

Metabolomics Primary Metabolism	Annotated Metabolites Metabolite Name	Comparison 1: Metabolomic profiles across samples within unchanging ODMA-producer		Comparison 2: Metabolomic profiles across samples within changing ODMA-producer		Comparison 3: Metabolomics profiles across ODMA-producer and ODMA non-producer	
		Univariate p-value*	Fold Change	Univariate p-value*	Fold Change	Univariate p-value*	Fold Change
	1,2-anhydro-myo-inositol NIST	0.2129 (W)	1.1149	0.6953 (W)	0.92874	0.3885	0.8773
	2-deoxytetrone	0.8394 (W)	0.99511	0.1663	0.94381	0.2718	0.69295
	2-hydroxyglutaric acid	0.8516	0.98204	0.403	0.85449	0.6632	1.0886
	2,3-dihydroxybutanoic acid NIST	0.3649	0.90482	0.8186	0.97769	0.3039	1.2377
	3-3-hydroxyphenyl-3-hydroxypropionic acid nist	0.2367 (W)	1.3534	0.5031	0.82287	0.264	0.62139
	3-hydroxy-3-methylglutaric acid	0.8553 (W)	1.0453	0.2761	0.92717	0.7925	0.96754
	3-hydroxyphenylacetic acid	0.1867	0.8332	0.2918	0.88457	0.0894	0.35177
	3,4-dihydroxyhydrocinamic acid NIST	0.7806	0.95812	0.5388	0.98267	0.5880 (W)	0.99541
	4-hydroxybenzoate	0.9872	0.99836	0.786	1.0088	0.9403	0.86596
	4-hydroxyhippuric acid NIST	0.1086	0.80798	0.3991	1.1986	0.5736	0.59658
	4-hydroxyphenylacetic acid	0.3064	0.90081	0.1317	1.256	0.9806	0.87809
	5-hydroxy-3-indoleacetic acid	0.1565	0.88894	0.192	0.94829	0.7239	0.90997
	aconitic acid	0.0883	0.89166	0.3869	0.97327	0.7787	0.93064
	adipic acid	0.2	1.1972	0.5785	0.96008	0.1394	1.7226
	alanine	0.7331	1.0602	0.0474	0.82199	0.1552	1.7668
	alpha-ketoglutarate	0.1983	0.81602	0.5566 (W)	0.77547	0.5144	1.1892
	ascorbic acid	0.2676	0.68856	0.7695 (W)	1.4687	0.6578	0.73107
	benzoic acid	1.189	0.2026	0.1963	0.96823	0.7892	1.1239
	catechol	0.5158 (W)	0.82735	0.9219 (W)	1.6175	0.1146 (W)	1.1082
	citric acid	0.3085 (W)	0.95101	0.2798	1.4077	0.0502	0.73055
	conduiritol-beta-epoxide	0.8702 (W)	0.87264	0.9671	1.1158	0.1827 (W)	0.35642
	creatinine	0.2312	1.3579	0.0879	0.41718	0.3542	2.2723
	dehydroascorbic acid	0.7611 (W)	0.82755	0.3008	0.70712	0.0675 (W)	1.6724
	deoxypentitol	0.7611 (W)	1.0271	1.0000 (W)	0.79874	0.7688	0.97349
	diglycerol	0.6457	0.91682	0.1656	0.73649	0.1019	1.8641
	erythritol	0.5158 (W)	1.0443	0.7695 (W)	0.9186	0.4231	0.80388
	erythronic acid lactone	0.4429	0.92252	0.8905	1.1236	0.0968 (W)	1.1698
	fructose	0.5561 (W)	1.0722	0.4226	1.1045	0.6426 (W)	0.93055
	fucose	0.9038	0.99097	0.7695 (W)	1.0056	0.2414 (W)	0.97938
	fumaric acid	0.4587	1.0606	0.9344	0.90438	0.9925	0.98929
	galactonic acid	0.0231	1.5446	0.5188	1.004	0.8235	0.8927
	galactose	0.1460 (W)	1.7131	0.1934 (W)	1.525	0.705	0.15126
	gluconic acid	0.0729	1.5788	1.0000 (W)	0.89319	0.0904	1.098
	gluconic acid lactone	0.9587	0.99255	0.8457 (W)	0.95455	0.5936	0.8644
	glucose	0.2801 (W)	1.514	0.4402	1.5404	0.7573 (W)	0.033494
	glyceric acid	0.5342	0.93554	0.9769	1.2113	0.3672	1.1408
	glycerol	0.0767 (W)	0.88451	0.8386	1.1011	0.1348 (W)	1.196
	glycerol-3-galactoside	0.3882	1.2241	0.5422	1.8579	0.6921	1.0017
	glycerol-alpha-phosphate	0.7457 (W)	0.95065	0.9874	1.2466	0.1574 (W)	1.2677
	glycine	0.2286 (W)	1.1697	0.9636	0.74092	0.2747	1.3859
	glycolic acid	0.6120 (W)	0.93826	0.3337	0.65255	0.1053	1.6017
	hexitol	0.9696	0.99706	0.7652	0.95484	0.6166	0.78028
	hexuronic acid	0.7922 (W)	0.98538	0.9219 (W)	1.3021	0.7252	0.71907
	hydroxyproline dipeptide NIST	0.5953	0.8972	0.4202	1.7016	0.3542	0.78066
	hypoxanthine	0.2772	1.1547	0.5305	0.91604	0.4151	1.2144
	indole-3-acetate	0.8652	1.0162	0.9573	0.93413	0.2323	1.331
	indoxyl sulfate	0.3387 (W)	0.88386	0.5289	0.96825	0.4378 (W)	0.93198
	isocitric acid	0.1706 (W)	0.89743	0.7289	1.204	0.9852	0.99557
	isohexonic acid	0.661	1.0782	0.5724	1.1391	0.6532	0.78578
	isothreonic acid	0.6554 (W)	0.97332	0.1898	0.96716	0.7711	0.92996
	lactic acid	0.4771 (W)	0.86377	0.4922 (W)	1.2083	0.8773 (W)	0.73481
	levoglucosan	0.4954	0.83925	0.0763	0.67205	0.7562	1.2759
	lysine	0.9829	0.99695	0.8272	0.78482	0.2926	2.2159
	lyxitol	0.0405 (W)	1.4181	0.1934 (W)	1.1872	0.7126	0.80428
	malic acid	0.0094	0.81678	0.2803	0.75176	0.8314	1.033
	myo-inositol	0.4400 (W)	1.1254	0.6466	0.77904	0.0212	0.50663
	n-acetyl-d-hexosamine	0.4898 (W)	1.1625	0.4316 (W)	1.6223	0.8104	0.69175
	N-acetylaspatic acid	0.1772 (W)	0.95285	0.7225	1.0765	0.599	1.0419
	N-acetylmannosamine	0.3707 (W)	1.3086	0.2324 (W)	1.0462	0.8168 (W)	0.66037
	N-carbamylglutamate	0.5254	0.92589	0.339	0.94577	0.1348 (W)	1.7796
	oxalic acid	0.1267	0.77754	0.4981	0.82356	0.4693	0.88287
	oxoproline	0.5699 (W)	0.95738	0.0371	0.92547	0.1574 (W)	1.1828
	p-cresol	0.5213	0.87117	0.4923	0.89751	0.1661	0.60435
	p-tolyl glucuronide	0.4647	0.83614	0.5435	0.81591	0.5458	1.3762
	phenol	0.4727	0.89731	0.7557	0.89834	0.0837	2.1414
	phosphate	0.6850 (W)	1.0526	0.8809	1.0322	0.7016	1.0966
	pinitol	0.1004 (W)	0.78124	1.0000 (W)	0.94903	0.6992 (W)	1.2762
	pseudo uridine	0.5158 (W)	0.84595	0.2133	1.7376	0.5880 (W)	1.0689
	pyrogallol	0.1996	0.74685	0.3828	0.90645	0.6285	0.79404
	quinic acid	0.0405 (W)	0.82459	0.1934 (W)	1.0596	0.4066	0.6024
	ribitol	0.8921	0.98176	0.3661	1.0016	0.3507 (W)	1.0128
	ribonic acid	0.7611 (W)	1.0049	0.7318	1.1431	0.8652	0.91986
	ribose	0.7457 (W)	0.99862	0.8051	1.0839	0.6079	0.95425
	saccharic acid	0.4589	1.1392	0.4121	1.2878	0.4621	0.68372
	sorbitol	0.4522 (W)	1.2692	0.2754 (W)	1.138	1.0000 (W)	2.2569
	succinic acid	0.5699 (W)	1.1344	0.8592	0.7656	0.0436	0.60672
	sucrose	0.6335	0.90369	1.0000 (W)	1.3822	0.2657	1.3244
	tagatose	0.7149	1.0738	0.1709	1.2932	0.3518	0.57897
	tartaric acid	0.2286 (W)	1.5764	0.5566 (W)	0.60603	0.0557 (W)	0.091355
	threitol	0.9829	0.99575	0.3750 (W)	1.1516	0.5880 (W)	0.77451
	threonic acid	0.9354 (W)	0.99924	0.2324 (W)	0.99454	0.0968 (W)	0.76752
	threonine	0.8748	0.97976	0.6278	0.93943	0.0566	1.4549

## Biogenic amines

tryptophan	0.5779	1.0702	0.4149	0.94581	0.3661	1.3468
tyrosine	0.776	0.97873	0.1903	1.051	0.1597	1.2619
UDP-glucuronic acid	0.1706 (W)	1.1909	0.8457 (W)	1.1057	0.4854 (W)	1.3912
uracil	0.4296	1.1024	0.6762	0.73503	0.5268	1.0684
urea	0.5978 (W)	0.92392	0.9802	1.5241	0.4854 (W)	0.9752
uric acid	0.1649	0.8761	0.154	1.2553	0.9385 (W)	1.2847
xanthine	0.3838	0.91037	0.2864	1.1897	0.2523	1.2468
xylitol	0.7457 (W)	1.1334	0.9219 (W)	0.80175	0.8168 (W)	3.0296
xylose	0.173	1.1742	0.5006	1.1969	0.0205	0.50058
xylose NIST	0.8236 (W)	1.0328	0.6953 (W)	0.94612	0.3929 (W)	1.1818
1_15N2-L-Arginine iSTD	0.6853	0.97849	0.2116	1.1388	0.0385	0.8163
1_D3-AC20 iSTD	0.0024 (W)	0.91969	0.7963	1.0215	0.7476	0.99779
1_D3-Creatine iSTD	0.1191 (W)	1.1649	0.8774	1.0748	0.9231	0.98751
1_D3-Creatinine iSTD	0.3184 (W)	1.0482	0.6953 (W)	1.0327	0.7926	0.83239
1_D3-DL-Alanine iSTD	0.3599 (W)	1.0199	1.0000 (W)	1.0209	0.3922	1.0026
1_D3-DL-Aspartic acid iSTD	0.3783	0.96615	0.5412	0.99616	0.9069	0.97645
1_D3-DL-Glutamic acid iSTD	0.5158 (W)	1.0207	0.7002	1.0132	0.7158	0.95445
1_D3-Histamine, N-methyl- iSTD	0.1772 (W)	0.93301	0.943	0.91696	0.491	1.0366
1_D3-L-Carnitine iSTD	0.0012 (W)	0.90418	0.9219 (W)	1.047	1.0000 (W)	1.0594
1_D5-L-Glutamine iSTD	0.4045 (W)	0.96294	0.142	1.0463	0.4378 (W)	1.0141
1_D9-Betaine iSTD	0.0037 (W)	0.92276	0.4316 (W)	1.0278	0.8168 (W)	0.91858
1_D9-Butyrobaine iSTD	0.0037 (W)	0.91599	0.4561	1.0044	0.1696	1.0246
1_D9-Choline iSTD	0.0175 (W)	0.92836	0.2752	1.0001	0.8168 (W)	1.0243
1_D9-Crotonobetaine iSTD	0.0087 (W)	0.92589	1.0000 (W)	0.99559	0.8773 (W)	0.98847
1_D9-TMAO iSTD	0.0175 (W)	0.8988	0.6953 (W)	1.0128	0.3114 (W)	1.0057
1_Val-Tyr-Val iSTD	0.0185 (W)	0.91922	0.6250 (W)	1.0032	0.8453	0.99289
2-oxo-2,3-dihydro-1H-indol-3-ylacetic acid	0.6918 (W)	0.84113	0.8572	0.61053	0.8168 (W)	1.024
3-Carboxypropyltrimethylammonium cation	0.1519 (W)	1.403	0.9603	0.39553	0.4387	2.7704
R-Butylcamitine	0.3387 (W)	0.906	0.5557	0.80009	0.5787	1.0806
S-Colinine N-oxide	0.98631	0.7151 (W)	0.1779	0.93569	0.0085	3.5055
gamma-Aminobutyric acid	0.7000 (W)	0.91298	0.2237	0.89876	0.4869	0.94136
1,3-Cyclohexanedione	0.1407	0.78432	0.3750 (W)	0.85728	0.8773 (W)	0.88206
1,3,7-Trimethyluric acid	0.9838 (W)	0.80842	0.0273 (W)	0.36896	0.6614	1.6504
1,4-Cyclohexanedicarboxylic acid	0.0764	1.2572	0.3832	0.88038	0.3747	0.90771
1-Acetylimidazole	0.7303 (W)	0.89961	0.0488 (W)	0.86445	0.6992 (W)	0.72385
1-Aminocyclohexanecarboxylic acid	0.472	0.84282	0.4535	0.84206	0.8999	0.45352
1-Methyladenosine	0.5978 (W)	0.83841	0.8457 (W)	1.014	0.5128	0.98336
1-Methylnicotinamide	0.9515 (W)	0.90709	0.4086	0.80836	0.1149	1.0666
1-Methyluric acid	0.1347 (W)	0.71624	0.7461	1.1774	0.8217	0.58093
2,2',2''-Nitrilotriethanol	0.1048 (W)	0.72738	0.302	0.67248	0.8292	3.2023
2,8-Quinolinediol	0.7457 (W)	1.0096	0.5399	0.80822	0.2986	0.9222
2-Acetylpyrazine	0.0405 (W)	0.72717	0.6953 (W)	0.96037	0.5874	1.6645
2-Amino-2-methyl-1,3-propanediol	0.3931 (W)	0.82994	0.6546	0.89256	0.9454	0.9266
2-Aminoethylphosphonic acid	0.0423 (W)	1.6124	0.8478	1.0996	0.0701	0.6176
2-Aminophenol	0.6839	1.069	0.4316 (W)	1.5711	0.3929 (W)	0.44126
2'-Deoxyguanosine	0.7922 (W)	0.92343	0.7922 (W)	0.77973	0.1654	0.59602
2-Hydroxy-4-methoxybenzaldehyde	0.2129 (W)	0.74405	0.1934 (W)	0.73277	0.0035	0.59602
2'-O-Methylguanosine	0.1004 (W)	0.97254	0.1602 (W)	1.0298	0.1414	0.8832
2'-O-Methylinosine	0.0262 (W)	1.536	0.5566 (W)	1.0165	0.5356 (W)	0.68256
2-Phosphonobutyric acid	0.0440 (W)	2.3911	0.7695 (W)	1.2127	0.6992 (W)	---
2-Propenenitrile, 3,4-1,1-dimethylethylphenylsulfonyl-, 2E-	0.1840 (W)	1.2045	0.9563	0.84934	0.3633	0.7762
2-Pyridone	0.7457 (W)	0.94647	1.0000 (W)	0.94695	0.8402	0.85694
2-Pyridylacetic acid	0.5352	1.2234	0.266	1.9591	0.8868	0.95371
2S-Amino-4E-pentadecene-1,3R-diol	0.9144	0.94861	0.8232	0.696	0.8198	0.52778
3-1-Pyrazolyl-alanine	0.1324	0.6757	0.2756	1.10179	0.8412	0.66469
3,4-Dimethoxybenzaldehyde	0.5425 (W)	0.90562	0.579	0.67982	0.7583	0.3406
3,5-Dihydroxyphenylglycine	0.9365 (W)	1.3758	0.9656	0.66662	0.8773 (W)	1.2089
3-Aminotyrosine	0.2206 (W)	1.3887	0.1602 (W)	0.80865	0.743	1.2944
3-Cysteinylacetaminophen	0.7404 (W)	0.9494	0.4198	2.2579	0.3468	0.0056891
3-Dehydrocamitine	0.0293 (W)	0.78353	0.321	0.92736	0.6420 (W)	0.7832
3-Guanidinopropionic acid	0.0693 (W)	0.57058	0.5839 (W)	1.7881	0.0702	1.0374
3-Hydroxyacetaminophen	0.2457	0.83043	0.4525	1.165	0.6429	0.6158
3-Hydroxyanthranilic acid	0.8872 (W)	0.87537	0.4212	0.79166	0.3054	0.41538
3-Hydroxybutylcamitine	0.1145	1.3004	0.3544	0.61585	0.022	2.4232
3-Hydroxyproline	0.7457 (W)	0.86519	0.6250 (W)	0.97076	0.012	0.61672
3-Hydroxysebacic acid	0.5158 (W)	0.95306	0.401	0.92967	0.4788	0.75002
3-Indoleacetic acid	0.4645 (W)	0.96601	0.8948	0.92697	0.2414 (W)	0.95253
3-Methylcrotonylglycine	0.5158 (W)	0.76338	0.1717	0.5921	0.4448	2.3134
3-Methylcytidine	0.5561 (W)	0.8167	0.1958	0.96493	0.035	0.41272
3-Methylhistidine	0.2519	0.86257	0.7254	1.0871	0.8632	1.0277
3-Methyl-L-histidine	0.0549 (W)	0.78423	1.0000 (W)	0.64596	0.1181	1.7862
3-Methylthiopropylamine	0.2514 (W)	1.6866	0.1726	1.3051	0.0968 (W)	0.56912
3'-O-Methylcytidine	0.9515 (W)	0.71912	0.3223 (W)	1.0131	1.0000 (W)	1.0463
3'-O-Methylguanosine	0.1004 (W)	1.005	0.9057 (W)	1.0298	0.581	0.8726
3'-O-Methylinosine	0.1403 (W)	0.90758	0.3750 (W)	1.104	0.6992 (W)	0.84038
3-Uridopropionic acid	0.5561 (W)	0.93353	0.7695 (W)	0.89536	0.4378 (W)	0.88621
4,4-Dimethyl-L-glutamic acid	0.7786 (W)	0.91646	0.7895 (W)	1.151	0.6428 (W)	0.63938
4,5,7-Trihydroxyisoflavone	0.7223 (W)	1.1394	0.2508	1.295	0.9581	0.81467
4,6-Diamino-5-formamidopyrimidine	0.5978 (W)	0.89072	0.5777	0.99402	1.0000 (W)	0.85787
4-Acetamidobutyric acid	0.4280 (W)	0.94728	0.7874 (W)	0.88557	0.1224	0.95038
4-Amino-1-butanol	0.8236 (W)	0.96803	0.9541	1.1116	0.8808	0.52533
4-Aminobenzoic acid	0.6263 (W)	0.81862	0.1188	1.0582	0.1827 (W)	0.3239
4-Aminomethylcyclohexanecarboxylic acid	0.0876 (W)	1.8613	0.4316 (W)	1.0918	0.0019	0.70511
4-Guanidinobutyric acid	0.6702 (W)	0.85911	0.8797	1.123	0.8964	0.81238
4-Hydroxy-6-methyl-2-pyrone	0.9948	0.99884	0.9084	0.62098	0.5001	1.4854

4-Hydroxybenzoic acid	0.1213	1.4814	0.5655	0.78254	0.1853	0.57229
4-Hydroxyhippuric acid	0.6554 (W)	0.67056	0.0371 (W)	0.5776	0.8669	0.32021
4-Hydroxyquinoline	0.2894 (W)	1.1902	0.5326	0.80965	0.0369 (W)	0.77563
4-Imidazoleacetic acid	0.4645 (W)	0.78426	0.3431	0.82643	0.4959	0.72403
4-Imidazoleacrylic acid	0.5561 (W)	0.97219	0.217	1.074	0.2922	0.91409
4-Methyl-1H-pyrazole	0.2215	0.89875	0.0794	0.96055	0.4264	0.93519
4-Methyl-5-thiazoleethanol	0.1142 (W)	0.54973	0.6075	1.3412	0.687	3.4015
4-Pyridoxic acid	0.1347 (W)	1.2613	0.753	0.97297	0.689	0.79176
4-Quinolincarboxylic acid	0.9677 (W)	0.85923	0.8212	0.92668	0.6992 (W)	0.4395
4-Thiouridine	0.5839 (W)	1.1372	0.9348	0.87516	0.053	3.1241
5,6-Dihydrouracil	0.1642 (W)	0.70683	0.8146	0.90417	0.6482 (W)	1.3664
5-Acetylamino-6-amino-3-methyluracil	0.1981 (W)	0.6265	1.0000 (W)	1.114	0.3762	1.0815
5-Amino-1-methyl-2-piperidinone	0.6120 (W)	0.77748	0.601	0.64025	0.9654	8.4044
5-Aminoimidazole-4-carboxamide	0.0208	0.7658	0.8118	1.0434	0.0024 (W)	1.4344
5-Aminosalicyclic acid	0.8394 (W)	0.83905	0.5566 (W)	0.79811	0.0673	1.087
5-Fluro-2-pyrimidone	0.2367 (W)	0.71333	0.874	1.0231	0.9819	1.1899
5-Hydroxy-3-indoleacetic acid	0.6408 (W)	0.91745	0.1655	0.71302	0.7249	0.87392
5-Hydroxymethyl-6-methyluracil	0.9193 (W)	0.91433	0.9155	0.80595	0.6382	0.93765
5-Hydroxytryptophan	0.3492 (W)	0.81671	0.0538	0.89491	0.1827 (W)	1.0263
5-Methoxy-3-indoleacetic acid	0.9191 (W)	0.89306	0.0641	0.92271	0.4639	0.28207
5-Methoxyuridine	0.2367 (W)	0.77732	0.1392	1.0883	0.0520 (W)	0.67854
5-Methyl-2-thiouridine	0.3104 (W)	0.77554	0.8287	1.0792	0.3172	1.5193
5-Methylthioadenosine	0.6850 (W)	0.88881	0.603	0.88355	0.7460 (W)	0.93492
6-Aminocaproic acid	0.1832	0.79964	0.8127 (W)	1.0681	0.8073	0.60783
6-Hydroxyflavone	0.1419 (W)	1.8056	0.2025	1.3213	0.1952	1.6507
7,8-Dihydrobiopterin	0.4771 (W)	1.3298	0.7919	1.0402	0.4887	0.89668
7-Methylguanosine	0.0879 (W)	0.68951	0.6065	0.6866	0.9358	3.016
7-Methylxanthine	0.5291 (W)	0.76656	0.6224	1.3048	0.1237	0.73837
8-Oxo-2'-deoxyadenosine	0.0629 (W)	2.2439	0.9332	0.42329	0.9744	1.0358
Abscisic acid	0.2894 (W)	1.1677	0.2088	0.74335	0.7204 (W)	0.46782
Acetaminophen glucuronide	0.5839 (W)	0.94341	0.4772 (W)	1.9937	0.2414 (W)	0.059919
Acetaminophen	0.3387 (W)	0.78798	0.3953	1.6636	0.7610 (W)	0.015088
Acetylcarnitine	0.1460 (W)	1.3935	1.0000 (W)	0.47861	0.6426 (W)	2.7411
Actrant	0.673	0.94723	0.6250 (W)	0.91419	0.015	0.82462
Adenine	0.1196	0.73815	0.1309 (W)	0.76457	0.2876	1.4438
Agmatine	0.1851 (W)	0.373	0.6953 (W)	1.8706	0.5781	0.52962
Ala-Ala	0.5621	0.91859	0.3002	0.98752	0.2268 (W)	0.81606
Ala-Ile	0.4045 (W)	0.82799	0.6726 (W)	1.0172	0.311	0.7358
Albuterol	0.2719 (W)	0.71715	0.8457 (W)	0.71804	0.2411	0.036742
Allantoic acid	0.5561 (W)	0.87778	0.9185	0.9483	0.4048 (W)	0.79844
alpha-Galactosamine-1-phosphate	0.2710 (W)	1.1897	0.1683	1.1556	0.4259	1.0905
Anastrozole	0.0223 (W)	2.2759	0.8962	0.6391	1.0000 (W)	0.49384
Androstane-3,17-diol	0.0463	0.78296	0.3750 (W)	0.98306	0.2671 (W)	0.90084
Anserine	0.3979	0.7654	0.477	0.44109	0.797	2.5974
Arginine	0.9032 (W)	1.1086	0.9217	0.79637	0.1831	0.94827
Arpiprazole	0.9442 (W)	0.99258	0.0623	0.75719	0.9334	2.7409
Asp-Arg	0.1403 (W)	0.66593	0.3423	0.87339	0.5330 (W)	0.77184
Aspartic acid	0.5158 (W)	0.85486	0.7893 (W)	1.0866	0.9169	0.82711
Asp-Glu	0.1579 (W)	0.7967	0.7124	0.83021	0.6992 (W)	0.78698
Asp-phe	0.2621 (W)	0.8107	0.2483	1.7313	0.1167	0.45394
Atomoxetine	0.1403 (W)	3.1905	0.4067	1.3874	0.9242	0.77419
Benzoic acid, 2-Z-3-3,4-dimethoxyphenyl-1-oxo-2-propen-1-ylamino-3-hydroxy-	0.5425 (W)	0.654	0.5548	0.66093	0.5004 (W)	0.45692
beta-Alanine	0.5922	0.92892	0.5566 (W)	0.9071	0.5356 (W)	1.1553
Betaine	0.3141	1.1145	0.2754 (W)	0.80812	0.4935	0.68705
Biotin	0.6325	0.80123	0.6488	0.55803	0.445	0.24074
Caffeine	0.2089	0.70266	0.2455	0.54378	0.4919	3.0491
Camitine	0.1976	1.2799	0.1782	0.51049	0.399	2.3195
Camosine	0.3639	0.74027	0.1748	0.85357	0.0313	0.81069
Cetraxate	0.2412	0.74992	0.2091	0.40304	0.5694	1.427
Choline	0.8377	0.97961	0.7899	0.90988	0.7339	0.80145
Cinanserin	0.5286 (W)	1.0594	0.0623	—	0.3735	0.029848
Citrulline	0.8078 (W)	1.1058	0.3618	0.88412	0.4660 (W)	1.1348
Cotinine	0.8236 (W)	1.1818	0.4087	0.68136	0.5014	5.5507
Creatine	0.0322	0.75446	0.9219 (W)	0.92498	0.8773 (W)	1.2851
Creatinine	0.0364 (W)	0.92153	0.7674	0.97938	0.3611	0.9998
CycloLeu-Pro	0.1313	0.73816	0.3948	1.3514	0.9888	0.59767
Cyclohexanamine	0.5561 (W)	0.94583	0.36	0.92078	0.1372	0.11138
Cyproheptadine	0.0164 (W)	1.2606	0.8457 (W)	0.72389	0.4854 (W)	0.73134
Cyromazine	0.0767 (W)	0.87275	0.2416	0.72571	0.7658	3.073
Cystathionine	0.3492 (W)	0.75451	0.2754 (W)	0.68562	0.8168 (W)	0.90294
Cystine	0.6263 (W)	0.99669	0.2893	1.5125	0.5429	0.98755
Cytosine	0.2367 (W)	0.78875	1.0000 (W)	1.0008	0.8492	0.82531
Daidzein	0.4562 (W)	1.5911	0.9969	2.5056	0.1496	0.73165
Decanoyl-L-carnitine	0.3184 (W)	0.98913	0.4938	0.82267	0.5125 (W)	1.1768
della-Hydroxylysine	0.4843	0.87814	0.2752	0.74679	0.5589	1.0089
Desmedipham	0.7853	0.90607	0.4505	0.77635	0.7673	2.457
Dextrophan	0.8551 (W)	0.89691	0.5056	—	0.6157	0.40446
D-Fructose	0.2988 (W)	1.7203	0.6008	1.4577	0.1796	0.28287
Diffufenzopyr	0.4492 (W)	0.73451	0.4124	1.736	0.4222	0.11303
DL-2-Methylglutamic acid	0.7922 (W)	1.0399	0.3963	1.2717	0.7458	0.7574
Dopamine	0.0010 (W)	0.49811	0.8404	0.93985	0.2106 (W)	0.71476
Doxepin	0.954	0.93467	0.8869	0.89596	0.6714	0.18559
D-Turanose	0.8682	0.96368	1.0000 (W)	1.155	0.6814	0.77094
Egonine	0.6277	1.1218	0.2569	0.53309	0.4627	2.5778
Ergothioneine	0.5699 (W)	1.1346	0.0488 (W)	1.6881	0.037	0.66356

Ethanolamine	0.5838 (W)	0.73525	0.2324 (W)	1.7881	0.1312	0.90737
Ethyldiethanolamine	0.8872 (W)	0.91152	0.8474	1.0501	0.5174	1.0293
Fluorene	0.1094 (W)	0.77214	0.5546	1.0725	0.8248	0.89693
Gabapentin related compound A	0.4522 (W)	0.88938	1.0000 (W)	0.86632	0.6712	0.94755
Galactosamine	0.8712 (W)	0.97765	0.4065	0.85453	0.7573 (W)	0.24854
gamma-Glutamylleucine	0.7294	0.96222	0.8087	1.0344	0.2813	0.79424
Glutamic acid	0.8872 (W)	1.195	0.7695 (W)	0.82077	0.6717	0.71795
Glutamine	0.7457	1.0428	0.6553	1.0408	0.3754	1.0298
Glycine	0.4936	0.91725	0.3334	0.89034	0.5442	0.87241
Glycine	0.6149 (W)	1.3182	0.6750 (W)	1.2961	0.8668	1.2014
Glycyl-leucine	0.4890 (W)	1.1678	0.5016	1.9222	0.5023 (W)	0.91308
Glycyltyrosine	0.9838 (W)	0.90391	0.382	0.84206	0.2078	0.98537
Gly-Gly-Gly	0.5838 (W)	0.93073	0.2324 (W)	1.7048	0.4378 (W)	1.1446
Gly-Ile	0.1519 (W)	0.64427	0.8457 (W)	1.3425	0.3915	1.2909
Gly-val	0.2801 (W)	1.54	0.4001	1.3137	0.9982	0.49025
Guanidinoacetic acid	0.1981 (W)	0.8782	0.115	0.83856	0.1894 (W)	1.0182
Guanidinosuccinic acid	0.7000 (W)	0.97628	0.7149	1.0526	0.9385 (W)	0.91744
Guanine	0.1191 (W)	1.1023	0.6266	0.81088	0.8678	0.84414
Hexadecyltrimethylammonium cation	0.6641	1.1069	0.3799	1.467	0.4121	0.58123
Hexanoyl-L-carnitine	0.7656	1.0228	0.4985	1.2069	0.6054	0.84405
H-gamma-glutamyl-glutamine	0.6026 (W)	1.5052	1.0000 (W)	1.0064	0.4205	0.66235
Hippuric acid	0.7611 (W)	0.91849	0.7564	0.90294	0.5769 (W)	1.8117
His-Pro	0.2147	0.84628	0.5566 (W)	1.2069	0.5049	0.80861
Histidine	0.8377	1.0229	0.5727	0.96444	0.1826	0.97867
Homocarnitine	0.1706 (W)	0.85908	0.382	0.89926	0.9672	1.0528
Homogentisic acid	0.021	1.3525	0.9744	0.76725	0.8759	1.571
Homoserine	0.3658	0.87261	0.7241	1.0059	0.0357	0.78234
Ibuprofen .beta.-D-glucuronide	0.9246 (W)	1.6694	0.8339 (W)	0.92932	0.7063	126.11
Ifenprodil	0.1579 (W)	0.52087	0.424	1.5855	0.9309 (W)	0.48604
Indole-3-acetamide	0.9193 (W)	1.0442	0.3223 (W)	0.66942	0.7936	1.3678
Indole-3-carboxaldehyde	0.2988 (W)	1.5491	0.1742	0.78453	0.6426 (W)	0.47448
Indolelactic acid	0.0443 (W)	2.221	0.8457 (W)	0.59476	0.2819	1.7443
Inosine	0.0961 (W)	0.76389	0.8457 (W)	1.1226	0.2266	0.86651
Isoleucine	0.7000 (W)	1.0626	0.6953 (W)	1.1019	0.4255	0.93902
Kynurenic acid	0.0523 (W)	0.75519	0.4344	1.1307	0.9385 (W)	0.86517
Kynurenine	0.6511	1.0692	0.8457 (W)	0.89871	0.4595	0.79922
Lactitol	0.4042 (W)	0.75411	0.9326 (W)	1.015	0.5006	1.286
L-Alanyl- .beta.-alanine	0.1265	0.61975	0.9219 (W)	0.8657	0.6271 (W)	0.7391
Latanoprost	0.7798 (W)	1.1621	0.5294 (W)	0.70357	0.5996	0.98197
Leu-Asp	0.4898 (W)	0.93651	0.9132	0.98458	0.1125 (W)	0.8799
Levetiracetam	0.1382	0.82077	0.1727	0.68273	0.8443	0.59089
L-Histidine	0.5284	1.0811	0.4167	0.84156	0.1836	1.6161
L-Homocitrulline	0.2534 (W)	1.2414	0.7871	0.81559	0.3648	1.3306
Liquiritigenin	0.6982 (W)	1.1757	0.2361 (W)	5.1601	0.1605	0.64771
Lisdexamfetamine	0.1403 (W)	0.83385	0.7201	0.96596	0.5023 (W)	0.97031
L-Lysine	0.852	1.0537	0.3474	0.60789	0.8078	1.1993
Lofexidine	1.0000 (W)	1.1251	0.0892	1.9631	0.6129	0.7038
Maltose	0.7457 (W)	0.96246	0.5292	0.9029	0.0849	0.7038
Methacholine cation	0.494	1.1015	0.3359	0.64488	0.9553	1.8576
Methionine	0.9032 (W)	1.127	0.9219 (W)	0.77067	0.0802	1.485
Methioninesulfoxide A	0.7871	1.0481	0.7742	0.95651	0.0339	0.78131
Methohexital	0.3085 (W)	0.828	0.7695 (W)	1.0115	0.7296	1.2197
Moclobemide	0.0290 (W)	0.36302	0.4771	1.4251	0.0785	0.18707
Muramic acid	0.1096 (W)	0.37824	0.6953 (W)	0.7052	0.1511	0.77544
N-2-Furoylglycine	0.3492 (W)	1.0589	0.4201	0.75529	0.7937	0.43503
N,N-Dimethylarginine	0.0803 (W)	0.81482	0.2533	0.9228	0.0742	0.96865
N- .alpha.-tert-Butoxycarbonyl-L-histidine	0.8292	1.0213	0.5796	0.90816	0.8474	1.0014
N2,N2-Dimethylguanosine	0.4645 (W)	0.80309	0.8457 (W)	1.0772	0.9333	0.92076
N2-Methylguanosine	0.3707 (W)	0.83335	0.7695 (W)	1.0386	0.5880 (W)	0.81177
N8-Acetylsermidine	0.5978 (W)	0.82448	0.6001	0.95207	0.4378 (W)	0.79511
N-Acetylaspargylglutamic acid	0.8712 (W)	0.91647	0.3028	0.90939	0.2427	1.0247
N-Acetylcytidine	0.3184 (W)	1.4302	0.3223 (W)	0.38912	0.9618	1.1424
N-Acetyl-DL-leucine	0.9677 (W)	0.85762	0.8571	0.92022	0.8168 (W)	1.0203
N-Acetylglucosamine	0.8712 (W)	0.94859	0.4237	1.1353	0.1827 (W)	1.0324
N-Acetylhistidine	0.8872 (W)	0.81056	0.9219 (W)	1.0236	0.6426 (W)	0.7511
N-Acetyl-leucine	1.1035	0.5886	0.5777	0.89086	0.2872	1.1567
N-Acetylmethionine	0.9354 (W)	1.0885	0.9803	1.0059	0.5678	0.63864
N-Acetylneuraminic acid	0.8314	1.0165	0.8161	1.0185	0.8051	0.85717
N-Acetylphenylalanine	0.4369	0.85324	0.4922 (W)	0.8338	0.4918	0.40373
N-Acetyltryptophan	0.5158 (W)	0.78938	0.5566 (W)	0.932	0.0932	0.76357
N-Benzoyloxycarbonylglycine	0.4645 (W)	0.68194	0.1551 (W)	1.7265	1.0000 (W)	0.21038
N-Carboxyethyl- .gamma.-aminobutyric acid	0.302	0.8071	0.6223	0.8589	0.0968 (W)	0.49337
N-Cinnamoylglycine	0.1126 (W)	2.0283	0.8339 (W)	0.79287	0.0121	0.96886
N-cyano-N'-1,1'-dimethylpropyl-N'-3-pyridinyl-guanidine	0.8078 (W)	1.0006	0.6953 (W)	0.93696	0.7603 (W)	1.1473
NEPSILON,N,NEPSILON,NEPSILON-TRIMETHYLLYSINE	0.1403 (W)	0.79935	0.3092	0.92587	0.6426 (W)	1.0677
N-epsilon-Acetyllysine	0.8872 (W)	0.94722	1.0000 (W)	0.87172	0.4581	0.93564
NG,NG-Dimethyl-L-arginine	0.2367 (W)	0.73197	0.3223 (W)	0.82448	0.8875	0.8898
Nialamide	0.2601	1.3717	0.6250 (W)	0.87708	0.2811	0.66461
Nicotine	0.5158 (W)	1.157	0.1602 (W)	1.2578	0.647	5.278
N-Isobutylglycine	0.0549 (W)	0.75299	0.4372	0.8396	0.6426 (W)	0.90909
N-Isovalerylglycine	0.5158 (W)	0.83287	0.9668	0.98685	0.8215	0.8745
N-Methyl- .gamma.-oxo-3-pyridinebutanamide	0.2129 (W)	1.3564	0.7695 (W)	1.1687	0.6857	4.2957
N-Methylalanine	0.6624	0.95167	0.564	0.90764	0.6426 (W)	0.95932
N-Methylanthranilic acid	0.102	1.5059	0.2582	1.6413	0.8774	0.31949
N-Methylglutamic acid	0.4771 (W)	0.86598	0.6953 (W)	0.78393	0.1102	0.52226

N-Methylhistidine	0.1294 (W)	0.89988	0.6250 (W)	0.95543	0.2749 (W)	1.1403
N-Methylisoleucine	0.8553 (W)	1.0101	0.0840 (W)	0.608	0.1218	0.98796
N-Methyllysine	0.5158 (W)	0.88491	0.8639	1.0193	0.8793	0.9079
N-Methylproline	0.4154	1.1943	0.8649	1.0668	0.5359	0.55345
N-Methylserine	0.5838 (W)	0.8922	0.9932	1.0053	0.2351	1.6844
N-Methylthreonine	0.6850 (W)	0.68862	0.7749	1.0952	0.2636	0.57402
N-Methyltyrosine	0.2594	0.69003	0.3750 (W)	1.5944	0.5603	0.13829
N-Methylvaline	0.0120 (W)	0.5826	0.2467	0.66854	0.0063 (W)	1.9607
N-omega-Acetylhistamine	0.782	0.94572	0.2333	0.68622	0.1094	1.4157
Octadecanedioic acid	0.5312 (W)	1.3141	0.9124	1.0469	0.3631	1.0695
Octopine	0.0097 (W)	2.4909	0.5839 (W)	0.94282	0.8212	---
Ornithine	0.5978 (W)	0.94481	0.6698	1.0888	0.9867	0.92227
Oxazepam	0.4352 (W)	1.2058	0.7998 (W)	0.80954	0.1348 (W)	0.20063
Oxybenzone	0.1952 (W)	1.8315	0.2118	3.9423	0.8554	1.793
Pantothenic acid	0.1278	1.3095	0.2754 (W)	0.88656	0.7242	1.6806
Pemoline	0.9773 (W)	1.0642	0.9326 (W)	1.0531	0.6026 (W)	2.0914
Phenethylamine	0.0062 (W)	0.7406	0.4343	1.1167	0.2106 (W)	0.36872
Phenylacetaldehyde B	0.2404	1.3568	0.9106	1.0784	0.9329	1.2205
Phenylacetylglutamine	0.5699 (W)	0.90031	0.9182	1.0157	0.2078	0.75682
Phenylacetylglutamine	0.7303 (W)	1.0262	0.7881	1.1413	0.6228	0.85278
Phenylalanine	0.8712 (W)	1.0491	0.6953 (W)	1.039	0.7592	0.75057
Phenylethanolamine A	0.0381	0.67348	0.4008	0.78155	0.2167	0.51037
Phlorobenzophenone	0.8373 (W)	0.9807	0.2807 (W)	2.9591	0.3793 (W)	0.4417
Phloroglucinol	0.071	0.59728	0.7392	0.8873	0.1336	0.52173
Piperacolic acid	0.3158	0.83285	0.8786	1.0458	0.0509	0.45849
Piperine	0.9326 (W)	1.0161	0.1056 (W)	2.4486	0.7610 (W)	0.044512
Pirimiphos-ethyl	0.0312	0.39803	0.3853	0.42159	0.0085 (W)	4.4179
Proline	0.3085 (W)	0.97171	0.6953 (W)	1.0006	0.6426 (W)	0.72373
Proline-hydroxyproline	0.5425 (W)	0.83711	0.388	0.85268	0.217	1.2892
Propionylcamitine	0.4522 (W)	1.306	0.1934 (W)	0.46913	0.0486	2.1884
Putrescine	0.2801 (W)	0.8135	0.1055 (W)	1.7143	0.4854 (W)	0.59493
Pyridoxamine	0.6702 (W)	1.0572	0.4007	1.0974	0.8857	0.79452
Pyridoxine	0.8712 (W)	0.96079	0.9892	1.0056	0.2666	0.57006
PyroGlu-Pro	0.8553 (W)	0.97287	0.8202	1.0596	0.2465	1.0755
Pyroglutamic acid	0.4522 (W)	1.1942	0.3595	0.82143	0.5068	1.0819
Quinolone	0.7611 (W)	0.88779	0.1565	0.68099	0.1909 (W)	0.64502
Ranitidine	0.6101 (W)	0.84773	0.1775 (W)	0.17448	0.5151 (W)	0.024989
Riboflavin	0.2429 (W)	1.3998	0.9219 (W)	0.98176	0.5069	2.1407
S-Adenosyl-homocysteine	0.8394 (W)	1.0515	1.0000 (W)	1.2124	0.8168 (W)	1.0308
S-Adenosyl-methionine	0.1981 (W)	0.74603	0.5737	0.8976	0.6721	0.7565
Scopoletin	0.0332	0.35747	0.3132	0.56846	0.9112	0.85299
Serine	0.7000 (W)	1.0289	0.7695 (W)	0.95351	0.3844	1.1729
Sucrose	0.9827 (W)	1.0332	0.1602 (W)	2.1644	0.1909 (W)	0.48953
Synephrine	0.3492 (W)	0.71111	0.2324 (W)	0.34983	0.6343 (W)	0.90687
Taurine	0.8236 (W)	1.3501	0.1602 (W)	0.38985	0.1348 (W)	2.479
Theophylline	0.7859	0.94262	0.2602	0.75916	0.1638	1.4092
Thiamine cation	0.4645 (W)	1.0415	0.8768	1.058	0.6152	0.77329
threo-Dihydropropion	0.3931 (W)	0.67724	0.0736	0.43225	0.5356 (W)	0.0044715
Threonine	0.6716	0.91841	0.8595	0.97228	0.3082	1.3868
TMAO	0.6120 (W)	1.0153	0.8457 (W)	0.82081	0.4245	1.1584
Triethylene glycol monobutyl ether	0.8872 (W)	0.99215	0.2324 (W)	0.53378	0.8168 (W)	2.1746
Trigonelline	0.5317	0.67373	1.0000 (W)	1.3889	0.0021	0.033222
Trimethylamine N-oxide	0.5425 (W)	1.1395	0.5536 (W)	0.58323	0.4732	1.0446
Troxipide	0.8236 (W)	0.89452	0.0840 (W)	0.65218	0.2835	1.5257
Tryptophan	0.9259	1.0128	0.9588	1.0072	0.5671	1.0294
Tyrosine	0.729	0.87467	0.5566 (W)	1.6826	0.1577	0.29723
Urocanic acid	0.4898 (W)	0.97971	0.5062	1.0805	0.5256	0.92911

\*p-value is calculated with t-test as a default. p-value with (W) is calculated by the Wilcoxon Mann Whitney test.  
 --- = no fold-change value output from Metaboanalyst