



Supplemental Figure 1. The fingerprint of GCs.

Supplemental Table 1. The MS condition of biochemical marker

		Q1Mass	Q3Mass	DP	EP	CE	CXP
	ID	(Da)	(Da)	(Volts)	(Volts)	(Volts)	(Volts)
	IS(Phe-d5)	171.1	125.2	63	8	21	24
1	Uric acid	169.1	169.1	20	10	5	10
2	Uridine	243.1	243.1	-20	-10	-5	-5
3	Hypoxanthine	137	94	40	10	18	10
4	Allantoin	157.1	114	-20	-10	-16	-5
5	2-deoxyguanosine	268	152	40	10	25	15
6	Xanthosine	285	153	40	10	20	10
7	Xanthine	153	109.9	40	10	14	10
8	Inosine	269.1	137	40	10	36	10
9	Adenosine	268.1	118.9	40	10	28	10
10	N-phenylacetyl glycine	194.2	91.1	40	9	20	17
11	Cholic acid	409.3	373.3	40	9	13	11
12	Taurine	126	126	20	10	5	10
13	Ursodeoxycholic acid(UDCA)	391.28	391.28	-20	-5	-5	-5
14	Glycocholic acid	464.3	464.3	-20	-10	-5	-5
15	Glycochenodeoxycholic acid(GCDCA)	450.4	450.4	20	10	5	5
16	LCA(lithocholic acid)	375.3	375.3	-10	-10	-10	-5
17	Taurocholic acid	514.3	514.3	-10	-10	-30	-5
18	Glycolithocholic acid(GLCA)	432.3	74	-10	-10	-64	-5
19	Taurochenodexy cholic acid	498.3	498.3	-10	-10	-10	-5
20	C20:4LPC	588.5	588.5	-20	-10	-5	-5
21	C16:1LPC	494.3	494.3	20	10	5	5
22	C18:1LPC	522.4	522.4	20	10	5	10
23	LPE(18:0)	482.3	482.3	10	10	5	10
24	LPC(16:0)	496.3	496.3	10	10	5	10
25	PC(16:0/0:0)	496.3	496.3	10	10	5	10
26	LPC(18:0)	524.4	524.4	10	10	5	10
27	PE(36:4)	740.6	740.5	10	10	5	10
28	PE(38:4)	768.6	768.6	10	10	5	10
29	LPC(20:1)	550.4	550.4	10	10	5	10
30	LPC(22:6)	568.3	568.3	10	10	5	10
31	PC(36:4)	782.5	782.5	10	10	10	10
32	PC(36:3)	784.6	784.6	10	10	10	10
33	PC(16:0/22:6)	806.6	806.6	10	10	10	10
34	PC(16:0/18:3)	756.6	756.6	10	10	10	10
35	2-hydroxyglutarate(2-HG)	147.1	129.2	-25	-10	-14	-10
36	Melavonic acid	147	147	-35	-10	-20	-5
37	Palmitic acid	255	255	-10	-10	-10	-5

38	3-hydroxybutyric	103	59	-40	-10	-15	-5
39	Ethylmalonic acid	131	86.9	-40	-10	-15	-5
40	Mesaconic	128.9	84.9	-40	-10	-15	-5
41	Acetylcarnitine	204.1	204.1	20	10	5	5
42	Aminohippuric acid	195.1	195.1	20	10	5	5
43	Palmitoyl-L-carnitine	400.3	400.3	20	10	5	5
44	Choline	104.2	60.3	40	10	17	10
45	Malondialdehyde(MDA)	235.1	159.1	25	10	5	5
46	Glutamic	147.1	130.1	80	10	5	10
47	Glutathione,Oxidized(GSSG)	613.2	355.3	98	10	34	10
48	Glutathione(GSH)	433.1	304.1	79	8	22	8
49	L-Histidine	154.1	154.1	-20	-5	-5	-5
50	L-Leucine	132.1	86.1	55	6	16	16
51	Isoleucine	132	132	20	10	5	5
52	L-Valine	118.1	118.1	20	10	5	5
53	Hippuric acid	180.1	180.1	20	10	5	5
54	Phenylalanine	166.1	120.1	40	10	15	10
55	Phenylpyruvic acid	165.1	165.1	20	10	5	5
56	Creatine	132	90	40	10	15	10
57	Spermidine	146.1	146.1	20	10	5	5
58	Creatinine	114.5	44	40	10	15	10
59	Proline	116.1	116.1	20	10	5	5
60	Alanine	90.1	44.2	40	10	15	10
61	L-Tryptophan	205.2	188.1	144	11	16	12
62	L-Kynurenine	209.1	192.1	45	8	14	13
63	Indole-3-lactic acid	204.1	204.1	-20	-10	-5	-5
64	Xanthurenic acid	204	204	-20	-10	-5	-5
65	5-hydroxytryptophan(5-HTP)	221.1	204.3	54	10	16	13
66	5-hydroxytryptamine(5-HT)	177.1	160.1	45	9	16	31
67	Ophthalmic acid(Opht A)	290.2	161.1	40	10	15	15
68	3-nitro-tyrosine(N-Tyr)	227.1	181	40	10	25	10
69	3-chloro-Ltyrosine(Cl-Tyr)	216	170	40	10	30	15
70	DL-o-tyrosine(o-Tyr)	182.1	136.1	40	10	20	10
71	Carnitine	162.1	162.1	20	10	5	5
72	S-(adenosyl)-L-homocysteine (SAH)	385.1	136	40	10	35	25
73	Glycine	76	30.1	40	10	15	10
74	4-(2-aminophenyl)-2,4-dioxobutanoic acid	208.1	162.1	40	10	15	10
75	4,6-dihydroxyquinoline	162.1	116	40	10	15	10
76	p-Cresol Glucuronide	283.08	107	-20	-10	-15	-10
77	Trigonelline	138.1	138.1	20	10	5	5
78	pyridoxic acid	182.1	182.1	-20	-10	-5	-5

79	N-acetyl-glucosamine	220.1	118.9	-22	-13	-10	-10
80	Pantothenic acid	218.1	218.1	-20	-10	-5	-5
81	Citric acid	191	111.2	-25	-10	-17	-6
82	Isocitrate	190.8	72.9	-20	-10	-30	-5
83	Oxaloacetate	130.8	86.9	-25	-10	-10	-5
84	Succinic acid	117	73	-40	-10	-15	-10
85	a-Ketoglutaric acid	145.1	101	-40	-10	-13	-6
86	Aconitic acid	173	85	-40	-10	-15	-10
87	Malic acid	132.9	115	-40	-10	-15	-10
88	Fumaric acid	115	70.9	-40	-10	-15	-10
89	1,6 –Fructose Diphosphate	339.1	97.1	-40	-7	-20	-5
90	Glucose-6-phosphate	259.02	97	-40	-10	-15	-10
91	Glucosamine-6-phosphate	260	126	40	10	15	10
92	Pyruic acid	87.3	87.3	-20	-5	-5	-5
93	Glucose	179.1	89.1	-20	-5	-8	-5
94	Lactate	89	89	-40	-10	-10	-5
95	Glucose-1-phosphate	258.9	79	-40	-10	-15	-10
96	ADP	426	328	-110	-10	-19	-5
97	.NAD	662.1	540	-83	-10	-20	-5
98	NADP	742.1	620.1	-105	-10	-20	-5
99	NADPH	746	729.1	40	10	20	10
100	NADH	331.4	78.8	-40	-10	-72	-5
101	8-Isoprostaglandin F2a(8-iso-PGF)	353.2	193.1	-100	-9	-40	-10
102	threonine	176	74	100	10	10	10
103	betaine	118.0	59.3	31	10	28	10
104	lysine	203	186	55	10	5	10
105	Ornithine	189	172	100	10	5	10
106	proline	172	70	100	10	15	10
107	3-indoxylsulfate	212.2	80	100	10	18	10
108	methylhistidine	170.1	124.1	100	10	20	10
109	β-alanine	90	44	100	10	20	10
110	methionine	206	104	100	10	18	10
111	N,N-dimethylglycine	104.1	104.1	100	10	10	10
112	urea	241	109	56	10	32	10
113	serine	162	60	100	10	10	10
114	pyroglutamic acid	128.0	82.1	100	-10	-20	-10
115	Benzene acetyl glycine	193.90	193.9	100	10	10	10
116	N6 - acetyl lysine	188.98	18.98	100	10	10	10
117	arginine	231	70	100	5	20	5
118	nicotinamide	123.1	80.0	60	5	30	5
119	E1	504.2	171.1	70	5	45	5
120	E2	506.2	171.1	70	5	48	5
121	16α-OHE1	520.2	171.1	75	5	45	5

122	16-ketoE2	520.2	171.1	75	5	45	5
123	E3	522.2	171.1	75	5	45	5
124	16-epiE3	522.2	171.1	75	5	45	5
125	17-epiE3	522.2	171.1	75	5	45	5
126	2-MeOE1	534.2	171.1	75	5	45	5
127	3-MeOE1	534.2	171.1	75	5	45	5
128	4-MeOE1	534.2	171.1	75	5	45	5
129	2-MeOE2	536.2	171.1	75	5	45	5
130	4-MeOE2	536.2	171.1	75	5	45	5
131	2-OHE1	753.3	170.1	85	5	50	5
132	4-OHE1	753.3	170.1	85	5	50	5
133	2-OHE2	755.3	170.1	85	5	50	5
134	4-OHE2	755.3	170.1	85	5	50	5

Supplemental Table 2. Results obtained to evaluate the accuracy of the developed UPLC-MS / MS method (n=6).

Sample	Compound	Concentration	Intra-day		Inter-day	
			Accuracy (%)	Precision (%)	Accuracy (%)	Precision (%)
Serum	GSH	750(ng/ml)	98.25	5.78	111.22	3.54
		1000(ng/ml)	110.2	4.12	86.71	4.95
		5000(ng/ml)	88.17	3.17	91.18	3.71
	GSSG	1500(ng/ml)	85.33	3.17	89.36	6.78
		2000(ng/ml)	89.09	5.84	93.22	5.55
		10000(ng/ml)	86.24	6.04	110.31	6.49
	L-Leucine	750(ng/ml)	114.55	3.45	102.57	5.92
		1000(ng/ml)	112.36	10.12	112.36	11.21
		5000(ng/ml)	98.54	5.42	101.28	9.54
	L-Kynurenine	37(ng/ml)	85.63	6.78	91.56	8.12
		50(ng/ml)	88.24	5.98	101.39	6.19
		250(ng/ml)	114.23	5.12	85.16	8.87
	L-Tryptophan	4500(ng/ml)	108.24	11.3	88.31	6.51
		6000(ng/ml)	98.32	6.57	84.17	5.59
		30000(ng/ml)	95.17	5.19	90.17	4.23
	5-HTP	1.5(ng/ml)	112.88	10.28	85.20	2.98
		2(ng/ml)	111.57	8.99	91.13	5.69
		10(ng/ml)	88.02	5.12	107.68	12.01
	Cholic acid	300(ng/ml)	112.36	6.38	86.38	9.52
		400(ng/ml)	109.54	5.44	85.96	10.81
		2000(ng/ml)	84.28	5.29	113.48	13.29
	5-HT	6(ng/ml)	94.19	6.38	109.33	9.19
		8(ng/ml)	109.29	4.55	87.89	5.55
40(ng/ml)		114.11	3.91	88.36	4.36	
Urine	N-phenylacetylglucylin	1800(ng/ml)	87.28	8.99	85.29	10.11
		2500(ng/ml)	91.06	4.36	94.95	5.29
		12500(ng/ml)	107.22	4.91	111.12	3.61
	GSH	75(ng/ml)	95.32	6.71	105.61	4.21
		100(ng/ml)	109.23	5.13	89.21	4.17
		500(ng/ml)	90.22	4.58	98.21	6.32
	GSSG	150(ng/ml)	114.32	3.17	89.36	6.78
200(ng/ml)		89.09	6.01	86.14	5.69	
1000(ng/ml)		89.31	7.24	99.23	6.88	
L-Leucine	750(ng/ml)	109.25	11.36	110.34	8.24	
	1000(ng/ml)	85.69	8.47	92.43	9.19	
	5000(ng/ml)	89.36	6.15	95.67	5.27	
L-Tryptophan	4500(ng/ml)	92.34	9.21	89.23	9.25	

	6000(ng/ml)	105.69	5.68	104.25	10.68
	30000(ng/ml)	86.11	4.44	96.25	5.68
	1.5(ng/ml)	85.68	11.31	88.21	6.17
5-HTP	2(ng/ml)	112.36	9.22	98.25	6.74
	10(ng/ml)	90.36	6.34	111.39	10.58
	300(ng/ml)	98.14	5.11	90.14	5.69
Cholic acid	400(ng/ml)	85.36	7.65	86.36	10.14
	2000(ng/ml)	91.25	8.33	114.01	10.36
	6(ng/ml)	98.12	5.98	111.32	8.64
5-HT	8(ng/ml)	111.98	5.17	89.69	4.98
	40(ng/ml)	85.23	3.25	91.58	6.91
	1800(ng/ml)	91.02	7.51	90.36	10.11
N-phenylacetylglycin	2500(ng/ml)	95.98	8.68	109.25	5.29
	12500(ng/ml)	111.36	6.72	101.09	4.55

Supplemental Table 3. Matrix variation on the assay.

Sample	Parameters	GSH		GSSG		L-Leucine		L-Kynurenine		L-Tryptophan		5-HTP		Cholic acid		5-HT		N-phenylacetylglucine		
		Base line	Spiked	Base line	Spiked	Base line	Spiked	Baseline	Spiked	Baseline	Spiked	Baseline	Spiked	Baseline	Spiked	Baseline	Spiked	Baseline	Spiked	
Plasma	Analyte spiked concentration(ng/ml)		1000		2000		1000		50		6000		2		400		8		2500	
	A	Measyred mean concentration (ng/ml; n=5)	2000	3120.3	4000	6221.38	2000	3110.2	100	152.3	12000	18542.1	4	5.85	800	1219.23	16	25.12	5000	7809.23
		CV%		3.14		4.15		2.69		4.59		3.69		6.15		3.44		5.17		4.69
		Spiked recovery (%)		112.0		111.1		111.0		104.6		109.0		92.5		104.8		114.0		112.4
	B	Measyred mean concentration (ng/ml; n=5)	4000	5593.5	8000	10894.2	4000	5126.39	200	261.36	24000	32591.4	8	11.23	1600	2123.56	32	41.25	10000	14102.4
		CV%		2.88		3.56		4.07		2.19		3.45		7.12		5.13		6.98		3.14
		Spiked recovery (%)		114.8		111.2		103.2		105.7		110.8		115.4		107.7		103.9		116.0
	C	Measyred mean concentration (ng/ml; n=5)	8000	9180.23	16000	18256.5	8000	9156.38	400	451.23	48000	55084.4	16	18.22	3200	3660.57	64	73.48	20000	22900.3
		CV%		4.12		3.17		3.47		3.21		3.54		3.42		4.19		3.57		3.86
		Spiked recovery (%)		118.0		112.8		115.6		102.5		118.1		111.0		115.1		118.5		116.0
	Urine	Analyte spiked concentration(ng/ml)		100		200		1000		50		6000		2		400		8		2500
		A	Measyred mean concentration (ng/ml; n=5)	200	309.2	400	625.43	2000	3188.6	100	144.26	12000	17651.2	4	5.22	800	1189.14	16	24.33	5000
		CV%		3.10		4.65		6.51		5.29		6.32		4.32		6.53		8.77		8.74
		Spiked recovery (%)		110.10		108.6		113.4		111.23		113.3		82.6		114.2		113.25		116.5
B		Measyred mean concentration (ng/ml; n=5)	400	533.2	800	1112.6	4000	5188.21	200	252.6	24000	29566.3	8	12.67	1600	2078.21	32	40.87	10000	14626.78
		CV%		3.15		6.46		6.08		4.28		6.55		8.10		8.76		7.15		5.47
		Spiked recovery (%)		112.1		86.4		111.8		107.51		88.14		111.6		116.1		96.69		113.46
C		Measyred mean concentration (ng/ml; n=5)	800	918.25	1600	1867.9	8000	9201.42	400	440.32	48000	55243.2	16	18.96	3200	3566.35	64	71.33	20000	21546.5
		CV%		5.13		3.87		4.59		3.99		3.81		4.43		5.16		4.98		8.34

Spiked recovery (%)

98.23

114.2

109.8

89.54

106.43

98.54

103.22

83.67

118.97
