	0.6906	0.5810	0.9614	1.0718	1.1346	1.1518
2067		1-stearoyl-2-oleoyl-GPI (18:0/18:1)*	LC/MS pos late	52467				1.33	0.1000	0.2819	1.0188	1.3503	1.3149	1.4146
2068		1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	LC/MS pos late	52726		HMDB09809		1.04	0.8630	0.6152	1.0052	1.0444	1.0495	1.1420
2079		1-stearoyl-2-arachidonyl-GPI (18:0/20:4)	LC/MS pos late	52468		HMDB09815		1.00	0.9767	0.6453	1.0081	1.0125	1.0142	0.9800
2102			1-palmitoyl-GPA (16:0)	LC/MS neg	52449	C04036	HMDB00327	6419701	1.30	0.0198	0.1237	0.8180	1.1367	1.0759

2106			1-linoleoyl-GPA (18:2)*	LC/MS neg	34428		HMDB07856		1.27	0.3053	0.4447	0.8881	1.1276	1.0614	1.1462
2110			1-arachidonoyl-GPA (20:4)	LC/MS neg	52690				1.15	0.6201	0.5637	1.2608	1.4525	1.4027	1.3471
2117			1-palmitoyl-GPC (16:0)	LC/MS pos late	46325		HMDB10382	86554	1.01	0.6963	0.5809	1.0106	1.0244	1.0384	1.0186
2118			2-palmitoyl-GPC (16:0)*	LC/MS neg	33965		HMDB61702	15061532	1.10	0.3733	0.4633	1.0400	1.1405	1.1232	1.0033
2119			1-palmitoleoyl-GPC (16:1)*	LC/MS pos late	35253		HMDB10383	24770461	1.14	0.3672	0.4613	1.1076	1.2660	1.2757	1.2752
2125			1-stearoyl-GPC (18:0)	LC/MS pos late	33230		HMDB10384	497299	0.98	0.8219	0.6058	1.0202	1.0037	1.0301	0.9519
2127			1-oleoyl-GPC (18:1)	LC/MS pos late	33961		HMDB02815	16081932	1.07	0.3560	0.4591	0.9787	1.0432	1.0433	0.9961
2130			1-linoleoyl-GPC (18:2)	LC/MS pos late	48258	C04100	HMDB10386	11988421	0.97	0.5737	0.5478	1.0216	0.9895	0.9883	0.9811
2132			1-linolenoyl-GPC (18:3)*	LC/MS pos late	34419		HMDB10388		1.02	0.9447	0.6369	0.9996	1.0176	1.0002	0.9999
2148			1-arachidonoyl-GPC (20:4n6)*	LC/MS pos late	45951	C05208	HMDB10395		0.99	0.8997	0.6250	1.0175	1.0092	1.0290	0.9810
2159			1-lignoceroyl-GPC (24:0)	LC/MS pos late	33228		HMDB10405		1.13	0.4390	0.4963	0.9206	1.0268	1.0746	1.0662
2169			1-palmitoyl-GPE (16:0)	LC/MS pos late	49617		HMDB11503	9547069	1.14	0.1636	0.3488	0.9408	1.0788	1.0714	1.0874
2176			1-stearoyl-GPE (18:0)	LC/MS pos late	35531		HMDB11130	9547068	1.08	0.4138	0.4884	1.0064	1.0917	1.0933	1.0945
2177	Lipid	Lysophospholipid	2-stearoyl-GPE (18:0)*	LC/MS neg	42388		HMDB11129		1.18	0.1331	0.3221	1.0258	1.2114	1.1713	1.1337
2178			1-oleoyl-GPE (18:1)	LC/MS pos late	41220		HMDB11506	9547071	1.04	0.5367	0.5363	1.0622	1.1089	1.0974	1.0986
2180			1-linoleoyl-GPE (18:2)*	LC/MS pos late	35628		HMDB11507	52925130	1.13	0.2856	0.4347	1.0054	1.1319	1.0960	1.1822
2191			1-arachidonoyl-GPE (20:4n6)*	LC/MS pos late	36800		HMDB11517	42807465	1.15	0.1331	0.3221	1.0149	1.1637	1.1229	1.1678
2211			1-palmitoyl-GPE (16:0)*	LC/MS neg	35186			3300276	1.04	0.7738	0.5995	0.9811	1.0233	0.9691	1.1257
2213			1-stearoyl-GPG (18:0)	LC/MS neg	45970				1.20	0.6943	0.5722	0.8211	0.9827	0.9473	0.9013
2215			1-oleoyl-GPG (18:1)*	LC/MS neg	34437				0.76	0.2257	0.3941	0.7111	0.5414	0.4951	0.4599
2217			1-linoleoyl-GPG (18:2)*	LC/MS neg	45968				1.37	0.2805	0.4336	1.0916	1.4922	1.4192	1.3791
2218			1-palmitoyl-GPI (16:0)	LC/MS neg	54885		HMDB61695		1.23	0.2804	0.4196	1.0523	1.2966	1.2799	1.3847
2221			1-stearoyl-GPI (18:0)	LC/MS pos late	35305		HMDB61696		0.92	0.5140	0.5251	1.0524	0.9673	0.9941	0.9375
2223			1-oleoyl-GPI (18:1)*	LC/MS neg	19324				1.15	0.2118	0.3810	0.9742	1.1189	1.1066	1.1281
2225			1-linoleoyl-GPI (18:2)*	LC/MS neg	36602				1.13	0.4288	0.4934	1.0480	1.1856	1.1608	1.2837
2229			1-arachidonoyl-GPI (20:4)*	LC/MS neg	36594		HMDB61690		1.16	0.2384	0.4063	1.0241	1.1887	1.1586	1.0962
2322			1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*	LC/MS pos late	34214		HMDB11342		1.26	0.0411	0.1800	0.9965	1.2560	1.1888	1.1133
2323			1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*	LC/MS pos late	52477		HMDB11343		1.25	0.0917	0.2700	1.0325	1.2870	1.2158	1.0941
2324			1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	LC/MS pos late	52677		HMDB11206	11146967	1.13	0.2295	0.3961	1.0068	1.1424	1.1248	1.1986
2325			1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*	LC/MS pos late	52716		HMDB11207		1.11	0.7334	0.5888	1.0295	1.1435	1.1005	1.1482
2326			1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	LC/MS pos late	52713		HMDB11352		1.10	0.4281	0.4934	1.0314	1.1339	1.0970	0.9789
2328			1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	LC/MS pos late	52673				1.04	0.9100	0.6250	1.0001	1.0395	1.0233	1.0331
2330			1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	LC/MS pos late	52478		HMDB11375		1.28	0.0698	0.2449	1.0579	1.3553	1.3004	1.1807
2331			1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*	LC/MS pos late	52614		HMDB11376		1.32	0.0706	0.2460	1.0200	1.3425	1.2967	1.1836
2334			1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	LC/MS pos late	52748		HMDB11220		1.10	0.4072	0.4827	1.0246	1.1300	1.1142	1.0928
2335			1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	LC/MS pos late	52689		HMDB11211		1.09	0.6712	0.5737	1.0350	1.1291	1.1000	1.1380
2339			1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	LC/MS pos late	52682		HMDB05779	9547058	1.10	0.4687	0.5059	1.0514	1.1543	1.1457	0.9935
2354			1-(1-enyl-palmitoyl)-GPC (P-16:0)*	LC/MS pos late	52475		HMDB10407	10917802	1.06	0.5860	0.5529	1.0598	1.1278	1.1347	1.0512
2355			1-(1-enyl-palmitoyl)-GPE (P-16:0)*	LC/MS pos late	52474				1.04	0.7489	0.5938	1.0425	1.0839	1.0784	0.9788
2357			1-(1-enyl-oleoyl)-GPE (P-18:1)*	LC/MS pos late	39270				1.06	0.6567	0.5708	1.0557	1.1235	1.1295	1.0091
2359			1-(1-enyl-stearoyl)-GPE (P-18:0)*	LC/MS pos late	44621				1.05	0.7468	0.5938	1.0918	1.1487	1.1721	0.9961
2362			glycerol	LC/MS neg	39271	C00116	HMDB00131	753	1.15	0.1380	0.3283	1.0230	1.1789	1.1296	1.2386
2363			glycerol 3-phosphate	LC/MS pos early	15122	C00093	HMDB00126	754	1.08	0.3626	0.4613	1.0562	1.1429	1.1020	1.1720
2369			1-myristoylglycerol (14:0)	LC/MS neg	43947	C01885	HMDB11561	79090	0.84	0.5278	0.5310	1.1599	0.9676	1.0222	1.1187
2372			1-palmitoylglycerol (16:0)	LC/MS neg	35625		HMDB31074	14900	0.74	0.8480	0.6084	2.4992	1.8433	1.6974	1.7563
2373			1-palmitoleoylglycerol (16:1)*	LC/MS neg	21127		HMDB11565		1.04	0.7494	0.5938	1.2758	1.3224	1.4370	1.5418
2376			1-oleoylglycerol (18:1)	LC/MS neg	52431		HMDB11567	5283468	0.86	0.9363	0.6345	1.2496	1.0705	1.0938	0.9976
2377			1-linoleoylglycerol (18:2)	LC/MS neg	21184			5283469	0.90	0.9090	0.6250	1.2529	1.1245	1.1005	1.1309
2378			1-linolenoylglycerol (18:3)	LC/MS neg	27447		HMDB11569	53480978	0.51	0.0090	0.0953	1.4045	0.7167	0.8626	0.7278
2382			1-dihomo-linolenylglycerol (20:3)	LC/MS neg	34393				1.06	0.4944	0.5147	1.0424	1.1072	1.0613	1.1454
2383			1-arachidonylglycerol (20:4)	LC/MS neg	48341	C13857	HMDB11549	5282281	0.91	0.8460	0.6083	1.1501	1.0498	1.0528	1.0007
2386			1-docosahexaenylglycerol (22:6)	LC/MS neg	34397		HMDB11587		0.99	0.7948	0.6033	1.0422	1.0274	1.1035	1.0559
2388			2-palmitoylglycerol (16:0)	LC/MS neg	35153		HMDB11533	123409	0.75	0.5472	0.5430	1.6566	1.2433	1.1603	1.3344
2391			2-oleoylglycerol (18:1)	LC/MS neg	33419		HMDB11537	5319879	0.77	0.4734	0.5079	1.2087	0.9302	0.9562	0.9444

2392		2-linoleoylglycerol (18:2)	LC/MS neg	21232		HMDB11538	5365676	0.82	0.6481	0.5690	1.2214	0.9972	0.9981	1.0302
2395		2-docosahexaenoylglycerol (22:6)*	LC/MS neg	32506		HMDB11557		0.94	0.7965	0.6038	0.8806	0.8238	0.8784	0.7997
2402		1-dihomo-linoleoylglycerol (20:2)	LC/MS neg	48675				0.48	0.0587	0.2220	1.3005	0.8233	0.6922	0.7108
2404		diacylglycerol (12:0/18:1, 14:0/16:1, 16:0/14:1) [2]*	LC/MS pos late	35103				2.48	0.7736	0.5995	1.2698	3.1475	3.0311	5.1151
2405		diacylglycerol (14:0/18:1, 16:0/16:1) [1]*	LC/MS pos late	55001				1.26	0.7159	0.5865	2.0776	2.8237	2.7679	3.7978
2406		diacylglycerol (14:0/18:1, 16:0/16:1) [2]*	LC/MS pos late	54953				1.41	0.8994	0.6250	1.8308	2.5862	2.6854	3.7466
2407		diacylglycerol (16:1/18:2 [2], 16:0/18:3 [1])*	LC/MS pos late	54954				0.86	0.5641	0.5475	1.2690	1.0969	1.1928	1.2399
2418		palmitoyl-palmitoyl-glycerol (16:0/16:0) [1]*	LC/MS pos late	54966		HMDB07098		1.90	0.6267	0.5658	0.8967	1.7060	1.6174	2.7092
2419		palmitoyl-palmitoyl-glycerol (16:0/16:0) [2]*	LC/MS pos late	54991		HMDB07098		1.89	0.8434	0.6073	1.3431	2.5391	2.4086	4.0550
2422		palmitoyl-oleoyl-glycerol (16:0/18:1) [1]*	LC/MS pos late	54990	C13861	HMDB07102		1.07	0.9923	0.6500	1.5379	1.6480	1.6826	1.9889
2423		palmitoyl-oleoyl-glycerol (16:0/18:1) [2]*	LC/MS pos late	54943	C13861	HMDB07102		1.07	0.9572	0.6386	1.5294	1.6337	1.6762	1.9959
2424		palmitoyl-linoleoyl-glycerol (16:0/18:2) [1]*	LC/MS pos late	54942		HMDB07103	9543695	0.82	0.8301	0.6058	1.5512	1.2735	1.2038	1.2319
2425		palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*	LC/MS pos late	52633		HMDB07103		0.96	0.9569	0.6386	1.4123	1.3510	1.3567	1.5190
2427		palmitoleoyl-oleoyl-glycerol (16:1/18:1) [1]*	LC/MS pos late	52634		HMDB07131	9543694	0.83	0.5634	0.5475	1.5567	1.2928	1.5048	1.4511
2428		palmitoleoyl-oleoyl-glycerol (16:1/18:1) [2]*	LC/MS pos late	52632				0.79	0.6313	0.5662	1.7245	1.3576	1.4836	1.2699
2429		palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]*	LC/MS pos late	52631		HMDB07132		0.76	0.4022	0.4811	1.2945	0.9865	1.0888	1.0469
2431		palmitoyl-arachidonoyl-glycerol (16:0/20:4) [1]*	LC/MS pos late	54967		HMDB07112		0.90	0.7970	0.6033	1.7011	1.5378	1.5487	1.9204
2432		palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]*	LC/MS pos late	54957		HMDB07112		0.79	0.9216	0.6285	2.0127	1.8657	1.7124	1.7595
2433		palmitoleoyl-arachidonoyl-glycerol (16:1/20:4) [2]*	LC/MS pos late	54958				0.82	0.6158	0.5637	1.2800	1.0523	1.2447	0.9737
2440		oleoyl-oleoyl-glycerol (18:1/18:1) [1]*	LC/MS pos late	57406		HMDB07218		0.83	0.4525	0.5027	1.3871	1.1461	1.1992	1.1000
2441		oleoyl-oleoyl-glycerol (18:1/18:1) [2]*	LC/MS pos late	54945		HMDB07218		0.81	0.4821	0.5126	1.3772	1.1214	1.1922	1.0783
2443		oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	LC/MS pos late	54946		HMDB07219		0.70	0.1503	0.3419	1.5813	1.1107	1.1343	1.0221
2444		oleoyl-linoleoyl-glycerol (18:1/18:2) [2]	LC/MS pos late	46798		HMDB07219		0.76	0.3578	0.4591	1.4330	1.0827	1.1217	0.9967
2448		linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]*	LC/MS pos late	46799		HMDB07248		0.65	0.1633	0.3488	1.5487	1.0143	1.0206	0.9614
2450		linoleoyl-linoleoyl-glycerol (18:2/18:3) [1]*	LC/MS pos late	54938		HMDB07249		0.48	0.0281	0.1494	2.0766	0.9954	1.0255	0.8893
2454		stearoyl-arachidonoyl-glycerol (18:0/20:4) [1]*	LC/MS pos late	54963				0.92	0.9618	0.6395	1.2177	1.1262	1.1280	1.0195
2455		stearoyl-arachidonoyl-glycerol (18:0/20:4) [2]*	LC/MS pos late	57450				0.90	0.4005	0.4811	1.1080	0.9928	1.0232	0.9189
2456		oleoyl-arachidonoyl-glycerol (18:1/20:4) [1]*	LC/MS pos late	57449		HMDB07228		0.82	0.8276	0.6058	1.2611	1.0396	1.0896	1.0263
2457		oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]*	LC/MS pos late	54960		HMDB07228		0.83	0.8431	0.6073	1.2543	1.0457	1.1164	1.0472
2458		linoleoyl-arachidonoyl-glycerol (18:2/20:4) [1]*	LC/MS pos late	54961		HMDB07257		0.69	0.2618	0.4196	1.4182	0.9849	1.0650	0.9058
2459		linoleoyl-arachidonoyl-glycerol (18:2/20:4) [2]*	LC/MS pos late	54955		HMDB07257		0.72	0.9812	0.6459	1.3319	0.9600	1.0390	0.9635
2462		linoleoyl-docosahexaenoyl-glycerol (18:2/22:6) [1]*	LC/MS pos late	54956				0.72	0.2871	0.4347	1.2598	0.9037	0.9801	1.0239
2486		sphinganine	LC/MS pos late	54949	C00836	HMDB00269	3126	1.17	0.0226	0.1329	0.9378	1.1002	1.0593	1.1861
2487	Sphingolipid Synthesis	sphinganine-1-phosphate	LC/MS pos late	17789		HMDB01383	520	1.35	0.0211	0.1290	0.9733	1.3093	1.2620	1.3814
2492		N-palmitoyl-sphinganine (d18:0/16:0)	LC/MS pos late	52605		HMDB11760	5283572	1.05	0.9327	0.6328	1.0399	1.0883	1.0710	1.2275
2493	Dihydroceramides	N-stearoyl-sphinganine (d18:0/18:0)*	LC/MS pos late	52604			5283573	1.28	0.4939	0.5147	1.1687	1.5002	1.4314	1.8213
2500		N-palmitoyl-sphingosine (d18:1/16:0)	LC/MS pos late	1759		HMDB04949	5283564	1.06	0.5232	0.5301	0.9871	1.0453	1.0543	1.1169
2503		N-stearoyl-sphingosine (d18:1/18:0)*	LC/MS pos late	44877		HMDB04950	5283565	1.03	0.9117	0.6250	1.2215	1.2623	1.1966	1.4318
2509		N-palmitoyl-sphingadineine (d18:2/16:0)*	LC/MS pos late	54979				1.18	0.0416	0.1802	0.9338	1.0993	1.0571	1.1584
2511		N-behenoyl-sphingadineine (d18:2/22:0)*	LC/MS pos late	57416				0.83	0.6158	0.5637	1.1628	0.9628	0.9584	0.9463
2512		N-nervonyl-sphingadiene (d18:2/24:1)*	LC/MS pos late	57372				0.92	0.7534	0.5938	1.1330	1.0424	1.0394	1.0975
2520		N-nervonyl-hexadecylsphingosine (d18:1/24:1)*	LC/MS pos late	57442				0.82	0.2831	0.4336	1.1482	0.9440	0.9968	0.9805
2525		ceramide (d18:1/14:0, d16:1/16:0)*	LC/MS pos late	57435				1.11	0.3343	0.4524	0.9920	1.1037	1.1065	1.2301
2526		ceramide (d18:1/17:0, d17:1/18:0)*	LC/MS pos late	57432				1.08	0.4620	0.5047	1.1938	1.2841	1.2198	1.4756
2528		ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)*	LC/MS pos late	57434				0.91	0.5840	0.5529	1.1204	1.0153	1.0158	0.9952
2534		glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	LC/MS pos late	57440				1.20	0.2557	0.4195	0.9500	1.1430	1.1676	1.1602
2535		glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	LC/MS pos late	53013				1.07	0.6338	0.5662	1.0186	1.0873	1.0863	1.0799
2541		glycosyl-N-(2-hydroxynervonyl)-sphingosine (d18:1/24:1(2OH))	LC/MS pos late	52234				0.94	0.9181	0.6278	1.1241	1.0578	1.0584	1.1028
2555		glycosyl ceramide (d18:1/20:0, d16:1/22:0)*	LC/MS pos late	57444				1.11	0.4630	0.5047	0.9772	1.0865	1.0634	1.0798
2559		glycosyl ceramide (d18:2/24:1, d18:1/24:2)*	LC/MS pos late	57595				1.09	0.6881	0.5810	1.0261	1.1233	1.1451	1.1203
2561		lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)	LC/MS pos late	57453				1.24	0.0163	0.1152	0.9233	1.1431	1.1290	1.2045
2565	Lactosylceramides (LCER)	lactosyl-N-nervonyl-sphingosine (d18:1/24:1)*	LC/MS pos late	53010				1.30	0.0598	0.2248	0.9561	1.2466	1.2328	1.2332
2572		myristoyl dihydrosphingomyelin (d18:0/14:0)*	LC/MS pos late	57370		HMDB12085		1.17	0.2752	0.4302	0.9055	1.0559	1.0590	1.1279
2573		palmitoyl dihydrosphingomyelin (d18:0/16:0)*	LC/MS pos late	57365			9909965	1.10	0.3527	0.4591	0.9551	1.0513	1.0642	1.1033

2574	Dihydrospingomyelins	behenoyl dihydrospingomyelin (d18:0/22:0)*	LC/MS pos late	52434		HMDB12091		1.06	0.8036	0.6040	1.1163	1.1792	1.2150	1.2056
2575		sphingomyelin (d18:0/18:0, d19:0/17:0)*	LC/MS pos late	57331		HMDB12087		1.11	0.7555	0.5938	1.0579	1.1772	1.1654	1.2963
2576		sphingomyelin (d18:0/20:0, d16:0/22:0)*	LC/MS pos late	57473				1.15	0.7905	0.6033	1.1274	1.2931	1.3176	1.4794
2577		palmitoyl sphingomyelin (d18:1/16:0)	LC/MS pos late	57476			9039941	1.05	0.3900	0.4792	0.9767	1.0275	1.0278	1.0292
2579		stearoyl sphingomyelin (d18:1/18:0)	LC/MS pos late	37506	C00550	HMDB01348	6453725	0.96	0.6372	0.5662	1.0551	1.0165	0.9975	1.0232
2580		behenoyl sphingomyelin (d18:1/22:0)*	LC/MS pos late	19503		HMDB12103		1.09	0.3925	0.4792	0.9776	1.0691	1.0741	1.1008
2581		tricosanoyl sphingomyelin (d18:1/23:0)*	LC/MS pos late	48492		HMDB12105		1.13	0.4670	0.5051	0.9792	1.1053	1.1025	1.1548
2582		lignoceroyl sphingomyelin (d18:1/24:0)	LC/MS pos late	52436				1.09	0.6401	0.5662	1.0141	1.1016	1.1134	1.1314
2583		sphingomyelin (d18:2/18:1)*	LC/MS pos late	57330				1.13	0.3367	0.4524	1.0035	1.1310	1.0851	1.0324
2584		sphingomyelin (d18:2/23:1)*	LC/MS pos late	57474				1.06	0.7434	0.5933	1.0005	1.0572	1.0601	1.1079
2585		sphingomyelin (d18:2/24:2)*	LC/MS pos late	57482				0.97	0.6261	0.5656	1.0118	0.9818	0.9550	0.9666
2587		sphingomyelin (d18:1/14:0, d16:1/16:0)*	LC/MS pos late	57479		HMDB12097	1143362	1.03	0.6201	0.5637	0.9869	1.0157	1.0329	1.0080
2588		sphingomyelin (d18:2/14:0, d16:1/14:1)*	LC/MS pos late	42463				1.02	0.7070	0.5845	1.0375	1.0570	1.0440	1.0689
2589		sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*	LC/MS pos late	47154				1.05	0.5267	0.5310	1.0302	1.0811	1.0669	1.1130
2590		sphingomyelin (d17:2/16:0, d18:2/15:0)*	LC/MS pos late	52433				1.05	0.6005	0.5629	0.9826	1.0308	1.0314	1.0353
2591		sphingomyelin (d18:2/16:0, d18:1/16:1)*	LC/MS pos late	57483				1.06	0.4433	0.4988	1.0188	1.0761	1.0575	0.9809
2592	Sphingomyelins	sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	LC/MS pos late	42459				1.01	0.8142	0.6058	0.9905	1.0045	0.9895	1.0451
2593		sphingomyelin (d18:1/18:1, d18:2/18:0)	LC/MS pos late	52615		HMDB12101	644382	1.00	0.9738	0.6446	1.1095	1.1045	1.0618	1.0713
2594		sphingomyelin (d18:1/19:0, d19:1/18:0)*	LC/MS pos late	37529				1.04	0.8324	0.6058	1.0334	1.0750	1.0624	1.1189
2595		sphingomyelin (d18:1/20:0, d16:1/22:0)*	LC/MS pos late	57475		HMDB12102		0.98	0.7147	0.5865	1.0379	1.0211	1.0126	1.0289
2596		sphingomyelin (d18:1/22:1, d18:2/20:0)*	LC/MS pos late	48490				0.98	0.7267	0.5865	1.0483	1.0262	0.9941	1.0001
2597		sphingomyelin (d18:1/20:2, d18:2/20:1, d16:1/22:2)*	LC/MS pos late	48491				0.94	0.4411	0.4984	1.1203	1.0498	0.9979	0.9791
2598		sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*	LC/MS pos late	57481				1.07	0.6972	0.5837	1.0359	1.1073	1.1264	1.1462
2599		sphingomyelin (d18:2/21:0, d16:2/23:0)*	LC/MS pos late	52465				1.05	0.6966	0.5837	1.0186	1.0735	1.0734	1.0873
2600		sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*	LC/MS pos late	57480		HMDB12104		0.95	0.4186	0.4904	1.0310	0.9621	0.9970	0.9519
2601		sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:2)*	LC/MS pos late	48493				0.97	0.5999	0.5478	0.9765	0.9489	0.9512	0.9809
2602		sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*	LC/MS pos late	57477				1.08	0.5350	0.5359	0.9985	1.0791	1.0861	1.0856
2603		sphingomyelin (d18:1/24:1, d18:2/24:0)*	LC/MS pos late	52435		HMDB12107		0.98	0.6887	0.5810	1.0083	0.9922	1.0023	0.9951
2604		sphingomyelin (d18:2/24:1, d18:1/24:2)*	LC/MS pos late	47153				0.99	0.6410	0.5662	1.0205	1.0057	1.0019	1.0009
2605		sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, d19:1/24:0)*	LC/MS pos late	52437				1.04	0.8370	0.6058	1.0097	1.0464	1.0203	1.0518
2606	Sphingosines	sphingosine	LC/MS pos late	57478	C00319	HMDB00252	5353955	1.27	0.0308	0.1527	0.9104	1.1546	1.1026	1.2396
2608		sphingosine 1-phosphate	LC/MS polar	17747	C06124	HMDB00277	5283560	1.17	0.0961	0.2782	0.9432	1.1035	1.0892	1.1229
2622	Mevalonate Metabolism	3-hydroxy-3-methylglutarate	LC/MS polar	34445	C03761	HMDB00355	1682	1.04	0.7198	0.5865	1.2755	1.3210	1.2700	1.1019
2637		cholesterol	LC/MS pos late	531	C00187	HMDB00067	11025406	1.05	0.7708	0.5991	1.0236	1.0714	1.1033	1.1279
2648		7-alpha-hydroxy-3-oxo-4-cholestenone (7-Hcca)	LC/MS neg	63	C17337	HMDB12458	3081085	1.27	0.0109	0.0987	1.0499	1.3307	1.2354	1.2101
2650		3beta,7alpha-dihydroxy-5-cholestenone	LC/MS neg	36776	C17335		3081084	1.01	0.7074	0.5845	1.0356	1.0482	0.9892	0.9445
2651	Sterol	3beta-hydroxy-5-cholestenone	LC/MS neg	36803	C17333		165511	1.33	0.0258	0.1424	0.9690	1.2887	1.2171	1.2180
2661		4-cholesten-3-one	LC/MS pos late	54805	C00599	HMDB00921	91477	0.91	0.3410	0.4524	1.1336	1.0326	1.0599	1.0383
2662		beta-sitosterol	LC/MS pos late	38125	C01753	HMDB00852	222284	1.52	0.0725	0.2494	0.8499	1.2938	1.1985	1.1012
2664		campesterol	LC/MS pos late	27414	C01789	HMDB02869	173183	1.41	0.1774	0.3574	0.9721	1.3730	1.3289	1.1448
2683		pregnenolone sulfate	LC/MS neg	33997		HMDB00774	160574	0.85	0.1938	0.3668	1.3918	1.1881	1.1007	1.0289
2687		17alpha-hydroxypregnenolone 3-sulfate	LC/MS neg	38170		HMDB00416	152971	0.74	0.1804	0.3620	1.1398	0.8425	0.7945	0.8301
2693	Pregnenolone Steroids	21-hydroxypregnenolone disulfate	LC/MS neg	37482			134595	0.95	0.5259	0.5310	1.1942	1.1377	1.1433	0.9416
2699		pregnenediol sulfate (C21H34O5S)*	LC/MS neg	46115				0.89	0.2810	0.4338	1.2941	1.1434	1.0874	1.0409
2700		pregnenediol disulfate (C21H34O6S2)*	LC/MS neg	32619				0.99	0.6886	0.5708	1.0612	1.0552	1.0081	0.9018
2711		Sulpha-pregnan-3beta,20beta-diol monosulfate (1)	LC/MS neg	32582				1.63	0.4595	0.5041	1.4923	2.4394	2.1390	2.8809
2714		Sulpha-pregnan-3beta,20alpha-diol monosulfate (2)	LC/MS neg	37196				1.61	0.7711	0.5991	1.3099	2.1094	1.8802	2.6125
2720	Progestin Steroids	Sulpha-pregnan-3beta,20alpha-diol disulfate	LC/MS neg	37200				2.18	0.8733	0.6195	1.3400	2.9194	2.5486	4.2027
2723		pregnenediol-3-glucuronide	LC/MS neg	37198		HMDB10318	123796	1.43	0.9089	0.6250	1.6706	2.3880	2.2053	2.8656
2728		pregnenolone/allopregnenolone sulfate	LC/MS neg	40708				1.46	0.8151	0.6058	1.0769	1.5721	1.3833	1.7759
2737		corticosterone	LC/MS neg	48394	C02140	HMDB01547	5753	0.71	0.5107	0.5251	1.1600	0.8192	0.8170	0.8281
2742	Corticosteroids	cortisol	LC/MS neg	5983	C00735	HMDB00063	5754	0.80	0.2425	0.4106	1.2109	0.9709	0.9965	0.9195
2744		cortisone	LC/MS neg	1712	C00762	HMDB02802	222796	0.94	0.5014	0.5199	1.0293	0.9662	0.9993	0.9610
2747		tetrahydrocortisone	LC/MS neg	1769	C05470	HMDB00903	5966	0.88	0.4405	0.4984	0.8534	0.7477	0.6793	0.8344

3495			adenosine	LC/MS neg	2831	C00212	HMDB00050	60961	1.12	0.1210	0.3082	0.9242	1.0319	1.0190	1.0199
3496			adenine	LC/MS pos early	555	C00147	HMDB00034	190	0.97	0.7353	0.5888	1.0499	1.0214	0.9998	1.0339
3501		Purine Metabolism, Adenine containing	N1-methyladenosine	LC/MS pos early	554	C02494	HMDB03331	27476	0.94	0.4941	0.5147	1.0227	0.9631	0.9699	0.8913
3502			N6-methyladenosine	LC/MS pos early	15650		HMDB04044	1869	1.28	0.0172	0.1182	0.9464	1.2076	1.1467	1.2526
3511			N6-carbamoylthreonyladenosine	LC/MS neg	37114		HMDB41623	161496	1.02	0.6254	0.5658	1.0795	1.0990	1.0729	0.9584
3521			N6-succinyladenosine	LC/MS neg	35157		HMDB00912	165243	1.06	0.4839	0.5126	1.1063	1.1709	1.1509	1.0474
3529			guanosine	LC/MS neg	48130	C00387	HMDB00133	6802	0.68	0.3617	0.4613	1.3899	0.9434	1.1128	1.2316
3532		Purine Metabolism, Guanine containing	7-methylguanine	LC/MS pos early	1573	C02242	HMDB00897	11361	0.94	0.4857	0.5126	1.0497	0.9878	0.9872	0.9220
3536			N2N2-dimethylguanosine	LC/MS pos early	35114		HMDB04824	92919	0.97	0.7964	0.6033	1.0877	1.0520	1.0441	0.9971
3550	Nucleotide		dihydroorotate	LC/MS polar	35137	C00337	HMDB03349	648	0.83	0.2947	0.4397	1.3086	1.0920	1.0897	0.9845
3551		Pyrimidine Metabolism, Orotate containing	orotate	LC/MS polar	601	C00295	HMDB00226	967	0.72	0.2752	0.4302	1.4380	1.0411	1.0147	0.9565
3553			orotidine	LC/MS polar	1505		HMDB00788	92751	0.27	0.3684	0.4613	4.1643	1.1039	1.0625	0.9848
3563			uridine	LC/MS neg	35172	C00299	HMDB00296	6029	1.13	0.0296	0.1494	0.9559	1.0830	1.0585	1.0076
3564			uracil	LC/MS polar	606	C00106	HMDB00300	1174	1.36	0.0001	0.0039	0.8620	1.1748	1.1373	1.1408
3565			isoadouridine	LC/MS neg	605	C02067	HMDB00767	15047	0.92	0.5380	0.5248	1.1482	1.0614	1.0521	0.9880
3568		Pyrimidine Metabolism, Uracil containing	5-methyluridine (ribothymidine)	LC/MS neg	33442		HMDB00884	445408	1.02	0.6614	0.5708	1.0289	1.0524	1.0066	1.0111
3579			Z-deoxyuridine	LC/MS neg	35136	C00526	HMDB00012	13712	1.48	0.0038	0.6038	0.9370	1.3152	1.2803	1.1564
3582			3-ureidopropionate	LC/MS pos early	1412	C02642	HMDB00026	111	1.14	0.3073	0.4461	0.9857	1.1280	1.1128	1.1502
3583			beta-alanine	LC/MS pos early	3155	C00099	HMDB00056	239	1.06	0.2533	0.4195	0.9648	1.0273	1.0211	1.0325
3584			N-acetyl-beta-alanine	LC/MS neg	55	C01073		76406	1.14	0.0997	0.2819	0.9713	1.1057	1.0371	1.0837
3594			cytidine	LC/MS neg	37432	C00475	HMDB00089	6175	0.75	0.1449	0.3340	1.2147	0.9107	0.9222	0.8597
3595		Pyrimidine Metabolism, Cytidine containing	cytosine	LC/MS pos early	514	C00380	HMDB00630	597	0.75	0.6907	0.5810	1.5359	1.1585	1.0775	1.2103
3596			3-methylcytidine	LC/MS pos early	573			159649	1.00	0.9738	0.6446	1.0539	1.0497	1.0292	1.0320
3598			N4-acetylcytidine	LC/MS neg	35132		HMDB05923	107461	0.79	0.4866	0.5126	1.0030	0.7959	0.8159	0.6889
3605			Z-O-methylcytidine	LC/MS pos early	35130			150971	0.99	0.8301	0.6058	1.0119	0.9990	0.9817	0.9759
3617		Pyrimidine Metabolism, Thymine containing	5,6-dihydrothymine	LC/MS neg	57564	C00906	HMDB00079	93556	1.19	0.1626	0.3488	0.8936	1.0610	1.0661	0.9840
3619			3-aminoisobutyrate	LC/MS pos early	1418	C05145	HMDB03911	64956	1.33	0.3347	0.4524	1.2128	1.6123	1.5703	1.6859
3637			quinoline	LC/MS pos early	1566	C03722	HMDB00232	1066	1.29	0.3545	0.4591	1.0201	1.3115	1.2745	1.3055
3641			nicotinamide	LC/MS pos early	1899	C00153	HMDB01406	936	1.10	0.3654	0.4613	0.9815	1.0802	1.0501	0.9746
3653		Nicotinate and Nicotinamide Metabolism	1-methylnicotinamide	LC/MS pos early	594	C02918	HMDB00699	10129685	1.04	0.9039	0.6250	1.0797	1.1254	1.1657	0.8960
3658			trigonelline (N'-methylnicotinate)	LC/MS pos early	27665	C01004	HMDB00875	5570	0.25	0.0000	0.0012	2.6560	0.6687	0.6092	0.5311
3660			N1-Methyl-2-pyridone-5-carboxamide	LC/MS pos early	32401	C05842	HMDB04193	69608	1.11	0.3207	0.4524	1.1157	1.2366	1.2396	1.0792
3661			N1-Methyl-4-pyridone-3-carboxamide	LC/MS pos early	40469	C05843	HMDB04194	440810	1.04	0.5945	0.5595	1.1335	1.1772	1.1762	0.9775
3665		Riboflavin Metabolism	riboflavin (Vitamin B2)	LC/MS neg	57594	C00255	HMDB00244	493570	0.72	0.7303	0.5872	2.0914	1.5081	1.5691	1.5755
3668		Pantothenate and CoA Metabolism	pantothenate	LC/MS neg	1827	C00864	HMDB00210	6613	1.04	0.9103	0.6250	1.0378	1.0791	1.0879	0.8751
3681			threonate	LC/MS polar	1508	C01620	HMDB00943	151152	1.16	0.1028	0.2856	0.9366	1.0851	1.0872	1.0301
3684		Ascorbate and Aldarate Metabolism	oxalate (ethanedioate)	LC/MS neg	27738	C00209	HMDB02329	971	1.10	0.1931	0.3668	0.9444	1.0383	1.0401	0.9580
3685			gulonate*	LC/MS polar	20694	C00257	HMDB03290	9794176	1.05	0.4298	0.4934	1.1075	1.1669	1.1018	1.0742
3687			alpha-tocopherol	LC/MS pos late	46957	C02477	HMDB01893	14985	0.84	0.0233	0.1341	1.0857	0.9103	0.9503	0.9157
3695			gamma-CEHC	LC/MS neg	1561		HMDB01931	133098	0.61	0.0043	0.0615	1.4697	0.8982	0.9574	0.8343
3696			gamma-CEHC glucuronide*	LC/MS neg	44676				0.59	0.0889	0.2674	1.0847	0.6405	0.7828	0.4098
3697		Tocopherol Metabolism	alpha-CEHC glucuronide*	LC/MS neg	42381				0.67	0.0849	0.2632	0.5580	0.3811	1.6654	0.3811
3698			alpha-CEHC sulfate	LC/MS neg	39346				0.59	0.1536	0.3451	1.0341	0.6098	1.3178	0.3678
3709	Cofactors and Vitamins		gamma-tocopherol/beta-tocopherol	LC/MS pos late	47696				1.02	0.9093	0.6052	1.0069	1.0255	0.9725	1.1609
3731			heme	LC/MS pos late	52473	C00032	HMDB03178	26945	2.55	0.2374	0.4058	0.6234	1.5919	1.3845	0.7645
3732			bilirubin (ZZ)	LC/MS pos late	41754	C00486	HMDB00054	5280352	1.02	0.9030	0.6250	0.9876	1.0066	0.9876	0.9585
3733			bilirubin (EE)*	LC/MS pos late	43807			5315454	1.06	0.8788	0.6207	1.0510	1.1114	1.0621	1.0420
3734		Hemoglobin and Porphyrin Metabolism	bilirubin (EZ or ZE)*	LC/MS pos late	32586		HMDB00488	5799469	0.97	0.6198	0.5637	1.0310	1.0050	1.0026	0.9560
3735			biliverdin	LC/MS pos late	47886	C00500	HMDB01008	5353439	1.56	0.3165	0.4524	1.2550	1.9605	1.7758	1.2959
3736			urobilinogen	LC/MS neg	2137	C05790	HMDB04157	26818	0.51	0.2962	0.4414	1.4816	0.7581	0.6663	0.5971
3738			L-urobilin	LC/MS pos late	32426	C05793	HMDB04159	5280818	0.90	0.7701	0.5991	0.6426	0.5782	0.4670	0.6835
3752			retinol (Vitamin A)	LC/MS pos late	40173	C00473	HMDB00305	445354	0.92	0.3186	0.4524	1.0681	0.9819	0.9895	0.9521
3754		Vitamin A Metabolism	carotene diol (1)	LC/MS pos late	1806				1.01	0.8004	0.6038	1.0537	1.0590	1.0765	1.1388
3755			carotene diol (2)	LC/MS pos late	57635				1.04	0.5795	0.5503	0.9851	1.0279	1.0236	1.0792

3756			carotene diol (3)	LC/MS pos late	57636				0.97	0.8310	0.6058	1.0064	0.9773	0.9957	0.9782
3758			beta-cryptoxanthin	LC/MS pos late	57637		HMDB33844	6384256	2.34	0.0617	0.2255	1.0525	2.4681	2.3271	2.9158
3771	Vitamin B6 Metabolism		pyridoxal	LC/MS pos early	57581	C00250	HMDB01545	1050	0.74	0.1679	0.3488	2.2180	1.6291	1.6450	1.1880
3772			pyridoxate	LC/MS neg	1651	C00847	HMDB00017	6723	0.64	0.0086	0.0047	1.7658	1.1264	1.0588	0.7066
3774			hippurate	LC/MS neg	31555	C01586	HMDB00714	464	0.52	0.0444	0.1866	1.7410	0.9012	0.8319	0.8014
3778			2-hydroxyhippurate (salicylurate)	LC/MS polar	15783	C07588	HMDB00840	10253	0.27	0.2056	0.3788	5.0419	1.3677	1.8714	0.9811
3780			3-hydroxyhippurate	LC/MS neg	18281		HMDB06116	450268	0.39	0.0039	0.0608	2.3223	0.8970	0.8607	0.7046
3782			4-hydroxyhippurate	LC/MS neg	39600		HMDB13678	151012	1.07	0.9149	0.6284	1.4973	1.6025	1.5490	1.6561
3786			benzoate	LC/MS neg	35527	C00180	HMDB01870	243	0.85	0.2604	0.4196	1.0568	0.8966	0.9161	0.8821
3798			4-hydroxybenzoate	LC/MS neg	15778	C00156	HMDB00500	135	1.29	0.1073	0.2870	0.9218	1.1866	1.0958	1.2092
3806			catechol sulfate	LC/MS neg	21133		HMDB59724	3083979	0.62	0.0135	0.1065	1.3413	0.8290	0.7512	0.7046
3809			guaiacol sulfate	LC/MS neg	35320		HMDB60013	22473	0.45	0.0004	0.0143	1.6297	0.7393	0.6747	0.7122
3810			3-methyl catechol sulfate (1)	LC/MS neg	46111				0.34	0.0025	0.0552	3.1599	1.0849	1.0168	1.3579
3812			4-methylcatechol sulfate	LC/MS neg	46165				0.85	0.8247	0.6058	1.4683	1.2517	1.2762	1.3818
3821			4-acetylphenol sulfate	LC/MS neg	46146			4684006	0.51	0.0795	0.2552	1.8592	0.9396	0.8565	1.3965
3824			4-ethylphenylsulfate	LC/MS neg	44620	C13637	HMDB62551		0.71	0.1253	0.3126	4.5771	3.2682	2.9174	4.9865
3825			4-vinylphenol sulfate	LC/MS neg	36089	C05627	HMDB62775	6426768	0.73	0.1681	0.3488	1.7447	1.2811	1.2192	1.3849
3837			3-methoxycatechol sulfate (1)	LC/MS neg	36088				1.19	0.6539	0.5708	1.1781	1.4051	1.4577	1.0104
3839			methyl-4-hydroxybenzoate sulfate	LC/MS neg	48783				0.46	0.4357	0.4983	3.4117	1.5594	1.9804	1.5227
3840			propyl 4-hydroxybenzoate	LC/MS neg	48429	D01422	HMDB32574	7175	0.97	0.8615	0.6152	1.0857	1.0572	1.0284	1.0633
3841			propyl 4-hydroxybenzoate sulfate	LC/MS neg	48480				1.15	0.7199	0.5805	0.9606	1.1075	1.1240	1.0037
3846			p-cresol sulfate	LC/MS neg	48460		HMDB11635	4615423	0.77	0.4976	0.6510	1.6391	1.2627	1.1925	1.4368
3853			o-cresol sulfate	LC/MS neg	36103			11615528	0.55	0.5561	0.5457	2.0532	1.1389	1.0499	0.9799
3857			3-(3-hydroxyphenyl)propionate sulfate	LC/MS neg	36845			187488	0.50	0.0125	0.1022	1.6244	0.8160	0.7682	0.7373
3860			3-(3-hydroxyphenyl)propionate	LC/MS neg	45415	C11457	HMDB00375	91	0.49	0.0037	0.0608	1.4436	0.7049	0.6693	0.5781
3862			3-phenylpropionate (hydrocinnamate)	LC/MS neg	36635	C05629	HMDB00764	107	0.55	0.1845	0.3648	1.1551	0.6327	0.5811	0.5705
3864			caffeine	LC/MS pos early	15749	C07481	HMDB01847	2519	0.25	0.0005	0.0172	3.1130	0.7918	0.6901	0.6236
3865			paraxanthine	LC/MS neg	569	C13747	HMDB01860	4687	0.45	0.0035	0.0608	1.8938	0.8554	0.7460	0.5219
3866			theobromine	LC/MS pos early	18254	C07480	HMDB02825	5429	0.94	0.4919	0.5147	1.3736	1.2904	1.1240	1.2906
3867			theophylline	LC/MS pos early	18392	C07130	HMDB01889	2183	0.41	0.0013	0.0319	2.1027	0.8566	0.7779	0.6898
3870			1,3-dimethylurate	LC/MS neg	18394		HMDB01857	70346	0.43	0.0013	0.0319	1.4533	0.6296	0.5740	0.4030
3871			1,7-dimethylurate	LC/MS neg	32391	C16356	HMDB11103	91611	0.40	0.0018	0.0423	1.6428	0.6579	0.5871	0.4183
3872			3,7-dimethylurate	LC/MS neg	34400	C16360	HMDB01982	83126	1.11	0.9808	0.6459	1.1835	1.3158	1.1700	1.1147
3873			1,3,7-trimethylurate	LC/MS neg	34399	C16361	HMDB02123	79437	0.26	0.0003	0.0118	1.8141	0.4757	0.4281	0.3360
3874			1-methylxanthine	LC/MS neg	34404	C16358	HMDB10738	80220	0.56	0.0042	0.0613	1.2844	0.7227	0.6374	0.5189
3875			3-methylxanthine	LC/MS neg	34389	C16357	HMDB01886	70639	0.80	0.1813	0.3626	1.4633	1.1738	1.0592	1.0348
3877			5-acetylamino-6-amino-3-methyluracil	LC/MS polar	32445	C16366	HMDB04400	88299	0.45	0.0085	0.0947	1.5948	0.7105	0.6458	0.4807
3878			5-acetylamino-6-formylamino-3-methyluracil	LC/MS polar	34424	C16365	HMDB11105	108214	0.56	0.0391	0.1741	1.5480	0.8681	0.7863	0.4986
3882			cotinine	LC/MS pos early	34401		HMDB01046	854019	0.50	0.4551	0.5037	15.6961	7.8826	9.9733	8.8569
3883			hydroxycotinine	LC/MS pos early	553		HMDB01390	10219774	0.21	0.8382	0.6058	0.3416	0.0722	0.1286	0.0307
3884			cotinine N-oxide	LC/MS pos early	38661		HMDB01411	9815514	0.76	0.2117	0.3810	0.5369	0.4055	0.4378	0.3965
3892			norricotine	LC/MS pos early	38662				0.74	0.1687	0.3488	0.4055	0.3002	0.3002	0.3002
3899			2-piperidinone	LC/MS pos early	38122		HMDB11749	12665	1.41	0.1133	0.2966	0.1079	1.4340	1.3401	1.7917
3893			2,3-dihydroxyisovalerate	LC/MS polar	43400	C04039	HMDB12141	677	0.17	0.0009	0.0257	3.9591	0.6703	0.8964	0.5409
3991			2-isopropylmalate	LC/MS polar	38276	C02504	HMDB00402	77	0.89	0.8373	0.6058	0.9789	0.8672	0.8179	1.2192
3992			2-oxindole-3-acetate	LC/MS pos early	15667		HMDB35514	3080590	1.05	0.1878	0.3668	0.7738	0.8228	0.8146	0.8657
4005			3-hydroxyindolin-2-one sulfate	LC/MS neg	40479				0.70	0.1901	0.3668	0.7912	0.5517	0.5222	0.6198
4012			batonicine	LC/MS pos early	48419	C08269	HMDB29412	164642	1.19	0.8502	0.6088	0.9329	1.1141	1.0873	1.5544
4017			gluconate	LC/MS polar	38100	C00257	HMDB00625	10690	0.92	0.9699	0.6502	1.1884	1.0967	1.0620	1.0042
4027			alliin	LC/MS pos early	587	C08265	HMDB33592	87310	0.48	0.0611	0.2255	2.2833	1.0869	0.9770	0.9844
4028			N-acetyllaiiin	LC/MS neg	41494				0.47	0.1247	0.3126	1.5707	0.7313	0.6769	0.6579
4061			cinnamoylglycine	LC/MS neg	45404		HMDB11621	706625	1.09	0.9573	0.6388	1.6304	1.7787	1.5402	1.6458
4086			dihydroferulate	LC/MS neg	38637			14340	1.42	0.6345	0.5682	1.4374	2.0462	1.9803	1.0810
4094			equol glucuronide	LC/MS neg	40481				0.77	0.1136	0.2966	0.6423	0.4920	0.4271	0.8325

4095			equol sulfate	LC/MS neg	41948				0.65	0.1112	0.2947	0.8961	0.5846	0.4964	1.0538
4096			ergothioneine	LC/MS pos early	40478	C05570	HMDB03045	3032311	0.63	0.0828	0.2612	1.3650	0.8571	0.9232	0.7960
4098			erythritol	LC/MS polar	37489	C00503	HMDB02994	222285	0.74	0.3177	0.4524	1.4840	1.0996	1.0611	0.9951
4103			ferulic acid 4-sulfate	LC/MS neg	20699		HMDB29200	6305674	0.88	0.4391	0.4983	1.3996	1.2386	1.1463	0.5024
4110			glycyrrhizinate	LC/MS neg	47114	C02283	HMDB11628	18526330	0.85	0.1995	0.3735	0.6923	0.5902	0.5902	0.5902
4125			homostachydrine*	LC/MS pos early	39789	C08283	HMDB33433	441447	0.80	0.2934	0.4392	1.1751	0.9381	0.9394	1.2653
4128			indolin-2-one	LC/MS pos early	33009	C12312		321710	1.06	0.5434	0.5403	0.9610	1.0166	0.9524	1.0872
4151			methyl indole-3-acetate	LC/MS pos early	43374		HMDB29738	74706	0.70	0.0181	0.1199	1.3542	0.9485	0.8520	1.2052
4154			N-(2-furoryl)glycine	LC/MS neg	1584		HMDB00439	21863	0.37	0.0112	0.0967	2.6460	0.9734	0.9324	0.8288
4159			naringenin 7-glucuronide	LC/MS neg	31536				1.90	0.3854	0.4749	0.4594	0.8744	0.7449	0.3910
4183			pipерine	LC/MS pos late	54924	C03882	HMDB29377	628024	0.94	0.3573	0.4591	1.6832	1.5759	1.4623	2.1093
4212			quinale	LC/MS polar	33935	C00296	HMDB03072	6508	0.30	0.0012	0.0319	3.7205	1.1156	0.9456	0.4748
4219			acesulfame	LC/MS neg	18335		HMDB33585	36573	2.44	0.3216	0.4524	1.3081	3.1938	2.7464	4.2246
4220			S-allylcysteine	LC/MS pos early	48569		HMDB34323	98280	0.45	0.1029	0.2856	1.5842	0.7162	0.6563	0.9800
4237			stachydrine	LC/MS pos early	43239	C10172	HMDB04827	115244	1.97	0.1370	0.3283	1.0642	2.0996	1.8623	1.7149
4245	Xenobiotics		tartrate	LC/MS neg	34384	C00898	HMDB00956	444305	0.60	0.9744	0.6446	1.7889	1.0701	1.0792	0.8358
4246			theanine	LC/MS pos early	15336	C01047	HMDB34365	439378	1.55	0.7017	0.5845	0.8367	1.2955	1.2014	1.2767
4249			thymol sulfate	LC/MS neg	22206	C09908	HMDB01878		2.13	0.2059	0.3788	1.8408	3.9201	8.3777	0.3305
4261			4-allylphenol sulfate	LC/MS neg	36095				1.84	0.6211	0.5637	1.8675	3.4427	3.0816	4.7984
4262			methyl glucopyranoside (alpha + beta)	LC/MS neg	37181				1.61	0.1836	0.3646	0.8992	1.4461	1.3603	0.8488
4289			4-vinylgalaic acid sulfate	LC/MS neg	46144				0.16	0.0404	0.1783	4.3193	0.6822	0.6350	0.6428
4290			pyrrolidine	LC/MS neg	48442		HMDB33143	122228	0.76	0.5984	0.5478	1.3860	1.0554	1.0140	0.8360
4293			daidzein sulfate (2)	LC/MS neg	48428				0.63	0.2275	0.3948	2.0940	1.3132	1.1760	1.7751
4295			eugeniol sulfate	LC/MS neg	48728			180632	0.14	0.0122	0.1013	3.9636	0.5588	0.9816	0.7254
4299			2-keto-3-deoxy-gluconate	LC/MS polar	48715	C00204	HMDB01353	161227	1.07	0.9406	0.6350	1.0314	1.1012	1.0630	0.8811
4301			isoeugenol sulfate	LC/MS neg	48141				0.74	0.5701	0.5478	0.7860	0.5706	0.6019	0.6168
4322			3,4-methylenediphenylate	LC/MS neg	48987				1.46	0.4714	0.5067	0.9600	1.3974	1.3181	1.1893
4375			caffeic acid sulfate	LC/MS polar	53026		HMDB41708		0.31	0.0023	0.0540	2.4962	0.7762	0.7653	0.4305
4379			tartronate (hydroxymalonate)	LC/MS neg	53254	C02287	HMDB35227	45	1.31	0.0038	0.0608	0.9499	1.2414	1.2004	1.1060
4412	Bacterial/Fungal		N-methylpiperidate	LC/MS pos early	20693			11286529	0.81	0.2050	0.3788	0.9276	0.7533	0.7224	0.6410
4436			4-acetamidophenol	LC/MS neg	47101	C06804	HMDB01859	1983	0.28	0.3306	0.4524	0.1404	0.0393	0.0393	0.0393
4437			3-(N-acetyl-L-cystein-S-yl) acetaminophen	LC/MS neg	12032			83967	1.00			1.0000	1.0000	1.0000	1.0000
4438			4-acetaminophen sulfate	LC/MS neg	45721	C06804	HMDB59911	83939	0.02	0.1681	0.3488	2.3665	0.0456	0.0456	0.0456
4439			4-acetamidophenylglucuronide	LC/MS neg	37475		HMDB10316	83944	0.43	0.3306	0.4524	0.1715	0.0741	0.0741	0.0741
4440			2-hydroxyacetaminophen sulfate*	LC/MS neg	15736			86290013	0.52	0.3306	0.4524	0.1971	0.1026	0.1026	0.1026
4441			2-methoxyacetaminophen sulfate*	LC/MS neg	33173			86290014	1.00			1.0000	1.0000	1.0000	1.0000
4442			2-methoxyacetaminophen glucuronide*	LC/MS neg	47031			14367271	1.00			1.0000	1.0000	1.0000	1.0000
4443			3-(cystein-S-yl)acetaminophen*	LC/MS pos early	33161			5233914	1.00			1.0000	1.0000	1.0000	1.0000
4463			salicylic acid glucuronide*	LC/MS neg	34365				0.31	0.0656	0.2333	1.7490	0.5371	0.7837	0.4252
4477			lidocaine	LC/MS pos late	33384	D00358	HMDB14426	3676	1.00			1.0000	1.0000	1.0000	1.0000
4478			N-ethylglycinexylidide	LC/MS pos early	35661	C16561	HMDB60656	24415	1.00			1.0000	1.0000	1.0000	1.0000
4519			flloxacin	LC/MS neg	33080	C07321	HMDB01929	4583	0.02	0.3306	0.4524	0.1070	0.0019	0.0019	0.0019
4601			metoprolol	LC/MS pos early	21320	D02358	HMDB01932	4171	1.00			1.0000	1.0000	1.0000	1.0000
4602			metoprolol acid mesilate*	LC/MS pos early	19037			62936	0.01	0.3306	0.4524	0.1063	0.0012	0.0012	0.0012
4603			alpha-hydroxymetoprolol	LC/MS pos early	34109		HMDB60994	114962	1.00			1.0000	1.0000	1.0000	1.0000
4617			warfarin	LC/MS neg	54738	C01541	HMDB01935		0.00	0.3306	0.4524	0.1057	0.0004	0.0004	0.0004
4619			hydrochlorothiazide	LC/MS neg	43335	C07041	HMDB01928	3639	1.00			1.0000	1.0000	1.0000	1.0000
4624			candesartan	LC/MS neg	39625	D00522 C07468	HMDB14934	2541	1.23	0.3343	0.4524	0.3838	0.4486	0.4345	0.3638
4625			valsartan	LC/MS neg	54749			5650	8.27	0.7499	0.5938	0.0535	0.4424	0.3688	0.8287
4626			lmesartan	LC/MS neg	48566	D05246	HMDB14420	158781	0.46	0.1630	0.3488	0.1920	0.0892	0.0892	0.0892
4627			enalapril	LC/MS pos late	53256			3222	1.00			1.0000	1.0000	1.0000	1.0000
4642			famotidine	LC/MS pos early	52949	D00318	HMDB01919	5702160	1.00			1.0000	1.0000	1.0000	1.0000
4644			omeprazole	LC/MS neg	42613	C07324	HMDB01913	4594	1.00			1.0000	1.0000	1.0000	1.0000
4652			metformin	LC/MS pos early	38600	C07151	HMDB01921	4091	0.84	0.3306	0.4524	0.4232	0.3553	0.3553	0.3553

4665																	
4674	Drug - Metabolic	rosuvastatin	LC/MS neg	38306	D01915	HMDB15230	446157	0.74	0.7227	0.5965	0.5043	0.3742	0.3668	0.3295			
4675		allopurinol riboside	LC/MS neg	40421				1.00			1.0000	1.0000	1.0000	1.0000			
4695		azypurinol	LC/MS polar	38321	D02365	HMDB00786	4644	1.00			1.0000	1.0000	1.0000	1.0000			
4734	Drug - Neurological	lanotrigine	LC/MS pos early	41726	D00354	HMDB14695 HMDB05043	3878	1.00			1.0000	1.0000	1.0000	1.0000			
4745		fluroxetine	LC/MS pos late	54762			60836	1.00			1.0000	1.0000	1.0000	1.0000			
4757	Drug - Psychoactive	quetiapine	LC/MS pos late	40450	C07397	HMDB05021	5002	1.00			1.0000	1.0000	1.0000	1.0000			
4772	Drug - Respiratory	diphenhydramine	LC/MS pos late	39787	C06960	HMDB01927	3100	1.00			1.0000	1.0000	1.0000	1.0000			
4776		salicylate	LC/MS neg	38669	C00805	HMDB01895	338	0.39	0.4263	0.4933	3.6577	1.4316	1.6402	1.1371			
4799	Drug - Topical Agents	hydroquinone sulfate	LC/MS neg	1515	C00530	HMDB02434	161220	1.06	0.7613	0.5968	1.5209	1.6075	1.5181	1.3403			
4841	Drug - Other	S-carboxymethyl-L-cysteine	LC/MS pos early	35322	C03727	HMDB29415	1080	0.10	0.0041	0.0613	5.6965	0.5632	0.6145	0.5167			
4848		diglycerol sulfate*	LC/MS neg	40700	C00059	HMDB01448	1118	0.93	0.3423	0.4524	1.0635	0.9875	0.9768	0.9300			
4851		D-sulfo-L-tyrosine	LC/MS neg	46960			514196	0.91	0.4881	0.5132	1.1253	1.0295	1.0189	0.9808			
4855		ethyl glucuronide	LC/MS neg	45413		HMDB10325	152226	0.09	0.0155	0.1152	3.8273	0.3540	0.3855	0.3508			
4867		3-acetylphenol sulfate	LC/MS neg	39603				0.48	0.0067	0.0791	1.0263	0.4950	0.4775	0.4659			
4869		2-aminophenol sulfate	LC/MS neg	48693		HMDB61116	181670	0.53	0.0296	0.1494	2.0453	1.0743	1.0142	0.6782			
4913		dimethyl sulfone	LC/MS pos early	43286	C11142	HMDB04983	6213	1.40	0.1091	0.2904	1.1653	1.6347	1.5325	2.0566			
4915		ectoine	LC/MS pos early	43424	C06231		126041	1.15	0.5135	0.5251	1.8424	2.1275	1.8428	2.9503			
4946	Chemical	perfluorooctanesulfonate (PFOS)	LC/MS polar	35651	C18142	HMDB59586	74483	1.15	0.3949	0.4798	1.0274	1.1837	1.1450	1.0713			
4955		succinimide	LC/MS polar	57564	C07273		11439	0.85	0.4851	0.5126	1.2888	1.0943	1.0432	0.9301			
4966		4-hydroxychlorothalonil	LC/MS neg	41888			34217	1.13	0.6044	0.5637	1.2067	1.3648	1.2988	1.2384			
4970		1,2,3-benzenetriol sulfate (2)	LC/MS neg	49441				1.81	0.7858	0.6012	0.8525	1.5392	1.6062	1.3206			
4972		2-methoxyresorcinol sulfate	LC/MS neg	49762				2.10	0.1713	0.3505	0.4923	1.0357	0.9521	1.1374			
4973		3-hydroxypyridine sulfate	LC/MS neg	49445				0.27	0.0002	0.0078	2.5205	0.6827	0.6042	0.6278			
4974		1,2,3-benzenetriol sulfate (1)	LC/MS neg	48448				3.53	0.0069	0.0791	0.4124	1.4576	1.5911	1.1603			
4983		6-hydroxyindole sulfate	LC/MS neg	48761				0.96	0.8015	0.6038	1.2551	1.2055	1.1572	1.2585			
4987		thioprotine	LC/MS pos early	48698			93176	1.01	0.7806	0.5968	1.0031	1.0175	1.0019	1.0185			