

Supplement data files

Figure S1 Changes in body weight during the experimental intervention period (n=7)

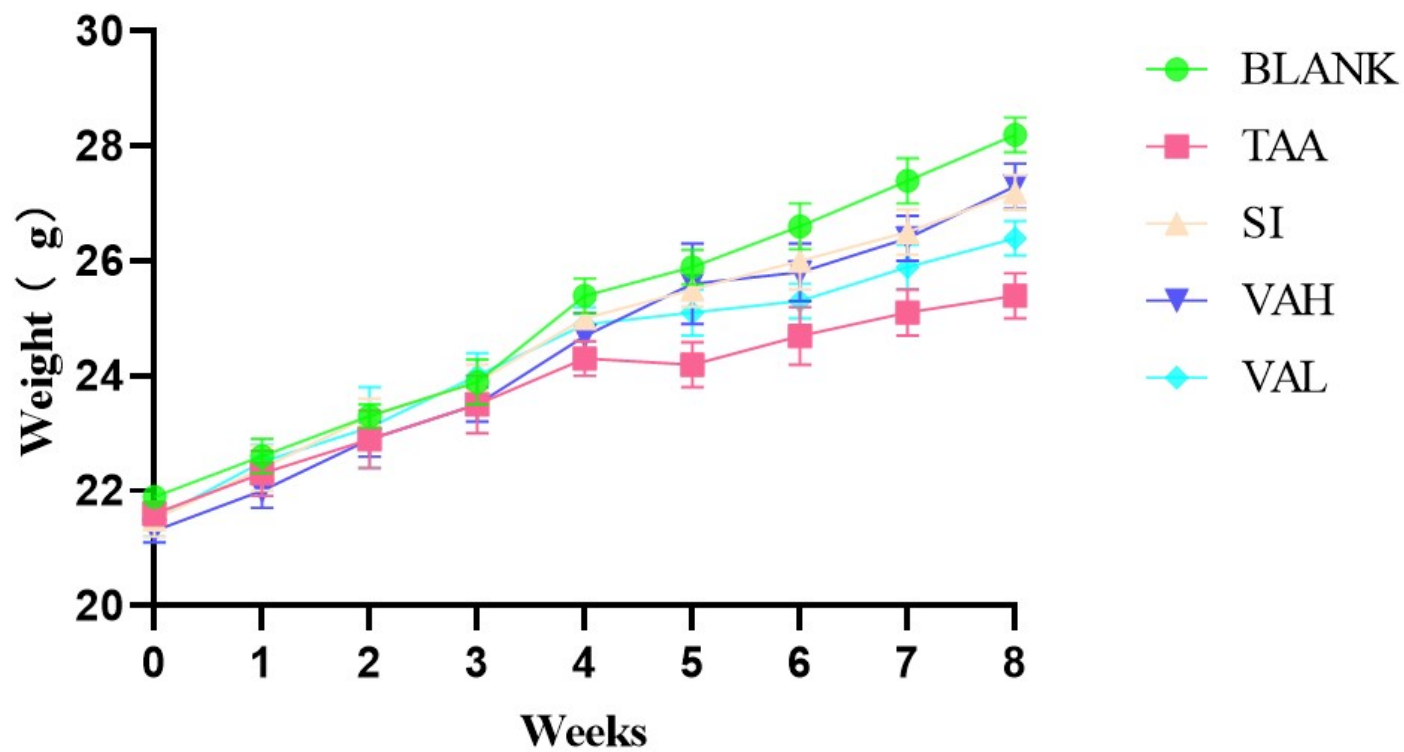


Table S1 The abundance of all significantly altered gut microbiota at the phylum, family, and genus levels (mean)

Name	BLANK	TAA	SI	VAH	VAL
p_Actinobacteria	0.001823985	0.003053193	0.008756452	0.002174243	0.004057707
p_Verrucomicrobia	0.000125564	0.138358545	0.01003192	0.045645896	0.028119775
p_TM7	7.26951E-05	0.002663283	0.004394747	0.001777725	0.004302226
p_Proteobacteria	0.045355115	0.032032092	0.018913936	0.014175539	0.013111547
f_S24-7	0.502177548	0.337661994	0.354553685	0.348255649	0.427499884
f_Lachnospiraceae	0.080559356	0.120039388	0.101548405	0.14792786	0.131485557
f_unclassified_Clostridiales	0.076818864	0.028668292	0.084372542	0.185167562	0.054369304
f_Lactobacillaceae	0.037067877	0.014757099	0.021920868	0.005234045	0.007930371
f_Deffribacteraceae	0.019264194	0.001110252	0.000165216	0.001182947	0.001189556
f_Turicibacteraceae	6.60864E-05	0.014188756	0.005293523	0.000158607	0.001698421
f_Porphryomonadaceae	0.003694231	0.006258385	0.004500486	0.001638943	0.003198583
f_unidentified_YS2	0.00092521	0.005709867	0.002702935	0.002702935	0.002623631
f_Leuconostocaceae	0.004044489	1.32173E-05	0.001817377	0	0
f_Peptostreptococcaceae	0.00024452	0.000964862	0.003178757	0.000403127	0.000548517
f_mitochondria	0.001790942	0	0.000726951	0	3.30432E-05
f_Christensenellaceae	0.000277563	0.000165216	9.2521E-05	0.000118956	0.000138781
f_unclassified_Burkholderiales	0.000337041	3.30432E-05	7.26951E-05	0.000105738	0
f_unidentified_Alphaproteobacteria	1.98259E-05	0.00024452	6.60864E-05	8.59124E-05	0.000112347
f_RF16	3.30432E-05	0.000105738	8.59124E-05	6.60864E-05	0
f_Micrococcaceae	6.60864E-06	2.64346E-05	0	9.2521E-05	5.28691E-05
f_Verrucomicrobiaceae	0.000125564	0.138358545	0.01003192	0.045645896	0.028119775
f_Anaeroplasmataceae	0.008412802	3.30432E-05	0.001989201	7.26951E-05	0.002127983
f_Enterobacteriaceae	0.001262251	5.28691E-05	0.000806254	0.000132173	0.000132173

f_Turicibacteraceae	6.60864E-05	0.014188756	0.005293523	0.000158607	0.001698421
g_Akkermansia	0.000125564	0.138318893	0.01003192	0.045645896	0.028119775
g_Turicibacter	6.60864E-05	0.014188756	0.005293523	0.000158607	0.001698421
g_Lactobacillus	0.036539186	0.01470423	0.021742435	0.005187785	0.007890719
g_unidentified_S24-7	0.502177548	0.337661994	0.354553685	0.348255649	0.427499884
g_unidentified_Clostridiales	0.092157524	0.069998744	0.085753749	0.124658829	0.106835319
g_unidentified_Bacteroidales	0.00082608	0.002194069	0.018570286	0.006271602	0.001857029
g_unclassified_Bacteroidales	0.001546422	0.006410383	0.00516135	0.00491683	0.004077533
g_unclassified_Helicobacteraceae	0.01348824	0.000627821	0.00209494	0.003912317	0.001863637
g_Bifidobacterium	0.000178433	0.002623631	0.007514027	0.001546422	0.003073019
g_Flexispira	0.006112995	0.002550936	0.001110252	0.000766603	0.000997905
g_unidentified_Bacteria	0.000819472	0.002015636	0.000951645	0.00102434	0.001110252
g_Dehalobacterium	0.000528691	0.000720342	0.001090426	0.002213895	0.001103643
g_AF12	0.001790942	0.001275468	0.000905384	0.000667473	0.000793037
g_unidentified_Streptophyta	0.002617023	0	0.001189556	0.000125564	0.000264346
g_Paraprevotella	0	0.000806254	0.001420858	0.001163121	0.000317215
g_Roseburia	3.30432E-05	0.001394424	0.000627821	0.000601386	0.000574952
g_unidentified_Coriobacteriaceae	3.30432E-05	0.000112347	0.000641038	0.000376693	0.000376693
g_Anacrotruncus	0.000343649	0	0.000151999	0.000403127	7.93037E-05
g_unclassified_Lactobacillales	0.000323823	9.91296E-05	0.000270954	6.60864E-06	0.000138781
g_unclassified_Lactobacillaceae	0.000515474	3.96519E-05	0.000171825	4.62605E-05	1.98259E-05
g_Burkholderia	0.000138781	0.000396519	5.28691E-05	3.96519E-05	3.96519E-05
g_unclassified_Erysipelotrichaceae	4.62605E-05	0.000185042	0.000132173	1.32173E-05	2.64346E-05
g_unclassified_Bradyrhizobiaceae	0	0.000231302	3.96519E-05	0	0
g_Comamonas	0.000204868	0	0	0	2.64346E-05
g_Rhodococcus	0.000185042	0	0	0	0

Table S2 The metabolites significantly up-or down-regulated in BLANK vs TAA (mean)

Name	BLANK	TAA	P. value	VIP	Trend
Dimethylglycine	96307873.61	69569613.33	0.004329004	1.565859637	↑
gamma-Aminobutyric acid	25014713.47	6635177.77	0.004329004	1.464493527	↑
Benzaldehyde	36907195.55	43846690.03	0.025974026	1.233907008	↓
2-Aminophenol	107212148.7	60221950.24	0.008658009	1.490194336	↑
Pyrrole-2-carboxylic acid	111102690.1	142581477.2	0.002164502	1.427382358	↓
2-Methylserine	40322331.25	57427425.89	0.025974026	1.231335051	↓
4-Hydroxybenzaldehyde	138473218.2	38626449.35	0.004329004	1.663295916	↑
1,1-Dimethylbiguanide	32947536.64	39576021.94	0.041125541	1.140969867	↓
gamma-Amino-gamma-cyanobutanoate	31876943.08	73807618.61	0.041125541	1.361820169	↓
Pipecolic acid	778640331.8	1803344524	0.041125541	1.33185724	↓
5-Amino-2-oxopentanoic acid	43259797.81	88038538.19	0.004329004	1.525777884	↓
L-Leucine	20149444.86	28559827.38	0.004329004	1.681518594	↓
Dopamine	210089456.4	380833783.8	0.041125541	1.148949324	↓
N-Acetylarylamine	16790497.86	10682982.43	0.004329004	1.624829282	↑
1-Hydroxymethylnaphthalene	18525960.52	202709506.1	0.004329004	1.66515668	↓
Phosphonoacetate	37166817.17	70187689.44	0.041125541	1.518062167	↓
(2R,5S)-2,5-Diaminohexanoate	16426000.24	13059911.65	0.041125541	1.248553019	↑
8-Hydroxyquinoline	97930819.69	311717432.3	0.004329004	1.376132931	↓

Name	BLANK	TAA	P. value	VIP	Trend
Pulegone	18696572.61	10427393.82	0.008658009	1.460499591	↑
2',4'- Dihydroxyacetophenone	18987228.21	10969302.42	0.041125541	1.060217813	↑
Tryptamine	4523746.67	1329248.08	0.004329004	1.696609302	↑
L-Rhamnono-1,4-lactone	22037143.03	12620908.45	0.002164502	1.663241771	↑
L-Carnitine	2833989746	6528207137	0.015151515	1.35224809	↓
3,4'- Dihydroxyphenylpropanoate	674127388.5	1082424522	0.002164502	1.702708191	↓
L-beta-Phenylalanine	52023018.78	35363988.25	0.008658009	1.582126324	↑
D-syneprine	126703331.5	90645817.56	0.008658009	1.61897545	↑
(S)-4-Hydroxymandelate	44621122.52	88325917.71	0.041125541	1.265325764	↓
(2S,5S)-trans- Carboxymethylproline	99131750.98	15626952.18	0.004329004	1.463971609	↑
Formiminoglutamic acid	84754704.8	43078813.55	0.008658009	1.309653361	↑
N-Formyl-L-glutamic acid	50976770.15	19691972.18	0.025974026	1.30572381	↑
2-Hydroxy-3-oxoadipate	26974297.8	21948699.81	0.002164502	1.617600344	↑
D-Alanyl-D-serine	3234401.26	12099784	0.041125541	1.216254931	↓
N-Formyl-L-methionine	64616260.83	28682869.2	0.025974026	1.033392188	↑
Cysteinylglycine	17949232.95	7368951.88	0.041125541	1.183277553	↑
Methyleugenol	59592451.24	168342569.2	0.004329004	1.58944772	↓
Acetylcholine chloride	6173691.92	18083948.14	0.025974026	1.239514146	↓
Dulcin	1314712.95	4317171.46	0.041125541	1.109184439	↓
(S)-beta-Tyrosine	5686826753	1847322815	0.041125541	1.326578395	↑
Epinephrine	4540787.97	3004888.48	0.015151515	1.410737085	↑

Name	BLANK	TAA	P. value	VIP	Trend
Phosphorylcholine	1336845876	4248831523	0.004329004	1.599349063	↓
5-Guanidino-3-methyl-2-oxopentanoate	145400661.3	52401901.38	0.008658009	1.605483955	↑
Isocitric acid	116217879.3	81408123.98	0.015151515	1.459583769	↑
L-Dopa	2156176.08	3263046.69	0.041125541	1.064271281	↓
N5-(L-1-Carboxyethyl)-L-ornithine	21512062.6	14424407.08	0.004329004	1.572349972	↑
Indolelactic acid	7094626.61	12225201.73	0.025974026	1.17538134	↓
Dethiobiotin	6301852.39	25428591.53	0.025974026	1.463596759	↓
beta-Alanyl-L-lysine	95091657.37	43780899.59	0.015151515	1.254501792	↑
Propionylcarnitine	71870245.79	19067853.14	0.008658009	1.448376228	↑
gamma-Glutamylalanine	25729366.92	37368304.67	0.002164502	1.714156757	↓
Capsidiol	8111240.59	1851895.36	0.002164502	1.721162308	↑
8-Methoxykynurenate	4145400.54	6221198.67	0.015151515	1.309257407	↓
Pyrimidodiazepine	11014553.73	8762824.41	0.025974026	1.226512524	↑
2-trans,6-trans-Farnesal	11595588.98	4913982.24	0.025974026	1.217736188	↑
Hydroxykynurenine	5924084.97	6811506.52	0.041125541	1.188484502	↓
N1-Acetylspermine	12861530.87	5790597.28	0.002164502	1.614293396	↑
Myristoleic acid	55971523.22	32147550.35	0.041125541	1.17441067	↑
Ergothioneine	1271164367	756021405.1	0.041125541	1.318138017	↑
Butyryl-L-carnitine	32141296.26	187959650.1	0.004329004	1.46684074	↓
Confertifolin	25681805.95	4508674.95	0.008658009	1.56648481	↑
Biotin	4436597.45	8308373.22	0.002164502	1.719448995	↓
Pindolol	476389683.6	37141163.23	0.015151515	1.319390789	↑
gamma-Glutamylcysteine	6819896.87	10391655.72	0.015151515	1.185800704	↓

Name	BLANK	TAA	P. value	VIP	Trend
10-Hydroxycarbazine	5627749.14	11920527.37	0.041125541	1.144316847	↓
Mannitol 1-phosphate	61580768.49	27488537.68	0.004329004	1.425407789	↑
Subaphylline	6783486.43	1660033.64	0.041125541	1.50065087	↑
Retinol	147849505.1	234412737.6	0.041125541	1.136381432	↓
Aurin	21275731.54	10824290.67	0.008658009	1.647136984	↑
(2R,3R)-3-Methylglutamyl-5-semialdehyde-N6-lysine	13095730.46	2111893.98	0.004329004	1.614250577	↑
Saccharopine	40853602.45	66819289.69	0.025974026	1.275376805	↓
Stearidonic acid	8053599.99	5295326.56	0.015151515	1.274420206	↑
Oleic acid	1536517457	626596805.3	0.004329004	1.475629633	↑
Glycitein	5795030.99	426116.82	0.004329004	1.693308005	↑
9-cis-Retinol	140410847.4	51692431.19	0.015151515	1.484911334	↑
9-OxoODE	87904860.06	36360126.05	0.015151515	1.399070086	↑
5'-Methylthioadenosine	362306826.3	270643658.1	0.041125541	1.26396429	↑
D-4'-Phosphopantothenate	31940926.5	40774904.03	0.041125541	1.197417124	↓
N(6)-[(Indol-3-yl)acetyl]-L-lysine	48947549.2	22743937.68	0.004329004	1.65433657	↑
Glutathione	2970831641	5114579822	0.015151515	1.216674368	↓
Nadolol	208493611.2	27705974.56	0.041125541	1.23778051	↑
Decanoyl-L-carnitine	49445759.02	36177161.68	0.041125541	1.368471367	↑
Enoxacin	41014473.3	10669730.12	0.025974026	1.042600798	↑
UMP	10533756.74	97041518.85	0.025974026	1.28827863	↓
Prostaglandin H2	164945160	290343283.1	0.041125541	1.141207946	↓
15(S)-HPETE	2014411.29	4161826.95	0.002164502	1.61150999	↓
2-Hydroxy-6-	55702790.88	40259364.47	0.041125541	1.1616853	↑

Name	BLANK	TAA	P. value	VIP	Trend
pentadecylbenzoic acid					
Prostaglandin G2	17346128.66	4595308.3	0.008658009	1.44901628	↑
Chelirubine	9645070.19	32600532.77	0.041125541	1.318130084	↓
Cortisol	25547320.59	7422790.34	0.002164502	1.732292653	↑
GMP	80576345.03	32146455.64	0.015151515	1.435515076	↑
Isolithocholic acid	230641618	69395722.18	0.008658009	1.35900608	↑
Risperidone	17495500.79	1556498.77	0.002164502	1.502729351	↑
S-Hexyl-glutathione	9345778.91	6237690.47	0.025974026	1.25195854	↑
5-Dehydroepisterol	17049938.1	8953670.13	0.025974026	1.393300462	↑
S-Succinylglutathione	16873181.51	8155859	0.008658009	1.327636687	↑
5alpha-Ergosta-7,22-diene-3beta,5-diol	47133598.43	12900523.09	0.004329004	1.50856746	↑
S-Glutathionyl-L-cysteine	41014611.48	77975485.23	0.025974026	1.237600815	↓
alpha-Tocopherol	89121142.07	28959996.05	0.004329004	1.607105319	↑
Isovitexin	289590868.7	133822832.5	0.025974026	1.095356317	↑
Retinoyl b-glucuronide	267047402.2	611343988.3	0.041125541	1.280348481	↓
26-Hydroxyecdysone	1508507182	111806528	0.015151515	1.595340893	↑
Taurochenodesoxycholic acid	233816147.7	69441000.58	0.015151515	1.308270012	↑
Deltaline	24646798.82	12874446.19	0.025974026	1.25294955	↑
Taurohyocholate	1508197135	7012701841	0.015151515	1.31349112	↓
Avermectin A2b aglycone	24109241.57	7802215.52	0.041125541	1.108903112	↑
(R)-3-Hydroxybutyric acid	904429355.6	626464396.7	0.004329004	1.63797745	↑
L-Serine	360430680.4	103920061.9	0.008658009	1.380711515	↑
Creatinine	17257921.97	652624.96	0.025974026	1.582434358	↑

Name	BLANK	TAA	P. value	VIP	Trend
D-Proline	7539784.05	5649147.97	0.025974026	1.364124506	↑
Mesaconate	5120737.45	12871677.44	0.008658009	1.653657154	↓
Phenyl acetate	88520276.71	120631852.5	0.008658009	1.434194779	↓
O-Phosphoethanolamine	61068883.11	37091295.41	0.041125541	1.045995319	↑
(S)-5-Amino-3-oxohexanoate	29616074.67	15291137.47	0.008658009	1.350235147	↑
Oxoglutaric acid	1639185.9	4124026.5	0.025974026	1.379853975	↓
L-Xylonate	133763879.1	34249990.91	0.008658009	1.568668371	↑
3-(2-Hydroxyphenyl)propanoic acid	4313506.81	2758869.51	0.004329004	1.570269652	↑
D-Xylose	3890984.99	12316271.4	0.015151515	1.328313081	↓
myo-Inositol	6302649.66	18938150.63	0.002164502	1.417085283	↓
D-Phenylalanine	47620799.26	22282792.35	0.008658009	1.508503162	↑
Thioguanine	186415051.4	128123546.4	0.025974026	1.326225364	↑
Suberic acid	54701657.9	26604520.36	0.041125541	1.239880765	↑
1H-Indole-3-acetamide	3987901.35	1038777.15	0.025974026	1.143225055	↑
Hippuric acid	38981836.37	13241293.89	0.025974026	1.49063554	↑
N6-Acetyl-L-lysine	33722683.1	14798914.17	0.041125541	1.139322723	↑
N-Acetylglutamic acid	641798146.1	1354539885	0.025974026	1.221410167	↓
N-Acetylmethionine	80967277.26	19817801.33	0.002164502	1.780889894	↑
5-Hydroxyindoleacetic acid	33087481.21	67523145.97	0.008658009	1.56147629	↓
D-Glucuronic Acid	62849788.02	39526393.26	0.015151515	1.335459705	↑
L-Arogenate	5847835.77	4532079.06	0.041125541	1.258422662	↑
N-Acetyl-D-glucosamine	25821840.92	10727220.18	0.015151515	1.304866285	↑

Name	BLANK	TAA	P. value	VIP	Trend
Nicotinate D-ribonucleoside	49244262.37	31247051.95	0.008658009	1.461200076	↑
1-Hexadecanol	2270928.52	7879784.54	0.002164502	1.786619354	↓
2,7-Dihydroxy-4'-methoxyisoflavanone	2508094.49	4604204.42	0.041125541	1.037882572	↓
Estradiol	17679622.04	1698228.73	0.041125541	1.576425999	↑
6-Phospho-2-dehydro-D-gluconate	1836071.84	1057438.12	0.002164502	1.694171497	↑
Hexadecanedioate	34852928.54	11110239.95	0.041125541	1.234857958	↑
13-OxoODE	24810295.87	13320825.41	0.004329004	1.582618219	↑
Arachidic acid	196625633.2	68169126.73	0.025974026	1.251889569	↑
12,13-DHOME	668757041.1	190013396.2	0.004329004	1.417552226	↑
CMP	42035676.78	84387796.11	0.041125541	1.332352019	↓
11-Dehydrocorticosterone	289003280.3	30721449.31	0.015151515	1.602581614	↑
PGA1	6682043.49	1225764.74	0.025974026	1.068142218	↑
Erucic acid	8565595.89	29308264.22	0.008658009	1.489102027	↓
Cellobiose	595399994.5	161724898.1	0.025974026	1.474433263	↑
3'-AMP	14725560.95	37376774.01	0.025974026	1.574412937	↓
Prostaglandin F3a	1839180.25	4881778.16	0.041125541	1.108596895	↓
Lipoxin A4	14541905.51	1145850.63	0.002164502	1.784099143	↑
Xanthohumol	3651880.93	245552.98	0.004329004	1.694420883	↑
Rosmarinic acid	9311073.72	1461237.75	0.025974026	1.370539429	↑
Deoxycorticosterone acetate	36786802.38	7952640.87	0.015151515	1.475801303	↑
Deoxycholic acid	3835360.65	8737576.72	0.041125541	1.197882247	↓
Mitragynine	48244131.39	10134384.22	0.008658009	1.618130055	↑
LysoPA(16_0_0_0)	18443218.73	11380029.42	0.025974026	1.295796765	↑

Name	BLANK	TAA	P. value	VIP	Trend
Alpha-Tocotrienol	125320058.9	21913378.84	0.008658009	1.610847923	↑
Abscisic acid glucose ester	661408.6	4361895.19	0.004329004	1.615995902	↓
Phosphonoformyl-CMP	4065570.13	10331981.04	0.041125541	1.169086344	↓
Folic acid	3713942.23	9516408.09	0.008658009	1.554774818	↓
Adenylsuccinic acid	3190710.8	4837957.53	0.025974026	1.279728778	↓
Perfluorooctanesulfonic acid	9566321.78	4914666.82	0.002164502	1.677335518	↑
Telmisartan	922917.89	132228.39	0.002164502	1.715240001	↑
Probucol	1333496.52	5057138.03	0.008658009	1.475824282	↓
Leukotriene C4	641634.06	245586.35	0.041125541	1.225977377	↑
2-(S-Glutathionyl)acetyl glutathione	7387612.89	15735253.02	0.041125541	1.087845948	↓

Table S3 The metabolites significantly up-or down-regulated in VAH vs TAA (mean)

Name	VAH	TAA	P. value	VIP	Trend
Triethylamine	8972218.51	21484548.63	0.002164502	1.634962968	↓
Dimethylglycine	87109667.7	69569613.33	0.015151515	1.385529383	↑
gamma-Aminobutyric acid	30747273.14	6635177.77	0.025974026	1.222165991	↑
Benzaldehyde	89103202.05	43846690.03	0.002164502	1.687223362	↑
Cytosine	68358070.36	28127053.17	0.004329004	1.447887365	↑
1-Pyrroline-2-carboxylic acid	9029362.2	37620699.41	0.004329004	1.212386461	↓
Betaine	258730926	370952953.8	0.015151515	1.175117973	↓

Name	VAH	TAA	P. value	VIP	Trend
2-Methylserine	27860772.88	57427425.89	0.002164502	1.501102565	↓
Styrene Oxide	14541979.56	46595937.19	0.025974026	1.316007045	↓
4-Hydroxybenzaldehyde	55987370.27	38626449.35	0.041125541	1.00034657	↑
Taurine	147908460.2	106993673.7	0.025974026	1.020195866	↑
Triacetate lactone	172175580.6	77798553.51	0.008658009	1.256437312	↑
gamma-Amino-gamma-cyanobutanoate	14228507.84	73807618.61	0.002164502	1.560096014	↓
Pipecolic acid	321712502.9	1803344524	0.002164502	1.443523959	↓
L-Leucine	22499582.84	28559827.38	0.004329004	1.541601306	↓
cis-4-Hydroxy-D-proline	5563798.82	18092216.7	0.025974026	1.020164171	↓
2-Hydroxyphenethylamine	32602080.93	26910106.98	0.041125541	1.033451724	↑
1-Hydroxymethylnaphthalene	5225454.1	202709506.1	0.002164502	1.678909187	↓
Ectoine	8003196.92	13782967.01	0.002164502	1.511748343	↓
8-Hydroxyquinoline	180643353.9	311717432.3	0.004329004	1.299912331	↓
L-2-Hydroxyglutaric acid	18644739.99	12212918.75	0.008658009	1.354001764	↑
Diethylphosphoric acid	6958352.97	11427776.04	0.008658009	1.217654306	↓
Uracil 5-carboxylate	78312306.47	14414073.15	0.002164502	1.727521601	↑
Tryptamine	8454968.6	1329248.08	0.002164502	1.713541941	↑
N(6)-Methyllysine	38750309.86	23326235	0.015151515	1.163654768	↑
L-Rhamnono-1,4-lactone	17846948.93	12620908.45	0.002164502	1.393682452	↑
L-Carnitine	3132876643	6528207137	0.025974026	1.345417245	↓
Caffeic acid	5869030.65	3756431.75	0.002164502	1.545362052	↑
S-Methyl-L-methionine	39714852.96	25808457.35	0.015151515	1.272729821	↑
3,4-	501269638	1082424522	0.002164502	1.576656961	↓

Name	VAH	TAA	P. value	VIP	Trend
Dihydroxyphenylpropanoate					
e					
Jasmone	51491199.4	14361176.77	0.015151515	1.294519462	↑
D-synephrine	123384628.3	90645817.56	0.002164502	1.648351103	↑
Pyridoxamine	6896273.34	3675876.19	0.002164502	1.390358072	↑
(S)-4-Hydroxymandelate	14905503.09	88325917.71	0.002164502	1.521588023	↓
Tetrahydrodipicolinate	119079955.7	66572186.73	0.008658009	1.306132054	↑
Gabapentin	31328094.35	180048386.8	0.002164502	1.597880206	↓
Iminoarginine	131782496.1	34030769.36	0.002164502	1.526226402	↑
Formiminoglutamic acid	71203073.59	43078813.55	0.041125541	1.10681219	↑
2-Hydroxy-3-oxoadipate	23800390.15	21948699.81	0.041125541	1.088678172	↑
Canavanine	106115856.7	7163817.87	0.002164502	1.569682027	↑
N-Formyl-L-methionine	137940172.4	28682869.2	0.004329004	1.347157401	↑
Methyleugenol	33235914.04	168342569.2	0.002164502	1.61159344	↓
(S)-beta-Tyrosine	13170669225	1847322815	0.002164502	1.43717117	↑
Epinephrine	4465115.54	3004888.48	0.041125541	1.405381587	↑
Phosphorylcholine	862344934	4248831523	0.002164502	1.738073819	↓
(Z)-But-1-ene-1,2,4-tricarboxylate	8240523.66	3886006.03	0.002164502	1.18767512	↑
3-Indoleacrylate	19679378.52	6354151.63	0.004329004	1.304457339	↑
N1-Acetylspermidine	42992823.6	16846746.01	0.002164502	1.357038986	↑
Homocitrulline	36267318.21	10785566.71	0.041125541	1.109209966	↑
Isocitric acid	65331735.98	81408123.98	0.015151515	1.132671852	↓
3-Carbamoyl-2-phenylpropionaldehyde	68171039.42	2250035.5	0.002164502	1.655096955	↑

Name	VAH	TAA	P. value	VIP	Trend
Indolepyruvate	12015922.57	17771615.24	0.002164502	1.470856451	↓
N5-(L-1-Carboxyethyl)-L-ornithine	28591066.5	14424407.08	0.004329004	1.47912818	↑
Indolelactic acid	7277997.84	12225201.73	0.002164502	1.535777525	↓
(-)-Jasmonic acid	18591057.24	5455931.93	0.015151515	1.286921996	↑
Propionylcarnitine	97760309.62	19067853.14	0.002164502	1.50205879	↑
N-Acetylserotonin	26747256.83	39108787.82	0.025974026	1.125942033	↓
Gamma-glutamyl-L-putrescine	16396554.81	7827128.19	0.015151515	1.111789189	↑
gamma-Glutamylalanine	15576958.97	37368304.67	0.002164502	1.73806156	↓
Capsidiol	5451463.21	1851895.36	0.008658009	1.473806333	↑
8-Methoxykynurenate	18997830.15	6221198.67	0.015151515	1.361573979	↑
2-trans,6-trans-Farnesal	15739598.69	4913982.24	0.002164502	1.507826494	↑
Hydroxykynurenine	3362379.33	6811506.52	0.002164502	1.099978211	↓
N2-Succinyl-L-ornithine	4016256.74	12682335.5	0.002164502	1.340486815	↓
Confertifolin	22414523.35	4508674.95	0.008658009	1.297451496	↑
Carbamazepine	43760511.56	16717658.02	0.002164502	1.17139649	↑
Felbamate	11344995.13	5220527.21	0.015151515	1.176677905	↑
Equol	64403582.67	30630989.82	0.008658009	1.264742561	↑
Lumichrome	508275623.3	346809934.2	0.015151515	1.286161354	↑
Ribavirin	103261722.9	57456771.79	0.041125541	1.212081847	↑
Cytidine	369449772.4	264050524.7	0.002164502	1.138378734	↑
Uridine	395532964.6	124575654	0.008658009	1.196319389	↑
Biotin	3624414.08	8308373.22	0.002164502	1.626264182	↓
Pindolol	80227052.61	37141163.23	0.004329004	1.388357831	↑

Name	VAH	TAA	P. value	VIP	Trend
gamma-Glutamylcysteine	5627454.58	10391655.72	0.002164502	1.312377842	↓
Muramic acid	1029973975	516798227.6	0.002164502	1.388315584	↑
Daidzein	7123184.69	1643166.41	0.041125541	1.242174532	↑
Linatine	12956389.09	19389719.02	0.015151515	1.303728428	↓
Mannitol 1-phosphate	100493100.4	27488537.68	0.002164502	1.639739723	↑
Subaphylline	3796522.46	1660033.64	0.004329004	1.313233388	↑
Honokiol	63674542.25	14147290.69	0.002164502	1.387991709	↑
Adenosine	612067720.2	275188972	0.025974026	1.034343986	↑
Baicalein	7602296.94	5091998.09	0.025974026	1.130977222	↑
Aurin	16317253.66	10824290.67	0.025974026	1.230180023	↑
(2R,3R)-3-Methylglutamyl-5-semialdehyde-N6-lysine	7715296.75	2111893.98	0.004329004	1.551909582	↑
(2R,3R)-3-Methylornithinyl-N6-lysine	9408132.94	4650419.89	0.025974026	1.099093405	↑
Saccharopine	40857085.41	66819289.69	0.015151515	1.141892578	↓
Stearidonic acid	13595155.23	5295326.56	0.004329004	1.397688835	↑
1-(3,4-Dihydroxyphenyl)-5-hydroxy-3-decanone	13191600.71	7111497.65	0.002164502	1.525961722	↑
Oleic acid	1490412646	626596805.3	0.015151515	1.352413255	↑
Glycitein	10501523.72	426116.82	0.002164502	1.727838485	↑
Retinal	26453402.07	7815250.17	0.025974026	1.405296683	↑
L-Octanoylcarnitine	15842431.59	4786438.05	0.004329004	1.500971401	↑
13-L-Hydroperoxylinoleic acid	259190789.4	82161105.86	0.002164502	1.512652314	↑
Sumatriptan	1312943.24	17890386.47	0.002164502	1.556406168	↓

Name	VAH	TAA	P. value	VIP	Trend
9-cis-Retinoic acid	44073226.35	16312552.82	0.002164502	1.422318044	↑
19(S)-HETE	183818256.3	34623934.42	0.002164502	1.6785718	↑
N(6)-[(Indol-3-yl)acetyl]-L-lysine	36477036.7	22743937.68	0.008658009	1.173157421	↑
4'-Oxonebramine	28318568.75	13717152.73	0.002164502	1.375520714	↑
Capsaicin	2113634.68	7587543.25	0.025974026	1.167084265	↓
Aflatoxin B1	36454647.02	626688.27	0.002164502	1.714357691	↑
Decanoyl-L-carnitine	24419404.04	36177161.68	0.025974026	1.196880341	↓
15(S)-HPETE	972938.26	4161826.95	0.002164502	1.646640325	↓
L-Alanyl-gamma-D-glutamyl-L-lysine	2572775.54	1678405.09	0.008658009	1.352169465	↑
2-Hydroxy-6-pentadecylbenzoic acid	147161550.3	40259364.47	0.002164502	1.692204874	↑
6-Ketoprostaglandin E1	141213945.5	37388487.37	0.041125541	1.369536367	↑
(13E)-11a-Hydroxy-9,15-dioxoprost-13-enoic acid	28312086.29	4991254.49	0.002164502	1.439502722	↑
Nitrendipine	83078618.05	29747233.65	0.004329004	1.397450192	↑
Chelirubine	483358.73	32600532.77	0.002164502	1.527438774	↓
Cortisol	34863306.96	7422790.34	0.002164502	1.722842539	↑
GMP	97432181.9	32146455.64	0.002164502	1.648501978	↑
Isolithocholic acid	433368702.6	69395722.18	0.025974026	1.27679546	↑
11b,17a,21-Trihydroxypregnenolone	41953615.56	20811514	0.002164502	1.305063877	↑
Risperidone	128154720.3	1556498.77	0.002164502	1.706719571	↑
5alpha-Ergosta-7,22-diene	33099424.61	12900523.09	0.025974026	1.269497572	↑

Name	VAH	TAA	P. value	VIP	Trend
3beta,5-diol					
Glutathionylspermidine	2882232.24	292596.01	0.002164502	1.406615789	↑
S-Glutathionyl-L-cysteine	15690009.93	77975485.23	0.002164502	1.542489621	↓
Hecogenin	4384710.16	1532053.23	0.002164502	1.172671906	↑
Gentamicin C1a	4220091.17	18220474.28	0.002164502	1.564411437	↓
Isovitexin	345557988.7	133822832.5	0.008658009	1.079089888	↑
3-Dehydroecdysone	51237820.34	207169699.3	0.002164502	1.388804994	↓
3-Epiccdysone	244064955.6	24519160.13	0.002164502	1.529607307	↑
26-Hydroxyecdysone	470054957.9	111806528	0.004329004	1.368159378	↑
Taurochenodesoxycholic acid	512828287.6	69441000.58	0.004329004	1.430554396	↑
Deltaline	20587227.02	12874446.19	0.041125541	1.068772269	↑
Protoporphyrinogen IX	6861316.68	23727536.83	0.002164502	1.549005422	↓
NADP	61770534.04	16575865.49	0.015151515	1.273102252	↑
2-Ketobutyric acid	78040687.98	36128869.88	0.002164502	1.33229699	↑
(R)-3-Hydroxybutyric acid	789532321.5	626464396.7	0.025974026	1.295324926	↑
L-Serine	355173443.4	103920061.9	0.008658009	1.254942381	↑
Uracil	9634822.35	18145335.35	0.002164502	1.162773147	↓
Creatinine	17352976.19	652624.96	0.002164502	1.709992448	↑
D-Proline	6926787.89	5649147.97	0.015151515	1.248517709	↑
Threonate	10670297.79	2875861.87	0.002164502	1.400686061	↑
Mesaconate	7368317.25	12871677.44	0.025974026	1.219687066	↓
Phenyl acetate	81075619.15	120631852.5	0.002164502	1.455420877	↓
Salicylic acid	5314938.13	529427.88	0.004329004	1.387099508	↑
O-Phosphoethanolamine	10997681.34	37091295.41	0.002164502	1.31808914	↓

Name	VAH	TAA	P. value	VIP	Trend
1H-Indole-3-carboxaldehyde	21875967.4	66276494.79	0.002164502	1.525519571	↓
Oxoglutaric acid	1458646.33	4124026.5	0.025974026	1.218210172	↓
L-Glutamic acid	758696790.1	1860520154	0.008658009	1.195525003	↓
L-Xylonate	147173715.3	34249990.91	0.002164502	1.417008509	↑
3-(2-Hydroxyphenyl)propanoic acid	3778722.12	2758869.51	0.015151515	1.187016887	↑
D-Xylose	2342744.08	12316271.4	0.004329004	1.363943672	↓
D-Ribose	31137248.66	92427526.03	0.008658009	1.377390161	↓
Aminoadipic acid	8040410.41	44843961.38	0.002164502	1.647435182	↓
beta-D-Glucosamine	33357128.93	17165077.68	0.025974026	1.162791037	↑
1D-chiro-Inositol	13392001.16	76863861.83	0.002164502	1.368376337	↓
Thioguanine	242030713.2	128123546.4	0.015151515	1.280284762	↑
Taurocyamine	25471112.04	14043117.85	0.004329004	1.420015022	↑
Homogentisic acid	1606266.94	1116972.71	0.041125541	1.040482281	↑
Dehydroascorbate	41114009.02	80295145.01	0.041125541	1.030738115	↓
Pyrophosphate	1130318636	219630241.6	0.004329004	1.318525303	↑
Hippuric acid	32576620.96	13241293.89	0.041125541	1.011049686	↑
1-Keto-D-chiro-inositol	1172426.83	3337711.02	0.015151515	1.163894057	↓
L-Tyrosine	399183585.6	291167855.1	0.002164502	1.215573164	↑
Hydroxyphenyllactic acid	11465907.82	17777903.1	0.004329004	1.356046508	↓
N6-Acetyl-L-lysine	23148712.21	14798914.17	0.041125541	1.128129907	↑
Kynurenic acid	6333760.39	4383517.26	0.008658009	1.164314605	↑
N-Acetylglutamic acid	537012561.5	1354539885	0.008658009	1.238209312	↓

Name	VAH	TAA	P. value	VIP	Trend
N-Acetylmethionine	66187362.79	19817801.33	0.041125541	1.139643538	↑
5-Hydroxyindoleacetic acid	24441561.1	67523145.97	0.002164502	1.565756258	↓
Citric acid	653610571.9	969541924.5	0.025974026	1.238217068	↓
D-Glucuronic Acid	24013379.36	39526393.26	0.008658009	1.184717748	↓
Gluconic acid	2395087121	772081751.4	0.002164502	1.533653719	↑
L-Tryptophan	936600076.6	331531331.5	0.002164502	1.012640544	↑
Galactaric acid	11226689.45	52759081.08	0.004329004	1.53298995	↓
D-Ribulose 5-phosphate	117997.46	603299.06	0.002164502	1.354882622	↓
12-Hydroxydodecanoic acid	18287590.92	4533846.52	0.002164502	1.63550596	↑
N-Acetylmannosamine	93812363.05	139530834	0.041125541	1.045173416	↓
N-Acetyl-D-glucosamine	24785604.71	10727220.18	0.004329004	1.208909454	↑
Carnosine	27751109.57	11975841.21	0.008658009	1.151457157	↑
Ribose 1-phosphate	15218864.68	100151027.2	0.008658009	1.380980191	↓
Melatonin	8901232.59	1996106.12	0.002164502	1.334442843	↑
Biopterin	867893.66	5236161.11	0.002164502	1.36794038	↓
1-Hexadecanol	1060339.31	7879784.54	0.002164502	1.724189729	↓
Pseudouridine	2044997.16	2866252.05	0.025974026	1.004300264	↓
(S)-Pinoembrin	4231631.77	262265.92	0.002164502	1.572055329	↑
2,7-Dihydroxy-4'-methoxyisoflavanone	8318535.53	4604204.42	0.008658009	1.280906576	↑
17a-Estradiol	425636033.8	781749279.7	0.041125541	1.114212829	↓
Estradiol	12666348.21	1698228.73	0.002164502	1.420543213	↑
6-Phospho-2-dehydro-D-gluconate	1447384.38	1057438.12	0.002164502	1.416911983	↑
Pendimethalin	103931.75	1286122.26	0.002164502	1.398622856	↓

Name	VAH	TAA	P. value	VIP	Trend
Cinchonidine	17572357.06	5213527.34	0.025974026	1.246498451	↑
13-OxoODE	31386525.2	13320825.41	0.002164502	1.648661671	↑
(-)-Epigallocatechin	172982271	93867490.12	0.025974026	1.038985462	↑
11-Dehydrocorticosterone	299366778.4	30721449.31	0.002164502	1.562734342	↑
Acebutolol	491972.89	2422727.28	0.004329004	1.373826213	↓
Esculin	1553417.52	4537467.08	0.008658009	1.466158827	↓
Mannobiose	27458316.33	12411374.62	0.002164502	1.076969168	↑
3'-AMP	9107350.08	37376774.01	0.004329004	1.530403993	↓
Lipoxin A4	12315348.41	1145850.63	0.002164502	1.53724612	↑
Xanthohumol	2988909.1	245552.98	0.002164502	1.528746232	↑
Deoxycorticosterone acetate	22420600.66	7952640.87	0.002164502	1.597188988	↑
N-Acetylactosamine	1833080.65	1058964.34	0.004329004	1.139534064	↑
CDP	10029782.05	5411035.62	0.015151515	1.176381277	↑
Mitragynine	33264320.57	10134384.22	0.041125541	1.031257761	↑
LysoPA(16_0_0_0)	39100409.77	11380029.42	0.002164502	1.472790747	↑
Phosphonoformyl-CMP	2751007.72	10331981.04	0.025974026	1.143933081	↓
Folic acid	2301379.44	9516408.09	0.002164502	1.632566167	↓
CDP-Ethanolamine	1350866.22	5958358.75	0.002164502	1.411784751	↓
Perfluorooctanesulfonic acid	16619718.28	4914666.82	0.002164502	1.61560906	↑
ATP	2775615.93	1250204.92	0.041125541	1.09012785	↑
Telmisartan	506455.59	132228.39	0.041125541	1.034905898	↑
Leukotriene C4	914086.98	245586.35	0.002164502	1.352931281	↑
Depospho-CoA	32496675.62	8220822.17	0.004329004	1.369725967	↑

Table S4 The metabolites significantly up-or down-regulated in VAL vs TAA (mean)

Name	VAL	TAA	P. value	VIP	Trend
Triethylamine	8670283.75	21484548.63	0.002164502	1.729542949	↓
Dimethylglycine	94045708.71	69569613.33	0.004329004	1.537230692	↑
gamma-Aminobutyric acid	22801784.54	6635177.77	0.004329004	1.398174076	↑
Benzaldehyde	78133569.51	43846690.03	0.002164502	1.723977919	↑
Hydroquinone	23068969.57	80730813.33	0.015151515	1.56799616	↓
Cytosine	66146006.22	28127053.17	0.041125541	1.326527358	↑
Betaine	188752240.4	370952953.8	0.004329004	1.370689036	↓
2-Methylserine	26794183.39	57427425.89	0.002164502	1.45237958	↓
L-2,4-diaminobutyric acid	5383753.59	4054014.43	0.015151515	1.414273089	↑
Styrene Oxide	15337357.44	46595937.19	0.025974026	1.39550594	↓
4-Hydroxybenzaldehyde	54868445.14	38626449.35	0.041125541	1.101395754	↑
gamma-Amino-gamma-cyanobutanoate	29870600.17	73807618.61	0.041125541	1.271529286	↓
Pipecolic acid	402065342.5	1803344524	0.004329004	1.429608964	↓
5-Amino-2-oxopentanoic acid	34173878.89	88038538.19	0.002164502	1.521410282	↓
L-Isoleucine	10486968125	7671320348	0.002164502	1.668110117	↑
L-Leucine	24677980.7	28559827.38	0.025974026	1.240932757	↓

Name	VAL	TAA	P. value	VIP	Trend
1- Hydroxymethylnaphthalene	18361420.56	202709506.1	0.002164502	1.47079269	↓
Phosphonoacetate	44127881.63	70187689.44	0.041125541	1.215621944	↓
8-Hydroxyquinoline	126792224.6	311717432.3	0.008658009	1.281067444	↓
L-2-Hydroxyglutaric acid	25584062.6	12212918.75	0.002164502	1.442314449	↑
Tryptamine	6426959.52	1329248.08	0.002164502	1.701097147	↑
S-Carboxymethyl-L- cysteine	12830209.36	26401152.51	0.008658009	1.459154135	↓
L-Carnitine	3648831845	6528207137	0.025974026	1.231362498	↓
3,4- Dihydroxyphenylpropanoate	613186560.1	1082424522	0.008658009	1.493379551	↓
L-beta-Phenylalanine	53496132.36	35363988.25	0.025974026	1.229502851	↑
D-synephrine	131122860	90645817.56	0.002164502	1.706692348	↑
Pyridoxamine	6926151.32	3675876.19	0.041125541	1.000349439	↑
(S)-4-Hydroxymandelate	22124441.3	88325917.71	0.025974026	1.425529125	↓
Tetrahydrodipicolinate	132098495.6	66572186.73	0.004329004	1.489251373	↑
Gabapentin	62672978.49	180048386.8	0.015151515	1.490747292	↓
Iminoarginine	126170620.8	34030769.36	0.002164502	1.565467885	↑
(2S,5S)-trans- Carboxymethylproline	99765636.82	15626952.18	0.025974026	1.367330507	↑
Deisopropylatrazine	5587215.57	598403.97	0.041125541	1.262602628	↑
Formiminoglutamic acid	76766909.17	43078813.55	0.008658009	1.348714649	↑
Canavanine	90542624.51	7163817.87	0.002164502	1.656961531	↑
N-Formyl-L-methionine	88982948.27	28682869.2	0.025974026	1.061245043	↑
Cysteinylglycine	19422965.92	7368951.88	0.004329004	1.329278624	↑

Name	VAL	TAA	P. value	VIP	Trend
Methyleugenol	48108559.48	168342569.2	0.004329004	1.430902641	↓
(S)-beta-Tyrosine	10483729541	1847322815	0.004329004	1.481559253	↑
Sorbitol	256072524.2	53243418.24	0.004329004	1.35800101	↑
Epinephrine	4454423.47	3004888.48	0.025974026	1.318516812	↑
Phosphorylcholine	679683811.5	4248831523	0.002164502	1.64203297	↓
N1-Acetylspermidine	40167759.45	16846746.01	0.015151515	1.28805176	↑
Homocitrulline	79728290.61	10785566.71	0.002164502	1.392650273	↑
3-Carbamoyl-2-phenylpropionaldehyde	60361091.75	2250035.5	0.002164502	1.708613557	↑
3-Methyl-L-tyrosine	612616344.4	205909332.2	0.025974026	1.158033879	↑
N5-(L-1-Carboxyethyl)-L-ornithine	25408087.32	14424407.08	0.002164502	1.489057253	↑
Propionylcarnitine	82183298.07	19067853.14	0.002164502	1.56557485	↑
gamma-Glutamylalanine	18288333.22	37368304.67	0.002164502	1.22580805	↓
Capsidiol	5357918.45	1851895.36	0.004329004	1.649108489	↑
2-trans,6-trans-Farnesal	17709660.49	4913982.24	0.002164502	1.573467875	↑
Hydroxykynurenine	4661451.44	6811506.52	0.002164502	1.629572017	↓
N1-Acetylspermine	10458411.15	5790597.28	0.002164502	1.501179017	↑
Illudin M	26124198.95	6829636.26	0.041125541	1.110584249	↑
Lumichrome	555164072.8	346809934.2	0.015151515	1.33168047	↑
Biotin	3656934.36	8308373.22	0.002164502	1.233470827	↓
gamma-Glutamylcysteine	5040110.53	10391655.72	0.002164502	1.29977491	↓
Muramic acid	1102071788	516798227.6	0.041125541	1.166128307	↑
Daidzein	6728042.21	1643166.41	0.002164502	1.668885149	↑
Linatine	10616851.33	19389719.02	0.002164502	1.316636911	↓

Name	VAL	TAA	P. value	VIP	Trend
Mannitol 1-phosphate	96122298.99	27488537.68	0.002164502	1.679886774	↑
Subaphylline	7436368	1660033.64	0.004329004	1.550786148	↑
Retinol	145660059	234412737.6	0.004329004	1.363953918	↓
(2R,3R)-3-Methylglutamyl-5-semialdehyde-N6-lysine	8011762.85	2111893.98	0.002164502	1.621014174	↑
(2R,3R)-3-Methylornithinyl-N6-lysine	13001607.61	4650419.89	0.008658009	1.354225103	↑
Saccharopine	36562288.72	66819289.69	0.015151515	1.187069027	↓
Stearidonic acid	11696372.18	5295326.56	0.002164502	1.463595214	↑
1-(3,4-Dihydroxyphenyl)-5-hydroxy-3-decanone	19574151.67	7111497.65	0.002164502	1.594686032	↑
Oleic acid	1231925848	626596805.3	0.015151515	1.323666834	↑
Stearic acid	5035331.34	5823152.72	0.041125541	1.193910537	↓
Glycitein	7904661.92	426116.82	0.002164502	1.791941049	↑
Retinal	37256497.41	7815250.17	0.002164502	1.621948479	↑
Sumatriptan	758155.09	17890386.47	0.002164502	1.81574701	↓
Metoclopramide	12091013.8	8317267.49	0.015151515	1.130322632	↑
19(S)-HETE	137686977.8	34623934.42	0.002164502	1.627736174	↑
N(6)-[(Indol-3-yl)acetyl]-L-lysine	52115302.4	22743937.68	0.004329004	1.53601378	↑
4'-Oxonebramine	29486794.88	13717152.73	0.002164502	1.555485604	↑
Aflatoxin B1	28622492.05	626688.27	0.002164502	1.717242952	↑
Prostaglandin D2	1555067.23	12721827.44	0.025974026	1.166408314	↓
15(S)-HPETE	1204802.72	4161826.95	0.002164502	1.541694327	↓
Prostaglandin E1	10432291.89	4922620.77	0.041125541	1.058954211	↑

Name	VAL	TAA	P. value	VIP	Trend
L-Alanyl-gamma-D-glutamyl-L-lysine	3446311.69	1678405.09	0.002164502	1.514461237	↑
21-Deoxycortisol	29878505.5	18568445.01	0.008658009	1.20222112	↑
2-Hydroxy-6-pentadecylbenzoic acid	138609684.6	40259364.47	0.002164502	1.70787549	↑
Prostaglandin G2	34537846.3	4595308.3	0.041125541	1.131457938	↑
(13E)-11a-Hydroxy-9,15-dioxoprost-13-enoic acid	35182843.97	4991254.49	0.002164502	1.593304869	↑
8-Isoprostane	13605765.87	7909989.26	0.025974026	1.19738224	↑
Nitrendipine	104478109.9	29747233.65	0.002164502	1.517797075	↑
Chelirubine	1610915.59	32600532.77	0.015151515	1.432368316	↓
Cortisol	36301375.56	7422790.34	0.002164502	1.818609492	↑
GMP	100937203.4	32146455.64	0.002164502	1.59176501	↑
Isolithocholic acid	352280049	69395722.18	0.002164502	1.437278058	↑
Riboflavin reduced	18131057.85	6245619.81	0.004329004	1.294786511	↑
Risperidone	126759932.7	1556498.77	0.002164502	1.805762305	↑
5alpha-Ergosta-7,22-diene-3beta,5-diol	35569323.54	12900523.09	0.004329004	1.3888214	↑
Glutathionylspermidine	8822917.98	292596.01	0.002164502	1.735809886	↑
S-Glutathionyl-L-cysteine	35184492.38	77975485.23	0.004329004	1.624303463	↓
alpha-Tocopherol	59314743.47	28959996.05	0.015151515	1.430610162	↑
Hecogenin	13442254.15	1532053.23	0.025974026	1.230878229	↑
Gentamicin C1a	8841626.53	18220474.28	0.025974026	1.222218685	↓
Isovitexin	393592424.4	133822832.5	0.002164502	1.314609588	↑
3-Dehydroecdysone	84576318.42	207169699.3	0.015151515	1.055199412	↓

Name	VAL	TAA	P. value	VIP	Trend
3-Epiecdysone	211585591.8	24519160.13	0.025974026	1.13099153	↑
26-Hydroxyecdysone	752040552.8	111806528	0.004329004	1.533273267	↑
Taurochenodesoxycholic acid	814244290.2	69441000.58	0.002164502	1.65956488	↑
Antibiotic JI-20A	3380764800	1592274596	0.004329004	1.383512143	↑
Deltaline	23161812.24	12874446.19	0.041125541	1.322302882	↑
Protoporphyrinogen IX	10860629.5	23727536.83	0.025974026	1.245216076	↓
Avermectin A2b aglycone	27342206.9	7802215.52	0.015151515	1.339426993	↑
L-Serine	423964738.6	103920061.9	0.004329004	1.515617764	↑
D-Proline	7734009.78	5649147.97	0.002164502	1.639185965	↑
Threonate	8580531.59	2875861.87	0.004329004	1.420949749	↑
Pyroglutamic acid	34514587.32	8319304.64	0.008658009	1.324557302	↑
Ketoleucine	30623911.06	12703654.88	0.008658009	1.424852537	↑
Salicylic acid	3874554.77	529427.88	0.041125541	1.275040074	↑
O-Phosphoethanolamine	13068305.86	37091295.41	0.004329004	1.239488127	↓
(S)-5-Amino-3-oxohexanoate	24308006.46	15291137.47	0.041125541	1.137963448	↑
1H-Indole-3-carboxaldehyde	23864911.9	66276494.79	0.002164502	1.592422776	↓
L-Xylonate	95415069.65	34249990.91	0.008658009	1.424847614	↑
D-Xylose	2802505.87	12316271.4	0.008658009	1.398685525	↓
D-Glucose	6006243.98	22748569.36	0.004329004	1.528815643	↓
myo-Inositol	4671453.26	18938150.63	0.002164502	1.594265746	↓
D-Galactose	5554945.41	13163309.18	0.008658009	1.368912111	↓
1D-chiro-Inositol	22426781.23	76863861.83	0.041125541	1.068764884	↓

Name	VAL	TAA	P. value	VIP	Trend
Indole-3-carboxylic acid	7273537.13	16092368.14	0.041125541	1.152197445	↓
3-Methylxanthine	15078342.52	26624218.12	0.015151515	1.082367329	↓
Thioguanine	289123931.9	128123546.4	0.004329004	1.450927052	↑
Homogentisic acid	1784440.9	1116972.71	0.025974026	1.243362037	↑
Capric acid	20131150.26	6282503.62	0.008658009	1.447321263	↑
Pyrophosphate	1081444838	219630241.6	0.015151515	1.389837885	↑
1-Keto-D-chiro-inositol	828166.98	3337711.02	0.004329004	1.497500233	↓
D-Mannose	1699353034	587155668.6	0.004329004	1.142807787	↑
L-Tyrosine	495541687.6	291167855.1	0.002164502	1.377182716	↑
Hydroxyphenyllactic acid	11019523.16	17777903.1	0.004329004	1.375033136	↓
N6-Acetyl-L-lysine	38207280.76	14798914.17	0.002164502	1.652064679	↑
10-Hydroxydecanoic acid	3452723.79	1297562.74	0.041125541	1.202416437	↑
Azelaic acid	28255967.23	8591416.41	0.002164502	1.678718905	↑
Kynurenic acid	9607119.41	4383517.26	0.002164502	1.52871691	↑
N-Acetylglutamic acid	405669751	1354539885	0.004329004	1.580203298	↓
5-Hydroxyindoleacetic acid	22211790.39	67523145.97	0.002164502	1.64006908	↓
Gluconic acid	2354950938	772081751.4	0.002164502	1.658255958	↑
Galactaric acid	19638746.14	52759081.08	0.015151515	1.372259093	↓
D-Ribulose 5-phosphate	251579.65	603299.06	0.041125541	1.231123139	↓
12-Hydroxydodecanoic acid	11151208.9	4533846.52	0.004329004	1.499212805	↑
N-Acetyl-D-glucosamine	42777505.04	10727220.18	0.002164502	1.531923805	↑
Biopterin	1455349.55	5236161.11	0.025974026	1.084805431	↓
1-Hexadecanol	1504048.17	7879784.54	0.002164502	1.822984509	↓
Pseudouridine	1669870.71	2866252.05	0.002164502	1.470770422	↓
Gemfibrozil	4033366.87	2728424.31	0.025974026	1.165972942	↑

Name	VAL	TAA	P. value	VIP	Trend
(S)-Pinocembrin	3375149.68	262265.92	0.002164502	1.584372446	↑
Genistein	2251725.64	8319631.39	0.002164502	1.457952874	↓
17a-Estradiol	283910038.8	781749279.7	0.004329004	1.503516012	↓
Estradiol	16946366.45	1698228.73	0.002164502	1.721983739	↑
Hexadecanedioate	20134787.01	11110239.95	0.041125541	1.012715938	↑
Cinchonidine	16709160.1	5213527.34	0.002164502	1.447698284	↑
5'-S-Methyl-5'-thioinosine	1739265.85	1082365.32	0.008658009	1.394024548	↑
(-)-Epigallocatechin	492839535.1	93867490.12	0.002164502	1.409456168	↑
9(S)-HPODE	6487275	13888812.46	0.041125541	1.122707986	↓
11-Dehydrocorticosterone	163901921.7	30721449.31	0.002164502	1.568207112	↑
Aspartylglycosamine	65078582.5	34920152.17	0.025974026	1.258160141	↑
8,9-DiHETrE	26768049.13	54317663.16	0.015151515	1.30876002	↓
Erucic acid	13687793.79	29308264.22	0.041125541	1.261326055	↓
Esculin	1571868.38	4537467.08	0.008658009	1.407902132	↓
3'-AMP	14662698.53	37376774.01	0.015151515	1.121923299	↓
S-(2-Hydroxyethyl)glutathione	33531211.99	5973437.36	0.025974026	1.230944075	↑
Xanthohumol	1969081.72	245552.98	0.002164502	1.55823159	↑
Rosmarinic acid	33728548.97	1461237.75	0.002164502	1.522981624	↑
Deoxycorticosterone acetate	21426811.84	7952640.87	0.002164502	1.63101027	↑
N-Acetyllactosamine	3390177.23	1058964.34	0.002164502	1.316857439	↑
Mitragynine	20574538.04	10134384.22	0.041125541	1.229017244	↑
25-Hydroxycholesterol	4660900.04	7810105.04	0.008658009	1.335927227	↓
Allocholic acid	117605534.3	31656556.92	0.004329004	1.555309592	↑
LysoPA(16_0_0_0)	28735695.61	11380029.42	0.004329004	1.432262723	↑

Name	VAL	TAA	P. value	VIP	Trend
Trehalose 6-phosphate	487757929.4	127049598.9	0.004329004	1.445227317	↑
Phosphonoformyl-CMP	1311207.7	10331981.04	0.015151515	1.485031631	↓
Folic acid	3436425.13	9516408.09	0.002164502	1.037226194	↓
CDP-Ethanolamine	1994788.21	5958358.75	0.004329004	1.414725468	↓
Perfluorooctanesulfonic acid	12134353.66	4914666.82	0.015151515	1.478890255	↑
Telmisartan	747673.4	132228.39	0.004329004	1.361965878	↑
Leukotriene C4	884172.46	245586.35	0.015151515	1.365176891	↑
NAD	9556997.65	42217108.25	0.015151515	1.196052652	↓
Dephospho-CoA	56300843.38	8220822.17	0.004329004	1.51547609	↑