

Table S1. Raw data of metabolomics-normal groups

Index	Platform	Name	N01pre	N02pre	N03pre	N04pre	N05pre	N06pre	N07pre	N08pre	N09pre	N01post	N02post	N05post	N06post	N07post	N08post	N09post	N10post	N11post
1	GC	2-Hydroxy-3-methylbutyric acid	47257	57278	47522	51007	31117	56307	55674	48178	49551	63619	23634	25909	47330	18920	68846	18396	30398	25344
2	GC	2-Hydroxybutyric acid	21709	29255	40942	20296	33997	29209	37748	23037	34241	88144	14217	11950	47441	8560	60515	5117	18705	11717
3	GC	2-Hydroxypyridine	37927	45534	73218	41334	31033	44599	89618	38040	41803	30130	64422	125123	46759	35218	34075	26324	36303	36441
4	GC	3-Methyl-2-oxovaleric acid	7717	8044	15660	12887	12306	13642	15617	12549	15151	10107	9449	3706	7634	5393	7543	5642	12738	7378
5	GC	Acetylglycine	13422	11908	4429	10439	12959	11905	3909	9769	11158	6535	2507	475	8854	4315	9998	3301	5744	5708
6	GC	Alpha-ketoisovaleric acid	695	798	864	812	747	735	716	723	815	775	292	562	602	487	518	518	582	490
7	GC	Aminomalonic acid	7805	9852	6726	5360	4526	5168	5220	5857	5699	6689	13820	8018	9320	10285	8925	8466	9052	7932
8	GC	Arachidonic acid	9734	8488	10631	5731	5297	6541	7613	7922	6376	4844	6801	5728	3856	4147	4986	3867	4898	3963
9	GC	Benzoic acid	1913	1882	2566	2954	4084	2759	6368	3576	2660	1606	3229	4420	2862	2557	2522	2428	2554	2203
10	GC	Beta-Alanine	2560	2146	932	1572	2711	1777	3625	1785	1400	2287	2328	1942	2124	1391	2365	1253	1552	1353
11	GC	Cholesterol	154172	139425	175819	137848	124146	143585	159087	158012	159329	146808	220012	215225	151290	163307	157341	155819	137602	138210
12	GC	cis-4-Hydroxy-L-proline	13139	11188	16521	9712	11841	9495	11109	10923	8353	9547	15436	17047	4339	18357	10481	18048	12084	19091
13	GC	Citrulline	5283	4678	4807	4630	6223	5495	5185	4561	5189	7075	4302	6344	5759	4701	7263	5039	4543	5062
14	GC	Creatinine	197598	131174	180699	178454	103830	170239	91114	182411	183795	136323	78262	82259	84953	75402	216509	86120	75831	83604
15	GC	D-Galactose	6961	5637	5920	3636	7660	5849	6964	4177	5159	6070	1689	2812	3459	3174	7076	1562	3001	2823
16	GC	D-Mannose	6542	2219	9011	4482	4828	1110	4466	3555	2759	3439	9211	6762	4575	5979	3962	9252	6294	7853
17	GC	Docosaehaenoic acid	4511	4356	5176	3167	2644	2949	3556	3086	2445	2718	2386	2686	1909	1692	2796	1159	1580	1403
18	GC	Dodecanoic acid	73361	88152	108703	48166	72097	82096	93322	67213	88035	45156	14210	16273	26056	14916	41644	19447	18331	15771
19	GC	D-Threitol	3678	3061	2908	2349	2787	2163	3440	2314	2367	4189	3822	3531	4262	2672	12083	2182	2947	2940
20	GC	D-Xylose	38890	48278	26687	47918	36927	61060	68584	66834	48013	27659	91509	70850	30289	50375	35427	44583	40446	43019
21	GC	Elaidic acid	141159	145492	186647	95806	135004	108463	146344	132204	108030	158301	105291	112184	124426	78749	165498	100813	100944	75433
22	GC	Ethanolamine	38716	29040	43495	27613	28062	25967	18841	24043	26227	15451	45154	31996	30010	25992	25496	25998	25662	26682
23	GC	Fumaric acid	3934	2503	4296	2273	4651	2532	4698	2394	2512	1998	4379	2444	1351	2843	1348	3366	3380	3016
24	GC	Galactonic acid	2866	2168	3254	2088	3234	2316	3463	1881	2191	2645	2563	1933	2111	1596	5356	1697	1588	1993
25	GC	Gluconolactone	48877	97860	24188	118857	100651	59636	109957	119677	50840	45121	92418	183593	63416	197285	130254	57009	105075	143360
26	GC	Glutaric acid	916	1037	1513	787	930	1297	1787	599	1138	1118	1041	819	932	669	842	561	521	776
27	GC	Glyceric acid	1665	1222	2079	1721	2300	2681	632	3238	2576	3385	3061	2670	1645	2536	4680	3680	6347	3196
28	GC	Glycerol	717099	273617	954907	637942	431168	367655	406610	552668	786686	469277	604310	642016	386474	475418	496313	595043	438762	570216
29	GC	Glycerol 3-phosphate	22752	20818	21720	15232	11396	13505	15701	12523	11348	10927	24755	21908	9993	15298	10921	13147	12249	13774
30	GC	Glycine	323552	244738	466608	231518	312372	254008	400314	272972	260594	252353	621874	623826	249548	444420	257328	429801	408689	488624
31	GC	Glycolic acid	58428	51555	61991	42214	47926	52941	82722	68821	47908	18131	69015	55382	16687	57842	16416	49305	75772	71970
32	GC	Heptadecanoic acid	685536	436044	734515	553263	786220	578292	707393	552313	581883	663640	723325	646613	594815	646135	515933	758007	551102	596642
33	GC	Isocitric acid	35971	164796	142175	150431	106070	125424	175989	112316	151977	89539	118260	142631	78468	100621	61532	71510	96673	166492
34	GC	Ketoleucine	880	725	1587	1387	1255	1467	1751	1398	1748	1060	827	773	587	397	807	382	1073	589
35	GC	L-Alanine	268145	160447	222814	200076	234026	200648	106262	212006	212190	201348	261810	275968	225541	324861	257102	502155	272483	366441
36	GC	L-Alpha-aminobutyric acid	8798	8811	9966	7080	10795	10567	5001	8918	11155	7857	7346	9207	11504	9006	8684	6648	8864	9567

37	GC	L-Arabinose	1429	1779	2202	1636	1892	2897	3909	2845	2094	2055	3007	1716	1845	2770	3849	3855	2590	3786
38	GC	L-Arabitol	1256	1980	3055	1981	4328	1482	8000	2226	1387	973	5628	5007	991	4435	1359	5579	3566	4109
39	GC	L-Arginine	8095	7264	8561	9271	15223	9333	8731	9090	9631	7845	7281	8601	7674	9034	10858	19893	10330	10334
40	GC	L-Aspartic acid	11050	5603	11988	7026	8445	7341	9674	6445	7303	12909	17899	13036	7693	11255	8840	11105	9406	13318
41	GC	L-Glutamic acid	5549	3324	6801	3281	4857	3420	5576	4013	3327	4445	8161	7159	3168	5325	3732	7762	5626	7109
42	GC	L-Glutamine	248241	279432	92017	294578	242263	271738	187328	283369	252521	144561	132938	132510	194512	339132	245070	278499	304614	364817
43	GC	Linoleic acid	43806	47243	56438	24092	26333	36828	35027	27964	31682	17952	13039	16130	10994	10531	20506	10087	11709	9194
44	GC	L-Lactic acid	340041	584671	1452330	2043675	416756	1427266	1024431	809976	1383026	1770471	1514890	703146	1745565	365232	460199	1772718	1148608	226972
45	GC	L-Leucine	103081	96359	142182	119017	140593	153535	102933	119723	131770	221795	74159	62334	130909	50554	112639	61514	94917	73903
46	GC	L-Lysine	139063	93828	162958	135158	127193	122404	146361	114510	124490	133267	199072	239120	110856	160855	131916	169203	145588	140568
47	GC	L-Methionine	22571	18527	28398	19811	19670	21840	24354	21774	19206	19850	28251	43304	16327	20269	19944	26331	21498	20912
48	GC	L-Phenylalanine	28181	25934	44670	29451	32695	33280	39571	31774	31965	50587	34903	46500	44889	19072	50092	28374	32729	26321
49	GC	L-Pipecolic acid	9722	7667	2462	7433	8286	7928	822	7402	8836	4780	1458	549	6784	4868	7754	6104	4376	5270
50	GC	L-Proline	122563	98637	112359	105195	96464	103362	34018	100465	105152	105960	97995	83172	88519	109759	124187	184211	120835	128375
51	GC	L-Serine	63084	49449	68056	51396	53505	56455	47658	55148	53291	68433	113423	100783	64678	89275	70214	92522	73005	77602
52	GC	L-Sorbose	81335	186593	37110	206703	170928	104937	193328	203763	79016	74647	220575	282045	111304	360136	246650	136711	207515	370894
53	GC	L-Threonine	64569	53001	76597	57691	56526	62589	61063	63100	66570	104441	83529	89354	90533	64546	111701	77564	73671	68883
54	GC	L-Tryptophan	77624	61478	90601	106015	67645	94731	85468	104245	92467	61801	139827	107617	67166	86867	58477	86468	121400	115852
55	GC	L-Tyrosine	58091	37011	53733	42881	44014	50732	56500	50493	50960	55090	88181	100352	40570	49168	59476	67884	46854	52191
56	GC	L-Valine	199215	171211	229346	212199	255575	276871	145047	237613	241684	346880	128799	122746	244592	101050	390443	156858	190371	161888
57	GC	Maleic acid	8228	8394	8587	6277	6708	8072	6953	2503	7566	7949	4370	4509	6358	4007	8999	2613	4064	5022
58	GC	Malic acid	32321	23802	42119	24222	21088	26471	29971	20550	25327	18380	41333	24292	13369	28851	13860	26030	31233	29452
59	GC	Methylmalonic acid	2049	2174	1938	1553	1493	1972	2285	1923	2373	2038	1521	1069	1829	1353	4111	1189	1276	1024
60	GC	MG(18:0(9Z)/0:0/0:0)	1341	1268	2099	1350	1487	2216	2192	1799	1763	1478	1056	1758	1835	1423	956	1184	1063	1068
61	GC	Myristic acid	94501	103690	134793	60981	79573	95027	102907	76140	93741	75018	20690	22240	45175	20761	79137	18172	22470	27500
62	GC	Myristoleic acid	4736	4812	6335	3147	3766	4136	3013	2834	3934	4136	1618	1386	2835	1801	5016	1087	1614	2249
63	GC	Nonadecanoic acid	1576	1583	1967	1160	1835	1333	2123	1574	1376	1222	1585	1242	1422	1255	1574	1177	1405	1377
64	GC	Oleic acid	19652	27426	23961	12201	14545	17570	17782	19677	19225	17307	10993	10020	15127	6736	18252	10242	10449	9944
65	GC	O-Phosphoethanolamine	4060	3623	6864	4239	7067	4083	6216	3874	4614	8628	6907	9031	6268	5212	6159	3853	4846	5836
66	GC	Oxalic acid	11153	13755	13190	15432	17519	19184	20675	20292	20999	29432	24251	15285	23461	21874	32955	21089	27305	20683
67	GC	Oxoglutaric acid	8369	7159	7397	6915	1823	7425	4225	5388	7768	4882	7487	2624	3604	5778	3709	2083	4869	5745
68	GC	Palmitic acid	655406	538480	555881	537811	619688	673801	633331	626269	636727	634980	370667	400918	477909	310468	676934	290127	377236	320054
69	GC	Palmitoleic acid	136203	141622	158149	87177	87536	113854	98558	81463	104991	118352	31823	37163	52995	34680	105707	25871	32434	45052
70	GC	Pantothenic acid	879	855	1047	333	809	832	967	350	784	1735	1422	1420	1176	565	2952	1077	638	546
71	GC	Pelargonic acid	3340	2911	6173	4157	4570	4542	6236	7336	2092	3305	4926	7171	6258	4634	3637	3330	5300	2687
72	GC	Petroselinic acid	268293	329105	336397	181246	213074	281766	260207	223456	230470	257103	102702	123124	123448	96792	227333	86854	116299	113068
73	GC	Phosphoric acid	425679	451165	530501	500915	590664	521109	576876	477133	604620	33088	518234	531686	486577	547291	63425	655737	629228	637862
74	GC	Pyroglutamic acid	269525	230457	423273	228983	203535	239268	310631	224288	219858	270552	446801	472485	239004	310088	251246	251743	264111	290392
75	GC	Pyruvic acid	44121	36161	61923	46638	43684	43188	62383	56975	45531	26577	53957	57880	21391	41804	14755	36352	27738	45406
76	GC	Rhamnose	9853	10246	10494	8886	7656	10538	11028	7272	8323	13842	10714	13331	13067	8441	28985	7243	9027	8908

77	GC	Sorbitol	4799	3410	4336	2769	2298	3716	4217	2526	3075	3243	1072	3617	3013	4304	671	1974	4105	5451
78	GC	Taurine	427852	244913	384070	242680	22717	245094	132881	13016	93227	446665	382662	277899	258628	272284	432428	5264	35283	106231
79	GC	Uracil	2700	1462	2825	2330	2582	1805	2694	1695	2139	2533	3210	3426	2580	2303	3599	2642	2612	3604
80	GC	Urea	131541	158824	122651	127698	10321	164126	195439	190195	192394	147973	172544	138206	132516	95451	134371	223776	117834	192198
81	GC	Uric acid	13791	11431	7463	9144	8705	10423	10930	9282	7248	9180	23455	12003	10914	10701	8930	10918	16933	11307
82	BA	CA	8.47	19.62	13.58	12.62	2.98	41.69	7.71	9.56	34.80	3.23	3.31	30.34	2.01	7.39	1.17	7.91	7.48	10.05
83	BA	aMCA	41.97	28.43	73.59	30.70	1.50	114.49	7.74	28.48	58.02	7.46	6.94	17.38	7.78	2.80	3.89	5.47	12.60	43.54
84	BA	bMCA	88.76	94.32	146.24	102.77	41.89	230.17	52.66	115.97	274.58	25.78	33.70	54.47	17.61	38.93	31.90	29.68	38.10	69.07
85	BA	wMCA	65.37	67.53	66.87	65.49	54.24	72.93	63.67	64.08	70.96	66.45	64.26	65.84	63.64	64.84	64.92	64.49	67.27	65.53
86	BA	DCA	33.89	83.84	77.36	37.86	207.13	33.96	3.80	15.34	38.23	6.73	6.54	13.91	1.13	8.73	3.72	3.37	4.59	14.77
87	BA	LCA	568.93	242.36	1719.38	267.31	377.11	1471.47	643.39	389.39	411.49	653.96	643.98	494.50	217.94	909.71	320.62	1884.05	962.59	813.54
88	BA	UDCA	11.07	32.23	21.31	5.64	2.24	16.39	2.38	5.17	20.11	3.10	2.75	3.97	1.27	0.39	1.29	2.02	1.36	4.20
89	BA	HDCA	41.28	266.93	241.04	49.57	89.92	393.41	22.88	55.83	318.03	12.78	18.98	46.88	5.83	17.81	6.98	9.79	3.44	21.72
90	BA	DHCA	49.44	43.22	156.22	42.73	49.44	44.91	49.48	44.29	40.94	62.75	108.43	82.37	39.22	139.90	85.13	231.96	77.77	125.63
91	BA	7_ketoDCA	185.00	109.61	440.01	52.03	57.77	312.72	134.83	58.41	85.26	288.15	117.05	110.91	74.10	143.40	167.94	678.20	380.83	497.91
92	BA	12_ketoCDCA	34.19	24.42	34.53	53.20	21.19	21.07	11.86	27.36	30.14	0.61	0.15	0.64	0.48	0.08	0.68	8.78	1.64	0.51
93	BA	dehydro_LCA	0.53	0.09	0.32	0.10	1.02	0.68	1.03	0.60	0.06	1.45	0.74	0.33	0.25	1.69	0.23	0.10	0.27	1.57
94	BA	23_nor_DCA	7.33	21.14	25.86	6.42	21.46	26.45	7.93	3.69	2.35	14.63	8.92	31.47	13.41	7.22	9.23	9.65	7.72	2.66
95	BA	6_ketoLCA	11.97	16.31	20.80	11.56	8.61	19.35	11.53	21.25	22.96	11.08	10.35	3.46	2.54	23.84	4.78	11.78	17.98	16.66
96	BA	7_ketoLCA	110.20	125.61	125.84	117.23	109.65	110.59	106.16	116.34	105.42	99.89	94.00	114.48	106.57	98.26	104.85	100.86	111.23	124.14
97	BA	12_ketoLCA	0.36	0.25	2.27	0.08	0.00	0.02	0.01	0.00	0.00	0.00	0.14	0.50	0.00	0.64	0.00	0.00	0.00	0.00
98	BA	apo_CA	0.25	1.56	6.52	0.12	0.10	6.35	0.84	0.09	5.16	0.33	0.76	1.35	0.19	0.09	0.18	0.08	1.70	0.46
99	BA	muroCA	1.46	7.68	0.38	1.90	4.92	1.91	3.29	4.59	1.48	3.28	2.52	8.10	3.84	2.52	5.02	9.74	7.13	13.86
100	BA	beta-UDCA	2.81	3.81	2.76	0.20	0.23	2.03	1.06	0.44	2.47	0.91	0.05	2.55	0.19	0.20	0.34	1.44	2.62	2.22
101	BA	3-ketoCA	123.18	156.16	186.03	120.48	124.98	197.27	109.21	127.80	175.51	104.69	104.68	123.09	102.81	112.96	104.31	105.18	104.30	113.05
102	BA	ACA	150.87	334.85	359.52	103.68	79.03	287.47	85.56	88.88	221.46	50.98	109.17	83.51	20.36	200.86	46.72	136.77	136.39	258.12
103	BA	TCA	424.15	135.24	633.48	166.07	209.31	776.42	435.98	139.82	307.77	1033.70	562.27	343.08	150.00	535.03	276.71	745.43	486.95	407.74
104	BA	TCDCA	4.03	2.17	2.53	2.58	2.61	3.53	3.45	3.37	2.34	3.94	3.09	2.49	2.58	2.95	3.04	3.33	3.53	2.68
105	BA	TaMCA	115.60	34.51	153.46	72.98	2.52	45.39	7.22	7.86	14.57	24.06	17.28	20.73	6.00	19.71	16.40	34.46	16.09	59.91
106	BA	TbMCA	1253.30	293.88	1495.84	843.63	479.46	1274.04	457.87	541.99	1006.92	637.20	349.63	458.71	182.62	525.89	263.15	384.99	473.08	758.36
107	BA	TwMCA	83.42	63.94	204.05	42.03	60.29	131.05	65.43	52.66	90.88	79.79	69.81	75.43	66.34	67.18	83.20	103.37	63.52	89.91
108	BA	TDCA	8.45	6.17	11.56	9.50	8.67	9.58	7.95	8.19	10.96	7.48	8.70	7.74	10.35	11.41	7.52	8.35	6.41	11.20
109	BA	TLCA	0.21	1.45	0.25	0.22	0.21	0.91	0.39	0.25	0.64	0.49	0.24	0.27	1.05	0.68	0.23	0.55	0.86	1.71
110	BA	TUDCA	117.72	216.82	238.66	128.37	142.80	582.12	130.61	148.06	549.06	78.34	81.45	134.32	12.31	67.61	25.40	59.41	59.62	103.45
111	BA	THCA	132.44	21.44	222.62	64.89	37.16	203.08	31.85	39.37	103.59	109.32	215.04	62.03	29.80	111.39	12.62	248.33	122.96	177.02
112	BA	THDCA	11.24	11.18	11.27	11.29	11.16	11.55	11.21	11.32	11.46	10.32	10.09	11.20	10.11	9.90	10.31	10.48	10.10	9.88
113	BA	GCDCA	543.82	419.78	584.41	298.65	67.32	1290.96	207.13	304.58	633.09	20.83	0.41	315.73	8.60	124.96	2.13	38.68	173.43	376.97
114	BA	GDCA	0.15	0.33	0.28	0.42	0.60	0.21	0.91	0.05	0.15	0.36	0.23	0.25	0.19	0.19	3.78	0.66	0.67	0.74
115	BA	GLCA	23.60	0.05	7.77	18.35	1.09	61.14	3.63	11.79	27.16	1.32	0.04	0.29	0.89	30.95	0.69	0.45	0.68	2.07
116	BA	GUDCA	163.70	145.07	156.91	163.06	140.07	188.79	153.36	162.69	199.54	148.82	156.86	149.15	139.16	154.50	140.26	145.19	141.65	151.37