

SUPPLEMENTARY TABLES

Supplementary Table 1. Metabolic differences in GC between group A and group C.

Metabolite	T	P-value	Log ₁₀ P-value	FDR	VIP	Foldchange	Log ₂ FC
Indole	-4.5677	9.04E-05	4.044	0.016995	2.8654	3.428414701	1.778
Maleic acid	4.2874	0.00019359	3.7131	0.016995	2.7606	0.357359826	-1.485
Se-Methylselenocysteine	-4.2841	0.00019535	3.7092	0.016995	2.7593	5.618608832	2.491
Vanillylmandelic acid	-3.9404	0.00049288	3.3073	0.03216	2.619	2.934616739	1.554
CMP	3.5798	0.0012801	2.8928	0.06682	2.4571	0.399632338	-1.324
4,5-Dihydroorotic acid	3.4071	0.0020054	2.6978	0.085415	2.3739	0.251218409	-1.993
O-Acetyls erine	-3.3207	0.0025045	2.6013	0.085415	2.3309	4.810236183	2.267
Gluconic acid	3.3033	0.0026181	2.582	0.085415	2.3221	0.461510061	-1.116
Glutathione	3.1904	0.0034891	2.4573	0.092316	2.2642	0.34135518	-1.551
Cytidine	-3.1497	0.0038663	2.4127	0.092316	2.2429	5.125313925	2.358
Isobutyric acid	-3.0903	0.0044877	2.348	0.092316	2.2114	4.994256605	2.321
Gentisic acid	3.0805	0.0045981	2.3374	0.092316	2.2062	0.047821721	-4.387
(R)-5,6-Dihydrothymine	2.6047	0.014556	1.837	0.23744	1.9366	0.286270468	-1.805
gamma-Aminobutyric acid	2.5564	0.016287	1.7882	0.25005	1.9076	0.148290947	-2.754
Sucrose	2.4686	0.019934	1.7004	0.28904	1.8539	0.377429704	-1.406
NAD	-2.4361	0.021462	1.6683	0.29483	1.8338	2.036908787	1.027
Uridine diphosphate glucuronic acid	2.3062	0.028716	1.5419	0.36332	1.752	0.490942118	-1.027
Oleic acid	2.2837	0.030179	1.5203	0.36332	1.7376	0.144795332	-2.788
5-Aminopentanoic acid	-2.1376	0.041418	1.3828	0.43813	1.6425	4.278440936	2.098
L-Formylkynurenine	-2.1315	0.041966	1.3771	0.43813	1.6384	2.748385324	1.459
Fructose 1,6-bisphosphate	-2.0575	0.049058	1.3093	0.44056	1.5892	2.159547359	1.111

Supplementary Table 2. Metabolic differences in FF between group A and group C.

Metabolite	T	P-value	Log ₁₀ P-value	FDR	VIP	Foldchange	Log ₂ FC
Isoproterenol	-6.9644	1.43E-07	6.8458	3.34E-05	1.8807	7.37E+05	19.492
Triethylamine	-6.2224	1.01E-06	5.9966	8.29E-05	1.7993	1.14E+06	20.126
gamma-L-Glutamyl-L-2-aminobutyrate	6.0979	1.41E-06	5.8518	8.29E-05	1.7839	0.247286036	-2.016
Tryptophanamide	-6.0953	1.42E-06	5.8487	8.29E-05	1.7836	4.270401845	2.095
N-Acetyl-D-glucosamine	5.8721	2.58E-06	5.5879	0.00012089	1.7546	0.474585924	-1.076
2-Aminoacrylic acid	-5.3574	1.04E-05	4.981	0.00034924	1.6805	14.21039917	3.829
4-Hydroxyphenylacetaldehyde	5.2649	1.34E-05	4.8713	0.00039337	1.6659	0.395350676	-1.339
Orciprenaline	-5.2202	1.52E-05	4.8184	0.00039499	1.6588	4.282288455	2.099
N-Acetylaspartylglutamic acid	4.8964	3.68E-05	4.434	0.00078318	1.6042	0.220191567	-2.184
Dihydrothymine	-4.7247	5.89E-05	4.2302	0.00097657	1.5731	19.52476717	4.288
Norepinephrine	-4.719	5.98E-05	4.2234	0.00097657	1.5721	102.5188891	6.68
L-Allothreonine	-4.7054	6.21E-05	4.2072	0.00097657	1.5695	2.54E+04	14.632
Guanine	4.6224	7.78E-05	4.1088	0.0010808	1.5539	0.183921576	-2.443
Dihydrouracil	4.6191	7.85E-05	4.105	0.0010808	1.5533	0.275095596	-1.862
N-Carbamoylputrescine	-4.5819	8.69E-05	4.0609	0.00113	1.5461	3.433476395	1.78

13-L-Hydroperoxylinoleic acid	-4.3593	0.0001593	3.7978	0.001962	1.5018	13.99678074	3.808
5-Guanidino-3-methyl-2-oxopentanoate	4.3391	0.00016829	3.7739	0.001969	1.4977	0.389878748	-1.359
9,12,13-TriHOME	4.2617	0.00020756	3.6829	0.0022076	1.4815	0.470278405	-1.089
1-Hydroxy-2-naphthoate	-4.2161	0.00023479	3.6293	0.0022892	1.4719	7.259001161	2.86
Guanosine	4.1625	0.00027136	3.5665	0.0025399	1.4603	0.380474071	-1.395
Quadrone	4.089	0.00033087	3.4803	0.0028615	1.4442	0.227603787	-2.136
Dehydroepiandrosterone	4.082	0.00033712	3.4722	0.0028615	1.4427	0.346860909	-1.528
L-Histidine trimethylbetaine	-4.0174	0.0004011	3.3968	0.0031904	1.4282	2.218721573	1.15
9-Riburonosyladenine	3.9965	0.00042419	3.3724	0.0031904	1.4235	0.439251515	-1.187
Linoleic acid	-3.986	0.00043629	3.3602	0.0031904	1.4211	2.089951513	1.064
Quinacrine	3.9617	0.00046558	3.332	0.0032758	1.4156	0.266865927	-1.906
Sorbitol	-3.9535	0.00047597	3.3224	0.0032758	1.4137	5.502366017	2.461
Vitamin D3	3.9396	0.0004939	3.3064	0.0033021	1.4105	0.202691746	-2.303
Ketoleucine	-3.9189	0.00052201	3.2823	0.003393	1.4057	3.788022274	1.922
L-Phenylalanine	3.8321	0.000658	3.1818	0.0040519	1.3854	0.214924347	-2.219
Biliverdin	-3.761	0.00079453	3.0999	0.004648	1.3684	2.479297863	1.31
15-Deoxy-d-12,14-PGJ2	3.6853	0.00097045	3.013	0.0055387	1.3499	0.493315574	-1.02
Carnosine	-3.521	0.0014926	2.8261	0.007938	1.3085	6.58E+04	16.007
Ritodrine	-3.5015	0.0015702	2.804	0.0081651	1.3034	1616.448985	10.659
Butyryl-L-carnitine	3.4557	0.0017688	2.7523	0.0089978	1.2915	0.267301061	-1.904
4-Quinolinecarboxylic acid	3.4448	0.0018192	2.7401	0.0090147	1.2886	0.361807591	-1.467
12-Keto-tetrahydro-leukotriene B4	-3.4362	0.0018604	2.7304	0.0090147	1.2864	4.30200043	2.106
14alpha-Hydroxy-5beta-cholest-7-ene-3,6-dione	-3.4273	0.0019037	2.7204	0.0090147	1.284	2.21E+05	17.752
N-Acetyl-L-2-amino-6-oxopimelate	3.3803	0.002149	2.6678	0.0098602	1.2715	0.415282392	-1.268
Acetylphosphate	3.3568	0.0022829	2.6415	0.010273	1.2652	0.29549081	-1.759
Qing Hau Sau	3.3461	0.0023462	2.6296	0.010359	1.2624	0.325913372	-1.618
Fomepizole	-3.3328	0.0024279	2.6148	0.010521	1.2588	4.853190973	2.279
cis,cis-Muconate	-3.2662	0.002878	2.5409	0.012244	1.2406	13.51460929	3.757
Docosapentaenoic acid (22n-3)	3.2134	0.0032919	2.4826	0.013514	1.226	0.241995983	-2.047
O-Phosphoethanolamine	-3.1679	0.0036926	2.4327	0.014671	1.2132	2.627913699	1.394
Phthalic acid	-3.1641	0.0037283	2.4285	0.014671	1.2122	2.820954047	1.497
2-Oxoarginine	3.1157	0.0042106	2.3757	0.015703	1.1984	0.250909547	-1.995
Adrenic acid	3.0881	0.0045124	2.3456	0.016285	1.1905	0.161561329	-2.63
D-Arabitol	-3.0756	0.0046548	2.3321	0.01642	1.1869	3.329448976	1.736
UMP	3.0716	0.0047016	2.3278	0.01642	1.1858	0.173767985	-2.525
Methyl jasmonate	-3.0515	0.004943	2.306	0.01701	1.18	3.239495934	1.696
9(S)-HPODE	3.0264	0.0052621	2.2788	0.017479	1.1726	0.268643886	-1.897
D-Glucose	-3.0196	0.0053507	2.2716	0.017479	1.1707	4.406062742	2.14
3-Aminopentanedioate	-2.9192	0.006853	2.1641	0.021373	1.1409	6.62E+04	16.015
Palmitic acid	-2.9144	0.0069352	2.1589	0.021373	1.1395	2.553952241	1.353
Alpha-dimorphecolic acid	-2.9136	0.0069479	2.1581	0.021373	1.1393	2.082075413	1.059
Succinic acid	2.9052	0.0070926	2.1492	0.021373	1.1367	0.29856985	-1.744
Adenosine	2.9034	0.0071244	2.1473	0.021373	1.1362	0.172532781	-2.536
L-Isoleucine	2.8921	0.0073237	2.1353	0.021422	1.1328	0.333055787	-1.587

2-Ketobutyric acid	2.8326	0.0084619	2.0725	0.024147	1.1147	0.398596939	-1.327
(R)-3-Hydroxybutyric acid	-2.7652	0.009954	2.002	0.027729	1.0939	4.006570776	2.003
5a-Pregnane-3,20-dione	2.743	0.010498	1.9789	0.028564	1.087	0.498753117	-1.004
Glycochenodeoxycholic acid	-2.7297	0.010837	1.9651	0.028864	1.0828	118.2718123	6.886
L-Asparagine	-2.7255	0.010944	1.9608	0.028864	1.0815	30.61474406	4.937
Oxoadipic acid	-2.7229	0.011012	1.9581	0.028864	1.0807	3.349186148	1.744
(S)-4-Amino-5-oxopentanoate	2.7195	0.011102	1.9546	0.028864	1.0797	0.269063122	-1.894
Mitragynine	2.703	0.011546	1.9376	0.029366	1.0745	0.494951495	-1.015
Pyroglutamic acid	-2.6426	0.013317	1.8756	0.033507	1.0553	3.647372068	1.867
Alpha-Linolenic acid	-2.6225	0.01396	1.8551	0.034387	1.0489	2.172165867	1.12
(R)-2,3-Dihydroxy-isovalerate	2.5819	0.01535	1.8139	0.036653	1.0358	0.440295879	-1.184
Myristic acid	2.5664	0.015915	1.7982	0.037616	1.0307	0.41322314	-1.276
L-4-Hydroxyphenylglycine	-2.4813	0.019362	1.7131	0.043825	1.0028	25.2016129	4.656