

Supporting Information

Cross-validation of metabolic phenotypes in SARS-CoV-2 infected sub-populations using targeted liquid chromatography-mass spectrometry (LC-MS)

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Table S1. Metabolite feature quality control performance metrics

Ref. index	Assay	Metabolite	Class	HMDB ID	QC %RSD		% missing values in samples		Failed QC (excluded from analysis)
					Spain (serum)	Australia (plasma)	Spain (serum)	Australia (plasma)	
1	Q300 metabolite array	10z-nonadecenoic acid	fatty acids	HMDB0013622	29.74	28.48	0	0	FALSE
2	Q300 metabolite array	2-hydroxy-3-methylbutyric acid	fatty acids	HMDB0000407	29.02	8.33	2.78	0	FALSE
3	Q300 metabolite array	2-hydroxybutyric acid	organic acids	HMDB0000008	26.96	7.38	0	0	FALSE
4	Q300 metabolite array	2-hydroxyglutaric acid	organic acids	HMDB0000694	25.47	19.86	0	0	FALSE
5	Q300 metabolite array	2-methyl-butyroylcarnitine	carnitines	HMDB0000378	25.22	12.89	0	0	FALSE
6	Q300 metabolite array	2-phenylpropionic acid	Phenyl-propanoic acids	HMDB0011743	13.65	9.91	0	3.13	FALSE
7	Q300 metabolite array	3-hydroxybutyric acid	organic acids	HMDB0000357	12.24	8.53	0	0	FALSE
8	Q300 metabolite array	3-hydroxy-isovaleric acid	fatty acids	HMDB0000754	17.44	19.13	0	0	FALSE
9	Q300 metabolite array	3-hydroxy-isovalerylcarnitine	carnitines	HMDB0062555	24.7	6.05	0	0	FALSE
10	Q300 metabolite array	3-methyl-2-oxovaleric acid	organic acids	HMDB0000491	18.59	19.86	0	0	FALSE
11	Q300 metabolite array	3-phenylpropionic acid	phenylprop anoic acids	HMDB0000764	19.36	27.07	0	0	FALSE
12	Q300 metabolite array	5-aminolevulinic acid	amino acids	HMDB0001149	18.35	17.43	0	0	FALSE
13	Q300 metabolite array	acetylcarnitine	carnitines	HMDB0000201	13.5	19.77	0	0	FALSE
14	Q300 metabolite array	acetylglycine	amino acids	HMDB0000532	18.51	8.73	0	0	FALSE
15	Q300 metabolite array	aconitic acid	organic acids	HMDB0000072	8.26	15.35	0	0	FALSE
16	Q300 metabolite array	alanine	amino acids	HMDB0000161	10.23	3.23	0	0	FALSE
17	Q300 metabolite array	alpha-aminobutyric acid	amino acids	HMDB0000452	16.12	6.04	0	0	FALSE
18	Q300 metabolite array	alpha-linolenic acid	fatty acids	HMDB0001388	23.21	15.6	2.78	0	FALSE
19	Q300 metabolite array	arachidonic acid	fatty acids	HMDB0001043	26.63	13.17	0	0	FALSE
20	Q300 metabolite array	arginine	amino acids	HMDB0000517	9.88	4.27	0	0	FALSE
21	Q300 metabolite array	asparagine	amino acids	HMDB0000168	27.43	10.39	0	0	FALSE

22	Q300 metabolite array	aspartic acid	amino acids	HMDB0000191	29.91	10.49	0	0	FALSE
23	Q300 metabolite array	azelaic acid	fatty acids	HMDB0000784	14.38	18.17	0	0	FALSE
24	Q300 metabolite array	beta-alanine	amino acids	HMDB0000056	11.23	11.47	0	0	FALSE
25	Q300 metabolite array	butyrylcarnitine	carnitines	HMDB0002013	28.46	9.86	0	0	FALSE
26	Q300 metabolite array	caproic acid	fatty acids	HMDB0000535	24.72	8.56	0	0	FALSE
27	Q300 metabolite array	carnitine	carnitines	HMDB0000062	11.76	3.58	0	0	FALSE
28	Q300 metabolite array	citric acid	organic acids	HMDB0000094	9.99	5.9	0	0	FALSE
29	Q300 metabolite array	creatine	amino acids	HMDB0000064	27.59	6.07	22.22	0	FALSE
30	Q300 metabolite array	d-glucose	carbohydrates	HMDB0000122	17.35	2.93	0	0	FALSE
31	Q300 metabolite array	dimethylglycine	amino acids	HMDB0000092	14.68	12.13	0	0	FALSE
32	Q300 metabolite array	docosahexaenoic acid	fatty acids	HMDB0002183	28.86	16.5	0	0	FALSE
33	Q300 metabolite array	erythronic acid	carbohydrates	HMDB0000613	21.14	5.21	0	0	FALSE
34	Q300 metabolite array	ethylmethylacetic acid	fatty acids	HMDB0002176	22.72	17.21	0	0	FALSE
35	Q300 metabolite array	glucaric acid	carbohydrates	HMDB0000663	29.02	12.61	6.94	0	FALSE
36	Q300 metabolite array	glutamic acid	amino acids	HMDB0000148	15.17	11.5	0	0	FALSE
37	Q300 metabolite array	glutamine	amino acids	HMDB0000641	17.9	5.54	0	0	FALSE
38	Q300 metabolite array	glutaric acid	organic acids	HMDB0000661	13.96	13.07	5.56	0	FALSE
39	Q300 metabolite array	glutaryl carnitine	carnitines	HMDB0013130	22.12	10.13	0	0	FALSE
40	Q300 metabolite array	glyceric acid	carbohydrates	HMDB0000139	19.94	3.38	0	0	FALSE
41	Q300 metabolite array	glycine	amino acids	HMDB0000123	13.07	3.66	0	0	FALSE
42	Q300 metabolite array	glycylproline	amino acids	HMDB0000721	24	26.57	1.39	0	FALSE
43	Q300 metabolite array	heptanoic acid	fatty acids	HMDB0000666	22.16	15.46	0	0	FALSE
44	Q300 metabolite array	hexanoylcarnitine	carnitines	HMDB0000705	22.4	8.2	0	0	FALSE

45	Q300 metabolite array	hippuric acid	benzenoids	HMDB0000714	19.09	4.71	0	0	FALSE
46	Q300 metabolite array	histidine	amino acids	HMDB0000177	13.39	5.05	0	0	FALSE
47	Q300 metabolite array	homoserine	amino acids	HMDB0000719	20.8	16.4	2.78	0	FALSE
48	Q300 metabolite array	indole-3-acetic acid	indoles	HMDB0000197	22.54	27.47	0	0	FALSE
49	Q300 metabolite array	indole-3-propionic acid	indoles	HMDB0002302	14.34	14.01	1.39	0	FALSE
50	Q300 metabolite array	indole-3-pyruvic acid	indoles	HMDB0060484	27.56	10.84	0	0	FALSE
51	Q300 metabolite array	isovaleric acid	fatty acids	HMDB0000718	21.06	25.91	11.11	0	FALSE
52	Q300 metabolite array	isovalerylcarnitine	carnitines	HMDB0000688	28.69	10.31	0	0	FALSE
53	Q300 metabolite array	ketoleucine	organic acids	HMDB0000695	17.54	13.12	0	0	FALSE
54	Q300 metabolite array	kynurenine	amino acids	HMDB0000684	28.57	10.77	0	0	FALSE
55	Q300 metabolite array	lactic acid	organic acids	HMDB0000190	13.94	12.79	0	0	FALSE
56	Q300 metabolite array	leucine	amino acids	HMDB0000687	13.11	3.82	0	0	FALSE
57	Q300 metabolite array	linoleic acid	fatty acids	HMDB0000673	17.86	11.6	0	0	FALSE
58	Q300 metabolite array	linoleyl carnitine	carnitines	HMDB0006469	16.88	8.46	0	0	FALSE
59	Q300 metabolite array	lysine	amino acids	HMDB0000182	11.92	4	0	0	FALSE
60	Q300 metabolite array	malic acid	organic acids	HMDB0000156	12.69	5.96	0	0	FALSE
61	Q300 metabolite array	malonylcarnitine	carnitines	HMDB0002095	17.04	16.54	0	0	FALSE
62	Q300 metabolite array	methionine	amino acids	HMDB0000696	10.79	21.43	0	0	FALSE
63	Q300 metabolite array	methylmalonic acid	organic acids	HMDB0000202	22.19	15.88	0	10.94	FALSE
64	Q300 metabolite array	myristoleic acid	fatty acids	HMDB0002000	22.39	11.85	0	0	FALSE
65	Q300 metabolite array	n-acetylaspartic acid	amino acids	HMDB0000812	13.82	21.59	0	0	FALSE
66	Q300 metabolite array	n-acetylneuraminic acid	carbohydra tes	HMDB0000230	17.33	10.93	0	0	FALSE
67	Q300 metabolite array	o-adipoylcarnitine	carnitines	HMDB0061677	29.39	14.92	0	0	FALSE

68	Q300 metabolite array	octanoic acid	fatty acids	HMDB0000482	29.89	6.49	0	0	FALSE
69	Q300 metabolite array	octanoylcarnitine	carnitines	HMDB0000791	14.5	11.97	6.94	0	FALSE
70	Q300 metabolite array	oleylcarnitine	carnitines	HMDB0005065	25.42	8.88	0	0	FALSE
71	Q300 metabolite array	ornithine	amino acids	HMDB0000214	12.46	3	0	0	FALSE
72	Q300 metabolite array	oxalic acid	organic acids	HMDB0002329	29.56	9.57	2.78	0	FALSE
73	Q300 metabolite array	oxoglutaric acid	organic acids	HMDB0000208	27.91	9.58	0	0	FALSE
74	Q300 metabolite array	palmitoylcarnitine	carnitines	HMDB0000222	21.1	12.04	1.39	0	FALSE
75	Q300 metabolite array	phenylacetic acid	benzenoids	HMDB0000209	16.52	11.87	0	0	FALSE
76	Q300 metabolite array	phenylacetylglutamine	amino acids	HMDB0006344	21.11	7.36	0	0	FALSE
77	Q300 metabolite array	phenylalanine	amino acids	HMDB0000159	21.17	17.01	0	0	FALSE
78	Q300 metabolite array	phenylpyruvic acid	benzenoids	HMDB0000205	22.09	6.1	0	0	FALSE
79	Q300 metabolite array	pipecolic acid	amino acids	HMDB0000716	14.83	15.65	0	0	FALSE
80	Q300 metabolite array	proline	amino acids	HMDB0000162	15.47	7.28	2.78	0	FALSE
81	Q300 metabolite array	propionic acid	fatty acids	HMDB0000237	22.17	15.97	2.78	0	FALSE
82	Q300 metabolite array	propionylcarnitine	carnitines	HMDB0000824	28.92	4.75	0	0	FALSE
83	Q300 metabolite array	pyroglutamic acid	amino acids	HMDB0000267	18.22	12.14	0	0	FALSE
84	Q300 metabolite array	pyruvic acid	organic acids	HMDB0000243	16.05	7.22	0	0	FALSE
85	Q300 metabolite array	sarcosine	amino acids	HMDB0000271	17.08	17.24	0	0	FALSE
86	Q300 metabolite array	sebacic acid	fatty acids	HMDB0000792	15.38	17.89	0	0	FALSE
87	Q300 metabolite array	serine	amino acids	HMDB0000187	16.31	4.29	0	0	FALSE
88	Q300 metabolite array	stearoylcarnitine	carnitines	HMDB0000848	18.67	23.16	0	0	FALSE
89	Q300 metabolite array	succinic acid	organic acids	HMDB0000254	13.12	10.76	0	0	FALSE
90	Q300 metabolite array	tetradecanoylcarnitine	carnitines	HMDB0005066	26.16	6.55	0	0	FALSE

91	Q300 metabolite array	threonic acid	organic acids	HMDB0000943	18.78	7.43	0	0	FALSE
92	Q300 metabolite array	threonine	amino acids	HMDB0000167	17.29	5.25	0	0	FALSE
93	Q300 metabolite array	tryptophan	amino acids	HMDB0000929	17.27	11.6	0	0	FALSE
94	Q300 metabolite array	tyrosine	amino acids	HMDB0000158	15.47	4.32	0	0	FALSE
95	Q300 metabolite array	valeric acid	fatty acids	HMDB0000892	22.74	13.25	1.39	0	FALSE
96	Q300 metabolite array	valine	amino acids	HMDB0000883	13.73	5.78	0	0	FALSE
97	Q300 metabolite array	1-methylhistidine	amino acids	HMDB0000001	77.01	10.34	5.56	0	TRUE
98	Q300 metabolite array	2-methylhexanoic acid	fatty acids	HMDB0031594	88.8	45.7	0	0	TRUE
99	Q300 metabolite array	2-phenylglycine	amino acids	HMDB0002210	145.41	168.79	65.28	0	TRUE
100	Q300 metabolite array	4-hydroxyproline	amino acids	HMDB0000725	45.36	7.07	40.28	0	TRUE
101	Q300 metabolite array	acetic acid	fatty acids	HMDB0000042	46.57	27.48	0	0	TRUE
102	Q300 metabolite array	adenosine monophosphate	nucleosides	HMDB0000045	61.47	83.12	0	0	TRUE
103	Q300 metabolite array	butyric acid	fatty acids	HMDB0000039	51.68	89.49	1.39	26.56	TRUE
104	Q300 metabolite array	citrulline	amino acids	HMDB0000904	7.04	3.66	86.11	0	TRUE
105	Q300 metabolite array	decanoic acid	fatty acids	HMDB0000511	103.4	5.22	20.83	0	TRUE
106	Q300 metabolite array	dodecanoylcarnitine	carnitines	HMDB0002250	44.69	22.81	0	0	TRUE
107	Q300 metabolite array	eicosapentaenoic acid	fatty acids	HMDB0001999	46.36	41.89	0	0	TRUE
108	Q300 metabolite array	fumaric acid	organic acids	HMDB0000134	41.67	63.04	0	0	TRUE
109	Q300 metabolite array	gamma- aminobutyric acid	amino acids	HMDB0000112	61.83	44.06	76.39	0	TRUE
110	Q300 metabolite array	homocitrulline	amino acids	HMDB0000679	84.86	47.94	4.17	0	TRUE
111	Q300 metabolite array	hydroxyphenyllactic acid	phenylprop anoic acids	HMDB0000755	100.64	16.38	13.89	0	TRUE
112	Q300 metabolite array	imidazolepropionic acid	fatty acids	HMDB0002271	43.01	122.64	0	0	TRUE
113	Q300 metabolite array	isoleucine	amino acids	HMDB0000172	na	5.09	98.61	0	TRUE

114	Q300 metabolite array	maleic acid	organic acids	HMDB0000176	43.43	64.88	0	6.25	TRUE
115	Q300 metabolite array	valerylcarnitine	carnitines	HMDB0013128	33.67	125.08	2.78	0	TRUE
116	Bile Acid	chenodeoxycholic acid	bile acids	HMDB0000518	1.67	3.65	0	0	FALSE
117	Bile Acid	cholic acid	bile acids	HMDB0000619	3.26	1.32	6.94	0	FALSE
118	Bile Acid	glycocheno- deoxycholic acid	bile acids	NA	7.52	3.7	0	0	FALSE
119	Bile Acid	glycocholic acid	bile acids	HMDB0000138	6.89	2.44	0	0	FALSE
120	Bile Acid	glycodeoxycholic acid	bile acids	NA	3.79	2.43	0	0	FALSE
121	Bile Acid	glycourso- deoxycholic acid	bile acids	HMDB0000708	3.65	0.89	0	0	FALSE
122	Bile Acid	taurochenodeoxych- olic acid	bile acids	HMDB0000951	5.72	2.82	0	0	FALSE
123	Bile Acid	taurocholic acid	bile acids	HMDB0000036	6.13	7.32	0	0	FALSE
124	Bile Acid	taurodeoxycholic acid	bile acids	HMDB0000896	2.93	2.83	0	0	FALSE
125	Bile Acid	ursodeoxycholic acid	bile acids	HMDB0000946	7.23	6.8	1.39	0	FALSE
126	Bile Acid	deoxycholic acid	bile acids	HMDB0000626	3.36	7.85	1.39	100	TRUE
127	Bile Acid	glycolithocholic acid	bile acids	HMDB0000698	10.84	45.26	20.83	100	TRUE
128	Bile Acid	lithocholic acid	bile acids	HMDB0000761	2.86	40.36	8.33	100	TRUE
129	Bile Acid	taurohydrodeoxy- cholic acid	bile acids	NA	na	5.71	100	0	TRUE
130	Bile Acid	tauroolithocholic acid	bile acids	HMDB0000722	na	12.87	100	0	TRUE

Table S2. Mass spectrometry multiple reaction monitoring (MRM) transition and chromatographic retention time details for the Q300 metabolomic array

Ref. index	Metabolite	Class	HMDB ID	Cone (V)	Collision (eV)	Ionization mode	Retention Time (min)	Precursor m/z	Product m/z	Internal Standard
1	10z-nonadecenoic acid	fatty acids	HMDB0013622	40	10	ES-	14.42	430.3	430.1	tridecanoic acid-d2
2	2-hydroxy-3-methylbutyric acid	fatty acids	HMDB0000407	40	10	ES-	5.39	254	235.9	hippuric acid-d5
3	2-hydroxybutyric acid	organic acids	HMDB0000008	40	20	ES-	4.34	237.8	151.8	propanoic acid-d3
4	2-hydroxyglutaric acid	organic acids	HMDB0000694	40	10	ES+	5.95	419.11	400.9	mandelic acid-d5
5	2-methylbutyryl-carnitine	carnitines	HMDB0000378	40	20	ES+	5.09	381.2	220.1	velarylcarnitine-c5-d3
6	2-phenylpropionic acid	phenylpropanoic acids	HMDB0011743	50	18	ES+	7.72	286	104.8	hydrocinnamic acid-d9
7	3-hydroxybutyric acid	organic acids	HMDB0000357	34	17	ES-	3.57	238	193.8	3-hydroxybutyric acid-d4
8	3-hydroxyisovaleric acid	fatty acids	HMDB0000754	40	10	ES-	4.29	252	193.9	beta-hydroxyisovaleric acid-d8
9	3-hydroxy-isovaleryl-carnitine	carnitines	HMDB0062555	40	20	ES+	3.66	397.2	220.1	velarylcarnitine c5-d3
10	3-methyl-2-oxovaleric acid	organic acids	HMDB0000491	30	10	ES+	9.94	401.1	247.9	ketoleucine-d3
11	3-phenylpropionic acid	phenylpropanoic acids	HMDB0000764	60	18	ES+	7.71	286.1	90.8	hydrocinnamic acid-d9
12	5-aminolevulinic acid	amino acids	HMDB0001149	46	25	ES-	3.38	265	136.8	valine-d8
13	acetylcarnitine	carnitines	HMDB0000201	40	10	ES-	2.77	383	323	acetylcarnitine c2-d3
14	acetylglycine	amino acids	HMDB0000532	50	18	ES-	2.86	322	126.8	valine-d8
15	aconitic acid	organic acids	HMDB0000072	30	18	ES-	6.41	443	245.9	mandelic acid-d5
16	alanine	amino acids	HMDB0000161	30	10	ES+	1.7	225	207.9	alanine-d4
17	alpha-aminobutyric acid	amino acids	HMDB0000452	46	18	ES-	2.65	237	136.8	valine-d8
18	alpha-linolenic acid	fatty acids	HMDB0001388	40	10	ES-	12.31	412.2	412.1	tridecanoic acid-d2
19	arachidonic acid	fatty acids	HMDB0001043	40	10	ES-	12.63	438.2	438.1	tridecanoic acid-d2
20	arginine	amino acids	HMDB0000517	40	12	ES+	0.8	310.2	293	arginine-15n2
21	asparagine	amino acids	HMDB0000168	40	18	ES+	3.3	403.1	194.8	tyrosine-d4
22	aspartic acid	amino acids	HMDB0000191	30	11	ES+	4.64	404.1	386.9	aspartic acid-d3
23	azelaic acid	fatty acids	HMDB0000784	40	10	ES-	7.91	459.2	288	hydrocinnamic acid-d9
24	beta-alanine	amino acids	HMDB0000056	40	11	ES+	1.58	225	195.9	alanine-d4
25	butyrylcarnitine	carnitines	HMDB0002013	40	20	ES+	4.35	367.2	220.1	velarylcarnitine c5-d3
26	caproic acid	fatty acids	HMDB0000535	30	25	ES-	7.84	250	136.8	caproic acid-d3
27	carnitine	carnitines	HMDB0000062	40	20	ES+	1.68	297.2	238.2	carnitine-d3
28	citric acid	organic acids	HMDB0000094	50	32	ES-	7.6	596.1	221.9	citric acid-d4
29	creatine	amino acids	HMDB0000064	50	18	ES+	1.94	267	113.8	alanine-d4
30	d-glucose	carbohydrates	HMDB0000122	40	12	ES-	3.43	313.9	205.8	d-glucose-d7
31	dimethylglycine	amino acids	HMDB0000092	50	18	ES+	1.56	239	151.8	serine-d3
32	docosahexaenoic acid	fatty acids	HMDB0002183	40	10	ES-	12.49	462.2	462.1	tridecanoic acid-d2
33	erythronic acid	carbohydrates	HMDB0000613	34	20	ES-	2.08	270	136.8	tyrosine-d4
34	ethylmethylacetic acid	fatty acids	HMDB0002176	40	10	ES-	6.23	238	56.7	valeric acid-d9
35	glucaric acid	carbohydrates	HMDB0000663	30	10	ES+	5.09	481.1	327.9	tryptophan-d5
36	glutamic acid	amino acids	HMDB0000148	40	12	ES+	3.32	265	114	tyrosine-d4
37	glutamine	amino acids	HMDB0000641	40	12	ES+	1.46	282	114	serine-d3

38	glutaric acid	organic acids	HMDB0000661	50	12	ES+	6.46	403.1	249.9	benzoic acid-d5
39	glutaryl carnitine	carnitines	HMDB0013130	40	20	ES+	5.21	546.2	220.1	velaryl carnitine c5-d3
40	glyceric acid	carbohydrates	HMDB0000139	40	18	ES-	2.39	239.9	136.8	tyrosine-d4
41	glycine	amino acids	HMDB0000123	30	18	ES-	1.34	209	136.8	glycine-d5
42	glycylproline	amino acids	HMDB0000721	40	18	ES+	2.28	308	126.8	tyrosine-d4
43	heptanoic acid	fatty acids	HMDB0000666	40	10	ES-	9	264.1	136.8	caproic acid-d3
44	hexanoyl carnitine	carnitines	HMDB0000705	40	20	ES+	6.21	395.2	220.1	velaryl carnitine c5-d3
45	hippuric acid	benzenoids	HMDB0000714	30	10	ES+	5.74	315.1	161.8	hippuric acid-d5
46	histidine	amino acids	HMDB0000177	40	12	ES+	0.77	291	273.9	histidine-15n3
47	homoserine	amino acids	HMDB0000719	30	10	ES+	1.82	255	237.9	serine-d3
48	indole-3-acetic acid	indoles	HMDB0000197	60	15	ES+	6.87	311	129.8	benzoic acid-d5
49	indole-3-propionic acid	indoles	HMDB0002302	30	14	ES+	7.33	325.1	129.8	hydrocinnamic acid-d9
50	indole-3-pyruvic acid	indoles	HMDB0060484	60	15	ES+	7.72	339	130	benzoic acid-d5
51	isovaleric acid	fatty acids	HMDB0000718	30	18	ES-	6.39	236	136.8	valeric acid-d9
52	isovaleryl carnitine	carnitines	HMDB0000688	40	20	ES+	5.25	381.2	220.1	velaryl carnitine c5-d3
53	ketoleucine	organic acids	HMDB0000695	30	10	ES+	10.05	401.1	247.9	ketoleucine-d3
54	kynurenine	amino acids	HMDB0000684	60	18	ES+	4.44	344.1	308.9	aspartic acid-d3
55	lactic acid	organic acids	HMDB0000190	30	14	ES+	3.39	226	164.8	lactic acid-d3
56	leucine	amino acids	HMDB0000687	46	22	ES-	4.25	265	136.8	leucine-d3
57	linoleic acid	fatty acids	HMDB0000673	40	10	ES-	12.72	414.3	414.1	tridecanoic acid-d2
58	linoleyl carnitine	carnitines	HMDB0006469	40	20	ES+	11.15	559.2	220.1	palmitoyl carnitine c16-d3
59	lysine	amino acids	HMDB0000182	30	10	ES+	0.77	282.1	83.8	lysine-d4
60	malic acid	organic acids	HMDB0000156	40	20	ES-	5.81	405.1	153.8	dmalic acid-d3
61	malonyl carnitine	carnitines	HMDB0002095	40	20	ES+	4.97	518.2	220.1	velaryl carnitine c5-d3
62	methionine	amino acids	HMDB0000696	40	23	ES-	3.6	283	136.8	methionine-d3
63	methylmalonic acid	organic acids	HMDB0000202	50	14	ES+	6.11	389.1	235.8	dmalic acid-d3
64	myristoleic acid	fatty acids	HMDB0002000	50	27	ES-	11.96	360.2	136.8	tridecanoic acid-d2
65	n-acetylaspartic acid	amino acids	HMDB0000812	60	12	ES+	5.72	446.2	292.9	tryptophan-d5
66	n-acetylneuraminic acid	carbohydrates	HMDB0000230	46	20	ES-	2.28	443.1	221.9	valine-d8
67	o-adipoyl carnitine	carnitines	HMDB0061677	40	20	ES+	5.57	560.2	220.1	velaryl carnitine c5-d3
68	octanoic acid	fatty acids	HMDB0000482	40	25	ES-	9.91	278.1	136.8	nonanoic acid-d3
69	octanoyl carnitine	carnitines	HMDB0000791	40	20	ES+	7.87	423.3	220.1	octanoyl carnitine c8-d3
70	oleyl carnitine	carnitines	HMDB0005065	40	20	ES+	11.53	561.2	220.1	palmitoyl carnitine c16-d3
71	ornithine	amino acids	HMDB0000214	40	10	ES+	0.75	268	70	ornithine-d6
72	oxalic acid	organic acids	HMDB0002329	30	18	ES-	6.59	359.1	149.8	adipic acid-d8
73	oxoglutaric acid	organic acids	HMDB0000208	50	26	ES-	9.47	550.1	232.9	nonanoic acid-d3
74	palmitoyl carnitine	carnitines	HMDB0000222	40	20	ES+	11.34	535.2	220.1	palmitoyl carnitine c16-d3
75	phenylacetic acid	benzenoids	HMDB0000209	30	23	ES+	6.89	272	78.8	benzoic acid-d5
76	phenylacetylglutamine	amino acids	HMDB0006344	30	18	ES-	5.82	398.1	279.9	mandelic acid-d5
77	phenylalanine	amino acids	HMDB0000159	60	10	ES+	4.76	301.1	283.9	phenylalanine-d8
78	phenylpyruvic acid	benzenoids	HMDB0000205	30	10	ES+	10.17	435.1	281.9	ketoleucine-d3
79	pipecolic acid	amino acids	HMDB0000716	46	20	ES-	2.77	263.1	136.8	alanine-d4
80	proline	amino acids	HMDB0000162	40	22	ES-	2.34	239.9	136.8	tyrosine-d4
81	propionic acid	fatty acids	HMDB0000237	30	18	ES-	4.41	208	136.8	propanoic acid-d3
82	propionyl carnitine	carnitines	HMDB0000824	40	20	ES+	3.62	353.2	220.1	velaryl carnitine c5-d3

83	pyroglutamic acid	amino acids	HMDB0000267	46	20	ES-	3.33	263	136.8	valine-d8
84	pyruvic acid	organic acids	HMDB0000243	30	18	ES-	8.34	357.4	136.8	citric acid-d4
85	sarcosine	amino acids	HMDB0000271	50	15	ES+	1.5	225	151.8	alanine-d4
86	sebacic acid	fatty acids	HMDB0000792	40	10	ES-	8.49	473.1	302	hydrocinnamic acid-d9
87	serine	amino acids	HMDB0000187	30	10	ES+	1.37	241	205.9	serine-d3
88	stearoylcarnitine	carnitines	HMDB0000848	40	20	ES+	11.64	559.2	220.1	palmitoylcarnitine c16-d3
89	succinic acid	organic acids	HMDB0000254	50	20	ES-	6	387	233.9	succinic acid-d4
90	tetradecanoylcarnitine	carnitines	HMDB0005066	40	20	ES+	12.26	507.2	220.1	palmitoylcarnitine c16-d3
91	threonic acid	organic acids	HMDB0000943	50	20	ES+	2.07	272	117.8	tyrosine-d4
92	threonine	amino acids	HMDB0000167	30	50	ES+	1.82	255	219.9	alanine-d4
93	tryptophan	amino acids	HMDB0000929	30	20	ES-	4.91	338	208.9	tryptophan-d5
94	tyrosine	amino acids	HMDB0000158	50	10	ES+	4.16	317.1	299.9	tyrosine-d4
95	valeric acid	fatty acids	HMDB0000892	30	18	ES-	6.62	236	136.8	valeric acid-d9
96	valine	amino acids	HMDB0000883	50	20	ES-	3.23	251	136.8	valine-d8
97	1-methylhistidine	amino acids	HMDB0000001	40	12	ES+	1.45	305	288.1	histidine-15n3
98	2-methylhexanoic acid	fatty acids	HMDB0031594	40	10	ES-	8.5	264.1	136.8	caproic acid-d3
99	2-phenylglycine	amino acids	HMDB0002210	50	18	ES+	3.35	287.1	270	methionine-d3
100	4-hydroxyproline	amino acids	HMDB0000725	40	22	ES-	2.02	256	136.8	tyrosine-d4
101	acetic acid	fatty acids	HMDB0000042	40	20	ES-	3.52	193.9	136.8	acetic acid-d3
102	adenosine monophosphate	nucleosides	HMDB0000045	30	18	ES+	2.39	483	135.9	tyrosine-d4
103	butyric acid	fatty acids	HMDB0000039	40	10	ES-	5.37	222	136.8	butyric acid-d3
104	citrulline	amino acids	HMDB0000904	40	15	ES-	1.64	309	265.9	alanine-d4
105	decanoic acid	fatty acids	HMDB0000511	50	20	ES-	11.33	306.12	136.8	decanoic acid-d2
106	dodecanoylcarnitine	carnitines	HMDB0002250	40	20	ES+	11.13	479.3	220.1	palmitoylcarnitine c16-d3
107	eicosapentaenoic acid	fatty acids	HMDB0001999	40	10	ES-	12.25	436.2	436.1	tridecanoic acid-d2
108	fumaric acid	organic acids	HMDB0000134	40	18	ES+	6.8	387	233.8	benzoic acid-d5
109	gamma-aminobutyric acid	amino acids	HMDB0000112	40	10	ES-	1.77	330	209.8	alanine-d4
110	homocitrulline	amino acids	HMDB0000679	30	11	ES+	3.13	325.1	307.9	alanine-d4
111	hydroxyphenyllactic acid	phenylpropanoic acids	HMDB0000755	40	22	ES-	4.78	318.1	299.9	aspartic acid-d3
112	imidazolepropionic acid	fatty acids	HMDB0002271	30	18	ES-	3.41	274	136.8	propanoic acid-d3
113	isoleucine	amino acids	HMDB0000172	46	22	ES-	4.09	265	136.8	leucine-d3
114	maleic acid	organic acids	HMDB0000176	40	20	ES-	6.65	385	233.9	adipic acid-d8
115	valerylcarnitine	carnitines	HMDB0013128	40	20	ES+	5.25	380.2	220.1	valerylcarnitine c5-d3
IS1	3-hydroxybutyric acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	30	18	ES-	3.52	242	193.8	NA
IS2	benzoic acid-d5	INTERNAL STANDARD	INTERNAL STANDARD	40	20	ES+	6.37	263.09	109.8	NA
IS3	beta-hydroxyisovaleric acid-d8	INTERNAL STANDARD	INTERNAL STANDARD	40	10	ES-	4.29	260.1	204.1	NA
IS4	caproic acid-d3	INTERNAL STANDARD	INTERNAL STANDARD	30	18	ES-	7.82	253	136.8	NA
IS5	carnitine-d3	INTERNAL STANDARD	INTERNAL STANDARD	40	20	ES+	1.67	300.2	238.2	NA
IS6	citric acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	30	18	ES-	7.71	600.1	223.9	NA
IS7	d-glucose-d7	INTERNAL STANDARD	INTERNAL STANDARD	40	12	ES+	3.36	321.1	209.019	NA
IS8	malic acid-d3	INTERNAL STANDARD	INTERNAL STANDARD	40	20	ES-	5.81	408.1	153.8	NA

IS9	glycine-d5	INTERNAL STANDARD	INTERNAL STANDARD	30	18	ES-	1.34	213	196	NA
IS10	hippuric acid-d5	INTERNAL STANDARD	INTERNAL STANDARD	30	10	ES+	5.74	320	167	NA
IS11	hydrocinnamic acid-d9	INTERNAL STANDARD	INTERNAL STANDARD	60	18	ES+	7.71	295.1	100.1	NA
IS12	ketoleucine-d3	INTERNAL STANDARD	INTERNAL STANDARD	30	10	ES+	10.05	404.1	251.1	NA
IS13	velarylcarnitine c5_d3	INTERNAL STANDARD	INTERNAL STANDARD	40	20	ES+	5.25	384.1	224.1	NA
IS14	acetylcarnitine-d3	INTERNAL STANDARD	INTERNAL STANDARD	40	10	ES-	2.77	386	326	NA
IS15	alanine-d4	INTERNAL STANDARD	INTERNAL STANDARD	30	10	ES+	1.69	229	212	NA
IS16	arginine-15n2	INTERNAL STANDARD	INTERNAL STANDARD	40	12	ES+	0.8	312	295	NA
IS17	aspartic acid-d3	INTERNAL STANDARD	INTERNAL STANDARD	30	11	ES+	4.64	407	389.8	NA
IS18	histidine-15n3	INTERNAL STANDARD	INTERNAL STANDARD	40	12	ES+	0.77	294	276	NA
IS19	lactic acid-d3	INTERNAL STANDARD	INTERNAL STANDARD	30	14	ES+	3.39	229	168.1	NA
IS20	leucine-d3	INTERNAL STANDARD	INTERNAL STANDARD	46	22	ES-	4.25	268	136.8	NA
IS21	lysine-d4	INTERNAL STANDARD	INTERNAL STANDARD	30	10	ES+	0.77	286	88	NA
IS22	methionine-d3	INTERNAL STANDARD	INTERNAL STANDARD	40	23	ES-	3.6	286	140	NA
IS23	palmitoylcarnitine c16-d3	INTERNAL STANDARD	INTERNAL STANDARD	40	20	ES+	11.34	538.1	223.1	NA
IS24	phenylalanine-d8	INTERNAL STANDARD	INTERNAL STANDARD	60	10	ES+	4.76	309.1	292.1	NA
IS25	serine-d3	INTERNAL STANDARD	INTERNAL STANDARD	30	10	ES+	1.36	244	208.9	NA
IS26	tryptophan-d5	INTERNAL STANDARD	INTERNAL STANDARD	30	20	ES-	4.91	343.1	214.1	NA
IS27	tyrosine-d4	INTERNAL STANDARD	INTERNAL STANDARD	50	10	ES+	3.34	321	304	NA
IS28	valine-d8	INTERNAL STANDARD	INTERNAL STANDARD	50	20	ES-	3.2	259	136.8	NA
IS29	mandelic acid-d5	INTERNAL STANDARD	INTERNAL STANDARD	30	18	ES-	5.86	291.14	136.8	NA
IS30	nonanoic acid-d3	INTERNAL STANDARD	INTERNAL STANDARD	30	18	ES-	10.64	295.1	136.8	NA
IS31	octanoylcarnitine c8-d3	INTERNAL STANDARD	INTERNAL STANDARD	40	20	ES+	7.87	426.1	223.1	NA
IS32	ornithine-d6	INTERNAL STANDARD	INTERNAL STANDARD	40	10	ES+	0.75	274.1	76.1	NA
IS33	propanoic acid-d3	INTERNAL STANDARD	INTERNAL STANDARD	30	18	ES-	4.41	211.1	136.8	NA
IS34	succinic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	30	18	ES-	6.05	391	236.9	NA
IS35	tridecanoic acid-d2	INTERNAL STANDARD	INTERNAL STANDARD	30	20	ES-	12.14	350.2	136.8	NA
IS36	valeric acid-d9	INTERNAL STANDARD	INTERNAL STANDARD	30	18	ES-	6.56	245	136.8	NA

Table S3. Mass spectrometry multiple reaction monitoring (MRM) transition and chromatographic retention time details for the quantitative bile acid method

Ref. index	Metabolite	Class	HMDB ID	Cone (V)	Collision (eV)	Ionization mode	Retention Time (min)	Precursor m/z	Product m/z	Internal Standard
116	chenodeoxycholic acid	bile acids	HMDB0000518	60	16	ESI-	5.67	391.3	391.3	chenodeoxycholic acid-d4
117	cholic acid	bile acids	HMDB0000619	60	20, 34	ESI-	4.79	407.3	407.3, 343.3	cholic acid-d4
118	glycochenodeoxycholic acid	bile acids	HMDB0000637	60	20	ESI-	4.78	448.3	448.3	glycochenodeoxycholic acid-d4
119	glycocholic acid	bile acids	HMDB0000138	60	20	ESI-	4.13	464.3	464.3	glycocholic acid-d4
120	glycodeoxycholic acid	bile acids	HMDB0000631	60	20	ESI-	4.96	448.3	448.3	glycodeoxycholic acid-d4
121	glycoursodeoxycholic acid	bile acids	HMDB0000708	60	20	ESI-	3.68	448.3	448.3	glycoursodeoxycholic acid-d4
122	taurochenodeoxycholic acid	bile acids	HMDB0000951	60	20, 60	ESI-	4.82	498.3	498.3, 80.1	taurochenodeoxycholic acid-d4
123	taurocholic acid	bile acids	HMDB0000036	60	20, 64	ESI-	4.19	514.3	514.3, 80.1	taurocholic acid-d4
124	taurodeoxycholic acid	bile acids	HMDB0000896	60	20, 60	ESI-	5.00	498.3	498.3, 80.1	taurodeoxycholic acid-d4
125	ursodeoxycholic acid	bile acids	HMDB0000946	60	16	ESI-	4.43	391.3	391.3	ursodeoxycholic acid-d4
126	deoxycholic acid	bile acids	HMDB0000626	60	16	ESI-	5.80	391.3	391.3	deoxycholic acid-d4
127	glycolithocholic acid	bile acids	HMDB0000698	60	20	ESI-	5.53	432.3	432.3	glycolithocholic acid-d4
128	lithocholic acid	bile acids	HMDB0000761	60	32	ESI-	6.56	375.3	375.3	lithocholic acid-d4
129	taurohyodeoxycholic acid	bile acids	NA	60	20, 60	ESI-	3.80	498.3	498.3, 80.1	taurohyodeoxycholic acid-d4
130	tauroolithocholic acid	bile acids	HMDB0000722	60	20, 60	ESI-	5.60	498.3	498.3, 80.1	tauroolithocholic acid-d4
IS37	chenodeoxycholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20	ESI-	5.66	395.3	395.3	NA
IS38	cholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20, 32	ESI-	4.79	411.3	411.3, 347.3	NA
IS39	glycochenodeoxycholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20	ESI-	4.77	452.3	452.3	NA
IS40	glycocholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20	ESI-	4.12	468.3	468.3	NA
IS41	glycodeoxycholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20	ESI-	4.96	452.3	452.3	NA
IS42	glycoursodeoxycholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20	ESI-	3.67	452.3	452.3	NA
IS43	taurochenodeoxycholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20, 62	ESI-	4.82	502.3	502.3	NA
IS44	taurocholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20, 65	ESI-	4.19	518.3	518.3, 80.1	NA
IS45	taurodeoxycholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20, 58	ESI-	4.99	502.3	502.3, 80.1	NA
IS46	ursodeoxycholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20	ESI-	4.42	395.3	395.3	NA
IS47	deoxycholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20	ESI-	5.80	395.3	395.3	NA
IS48	glycolithocholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20	ESI-	5.52	436.3	436.3	NA
IS49	lithocholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20	ESI-	6.55	379.3	379.3	NA
IS50	tauroolithocholic acid-d4	INTERNAL STANDARD	INTERNAL STANDARD	60	20, 60	ESI-	5.60	486.3	486.3, 80.1	NA

Table S4. Results from univariate statistical analysis

Ref. index	Metabolite	Australia (Kruskal-Wallis (KW) with post-hoc Dunn's test (DT), Three groups: healthy; SARS-CoV-2 neg; SARS-CoV-2 pos)									Spain, (Mann-Whitney (MW)), Two groups: healthy; SARS-CoV-2 pos)				
		KW <i>p</i>	BH <i>q</i>	Healthy Control Mean Conc. (sd) [μM]	SARS-CoV-2 Pos Mean Conc. (sd) [μM]	SARS-CoV-2 Neg Mean Conc. (sd) [μM]	QC Mean Conc. (sd) [uM]	Healthy Control - SARS-CoV-2 Neg	Healthy Control - SARS-CoV-2 Pos	SARS-CoV-2 Neg - SARS-CoV-2 Pos	MW <i>p</i>	BH <i>q</i>	Healthy Control Mean Conc. (sd) [μM]	SARS-CoV-2 Pos Mean Conc. (sd) [μM]	QC Mean Conc. (sd) [μM]
1	10z-non-adeceanoic acid	8.95E-01	9.54E-01	0.99 (0.55)	0.9 (0.48)	0.92 (0.63)	0.35 (0.08)	4.53E-01	3.67E-01	3.24E-01	1.97E-04	8.35E-04	0.54 (0.33)	1.09 (0.57)	0.96 (0.23)
2	2-hydroxy-3-methylbutyric acid	9.64E-01	9.87E-01	12.54 (4.3)	11.71 (7.77)	12.67 (12.52)	12.34 (0.84)	4.29E-01	4.64E-01	3.96E-01	1.55E-01	2.28E-01	7.16 (8.22)	10.07 (13.5)	16.5 (4.1)
3	2-hydroxy-butyric acid	4.20E-04	2.34E-03	68.97 (27.87)	126.98 (39.67)	70.58 (69.3)	48.78 (2.94)	3.52E-01	1.52E-04	5.97E-04	6.08E-04	2.21E-03	62.02 (43.92)	95.12 (78.59)	74.52 (17.2)
4	2-hydroxy-glutaric acid	5.31E-03	1.76E-02	3.81 (1.29)	4.74 (1.88)	3.85 (2.02)	1.86 (0.3)	1.89E-01	8.19E-04	1.11E-02	2.39E-03	6.18E-03	3.34 (2.31)	5.44 (4.86)	7.89 (1.37)
5	2-methyl-butylcarnitine	2.54E-01	4.48E-01	0.06 (0.02)	0.06 (0.05)	0.05 (0.04)	0.03 (0)	8.13E-02	4.61E-01	7.22E-02	2.55E-01	3.38E-01	0.07 (0.02)	0.05 (0.06)	0.05 (0.01)
6	2-phenylpropionic acid	6.07E-06	9.18E-05	0.32 (0.24)	0.01 (0.16)	0.2 (0.22)	0.16 (0.01)	3.18E-02	5.71E-07	1.12E-03	5.93E-04	2.21E-03	0.48 (0.38)	0.14 (0.24)	0.27 (0.03)
7	3-hydroxy-butyric acid	7.10E-01	8.32E-01	41.14 (76.22)	81.47 (51.96)	61.44 (179.04)	74.1 (5.18)	2.21E-01	2.61E-01	4.56E-01	5.13E-02	8.91E-02	36.16 (154.9)	51.89 (225.47)	138.29 (14.71)
8	3-hydroxy-isovaleric acid	1.17E-01	2.63E-01	0.35 (0.11)	0.49 (0.34)	0.33 (0.19)	0.44 (0.07)	4.94E-01	3.59E-02	3.46E-02	2.25E-01	3.10E-01	0.32 (0.08)	0.4 (0.22)	0.45 (0.07)
9	3-hydroxy-isovalerylcarnitine	5.22E-01	7.19E-01	0.03 (0.01)	0.03 (0.06)	0.03 (0.02)	0.02 (0)	1.53E-01	4.75E-01	1.75E-01	5.56E-01	6.33E-01	0.03 (0.01)	0.03 (0.02)	0.03 (0.01)
10	3-methyl-2-oxovaleric acid	5.68E-01	7.52E-01	130.49 (42.74)	116.22 (50.99)	119.1 (52.66)	60.39 (9.79)	1.48E-01	2.46E-01	3.70E-01	8.29E-04	2.58E-03	2839.1 (1046.92)	1841.94 (856.49)	1248.76 (198.83)
11	3-phenylpropionic acid	4.02E-06	8.52E-05	1.14 (0.86)	0.06 (0.51)	0.6 (0.74)	0.65 (0.15)	1.53E-02	3.25E-07	2.08E-03	6.74E-04	2.23E-03	0.98 (0.84)	0.32 (0.52)	0.57 (0.1)
12	5-aminolevulinic acid	3.26E-04	1.96E-03	3.17 (0.63)	4.06 (0.97)	3.03 (0.92)	4.09 (0.58)	4.47E-01	1.85E-04	3.01E-04	1.01E-04	4.88E-04	2.82 (0.74)	3.58 (1.5)	6.27 (0.99)
13	acetylcarnitine	3.88E-02	9.80E-02	14.31 (8.5)	23.02 (23.26)	18.58 (9.28)	8.39 (1.4)	3.95E-01	9.57E-03	1.87E-02	7.51E-01	8.12E-01	16.58 (7.49)	14.04 (9.27)	9.74 (1.13)
14	acetyl glycine	6.39E-01	7.78E-01	6.34 (2.89)	6.74 (4.38)	6.52 (3.48)	6.19 (0.44)	3.01E-01	3.32E-01	1.73E-01	2.30E-01	3.12E-01	7.51 (4.03)	8.13 (6.02)	8.35 (1.32)
15	aconitic acid	2.08E-01	3.88E-01	71.89 (21.07)	77.59 (23.06)	64.77 (24.68)	121.49 (15.23)	6.92E-02	4.51E-01	5.82E-02	3.35E-01	4.28E-01	47.75 (19)	56.34 (20.28)	45.01 (3.19)
16	alanine	2.54E-02	7.28E-02	472.56 (84.93)	495.3 (219.07)	380.9 (105.72)	418.94 (11.05)	2.65E-02	2.38E-01	4.65E-03	2.87E-02	5.16E-02	402.88 (83.53)	458.45 (137.64)	655.66 (57.44)
17	alpha-aminobutyric acid	3.46E-02	9.16E-02	29.56 (6.55)	37.03 (8.48)	25.96 (9.32)	21.76 (1.07)	1.84E-01	4.59E-02	5.20E-03	7.61E-02	1.22E-01	34.64 (10.88)	29.09 (13.93)	27.25 (3.76)
18	alpha-linolenic acid	4.92E-01	7.04E-01	12.16 (8.77)	8.62 (6.91)	11.29 (7.45)	9.59 (1.22)	3.70E-01	1.23E-01	2.01E-01	5.47E-02	9.36E-02	140.78 (118.96)	186.94 (194.08)	666.84 (119.9)
19	arachidonic acid	1.47E-01	3.06E-01	3.86 (1.36)	5.11 (1.8)	4.3 (2.41)	8.14 (0.88)	1.88E-01	2.52E-02	1.38E-01	1.25E-09	1.89E-08	97.62 (33.11)	192.7 (71.19)	440.43 (95.75)
20	arginine	3.32E-04	1.96E-03	116.81 (27.42)	69.25 (29.95)	93.37 (25.88)	108.48 (3.78)	1.01E-02	3.47E-05	4.36E-02	4.48E-01	5.45E-01	139.36 (32.53)	130.89 (43.95)	377.44 (31.95)
21	asparagine	1.17E-03	5.64E-03	67.97 (15.64)	51.48 (14.5)	58.78 (17.23)	45.6 (3.87)	2.93E-02	1.20E-04	3.38E-02	2.87E-02	5.16E-02	59.02 (15.7)	69.39 (26.25)	43.76 (10.28)

22	aspartic acid	5.60E-05	5.40E-04	5.8 (2.13)	9.43 (3.38)	7.3 (5.06)	14.11 (1.21)	7.88E-02	6.82E-06	1.49E-03	5.47E-05	3.04E-04	21.89 (10.52)	37.41 (17.81)	72.87 (16.88)
23	azelaic acid	6.29E-01	7.75E-01	0.25 (0.09)	0.24 (0.1)	0.24 (0.15)	0.27 (0.04)	3.10E-01	3.15E-01	1.68E-01	2.03E-01	2.91E-01	0.1 (0.08)	0.14 (0.05)	0.34 (0.04)
24	beta-alanine	2.58E-01	4.48E-01	3.34 (3.62)	3.74 (1.28)	3.25 (1.96)	5.16 (0.48)	1.95E-01	2.10E-01	5.00E-02	1.26E-03	3.72E-03	6.44 (2.05)	4.51 (2.11)	8.23 (0.8)
25	butyrylcarnitine	3.72E-03	1.36E-02	0.18 (0.16)	0.29 (0.19)	0.15 (0.14)	0.13 (0.01)	4.76E-01	1.93E-03	1.60E-03	5.78E-01	6.52E-01	0.22 (0.37)	0.2 (0.29)	0.09 (0.02)
26	caproic acid	4.98E-01	7.04E-01	1.16 (0.29)	1 (0.39)	1.21 (0.34)	0.62 (0.04)	4.48E-01	1.68E-01	1.38E-01	3.46E-03	8.52E-03	10.78 (6.42)	6.56 (2.95)	8.53 (1.81)
27	carnitine	4.01E-03	1.42E-02	47.81 (10.61)	53.36 (20.84)	44.86 (14.68)	35.96 (1.05)	9.62E-02	2.11E-02	4.77E-04	7.60E-01	8.13E-01	30.4 (7.1)	30.88 (18.54)	29.48 (3.03)
28	citric acid	6.74E-01	8.11E-01	135.68 (28.33)	142.51 (43.3)	124.14 (34.47)	110.36 (5.31)	1.95E-01	4.14E-01	2.67E-01	8.65E-01	9.08E-01	99.76 (27.12)	101.12 (35.08)	96.2 (8.23)
29	creatine	7.54E-01	8.69E-01	40.66 (24.15)	42.44 (49.06)	45.41 (21.82)	61.72 (3.06)	4.45E-01	2.38E-01	2.82E-01	4.80E-03	1.11E-02	31.04 (35.97)	59.03 (57.95)	59.99 (12.09)
30	d-glucose	1.84E-04	1.30E-03	4934.4 (912.2)	6433.71 (1289.63)	5069.97 (1377.85)	4329.36 (103.6)	2.97E-01	5.87E-05	4.35E-04	9.55E-01	9.82E-01	3508.96 (1045.74)	3299.31 (1971.36)	4807.99 (714.38)
31	dimethylglycine	7.34E-03	2.36E-02	3.6 (1.92)	4.65 (1.97)	3.09 (1.34)	3.36 (0.33)	5.31E-02	5.97E-02	8.64E-04	3.92E-01	4.87E-01	4.66 (1.78)	4.35 (9.26)	5.26 (0.66)
32	docosahexaenoic acid	2.05E-01	3.88E-01	3.04 (1.52)	3.01 (2.19)	3.86 (2.58)	1.99 (0.27)	3.74E-02	1.89E-01	1.96E-01	1.98E-03	5.24E-03	52.26 (32)	78.44 (58.46)	81.25 (18.16)
33	erythronic acid	2.98E-01	5.02E-01	8 (2.44)	10.73 (5.43)	6.92 (4.81)	5.78 (0.25)	4.45E-01	9.93E-02	7.78E-02	5.81E-06	3.85E-05	10.72 (4.47)	4.94 (3.01)	4.15 (0.76)
34	ethylmethylacetic acid	1.39E-01	3.00E-01	1.46 (0.15)	1.48 (0.11)	1.42 (0.09)	1.45 (0.21)	4.18E-02	4.96E-01	4.47E-02	9.64E-01	9.82E-01	1 (0.5)	1.01 (0.46)	19.65 (3.96)
35	glucaric acid	5.34E-01	7.26E-01	0.49 (0.32)	0.59 (0.24)	0.53 (0.17)	1.19 (0.12)	2.80E-01	1.32E-01	2.91E-01	9.92E-03	2.02E-02	0.11 (0.09)	0.17 (0.19)	0.14 (0.03)
36	glutamic acid	1.41E-03	6.49E-03	9.76 (7.99)	19.02 (8.93)	12.98 (8.17)	33.56 (3.15)	1.32E-01	1.90E-04	6.87E-03	5.33E-11	3.82E-09	11.46 (6.31)	26.85 (13.3)	74.13 (9.63)
37	glutamine	2.32E-03	9.47E-03	367.41 (89.23)	311.36 (50.55)	316.07 (55.08)	216.2 (9.77)	2.24E-03	8.33E-04	3.55E-01	2.27E-02	4.23E-02	109752.03 (14792.38)	98053.08 (23220.43)	46951.44 (7198.67)
38	glutaric acid	3.38E-01	5.23E-01	0.3 (0.14)	0.35 (0.34)	0.31 (0.08)	0.26 (0.02)	3.70E-01	1.38E-01	7.86E-02	8.50E-07	6.93E-06	0.08 (0.18)	0.25 (0.33)	0.42 (0.05)
39	glutaryl carnitine	1.71E-01	3.43E-01	0.09 (0.02)	0.08 (0.04)	0.09 (0.02)	0.08 (0.01)	4.63E-01	5.57E-02	4.62E-02	7.86E-01	8.33E-01	0.12 (0.06)	0.12 (0.2)	0.06 (0.01)
40	glyceric acid	1.47E-04	1.20E-03	3.86 (0.84)	5.15 (1.24)	3.85 (1.46)	6.57 (0.18)	4.94E-01	1.19E-04	1.27E-04	4.89E-01	5.83E-01	10.93 (4.11)	10.46 (5.1)	7.88 (1.35)
41	glycine	9.26E-01	9.72E-01	244.44 (57.83)	238.94 (60.32)	249.61 (62.72)	242.34 (7.24)	3.49E-01	4.45E-01	4.05E-01	2.08E-02	3.93E-02	283.58 (82.58)	346.84 (95.74)	486.17 (54.43)
42	glycylproline	6.42E-02	1.58E-01	0.12 (0.05)	0.09 (0.06)	0.11 (0.03)	0.1 (0.01)	3.36E-02	1.50E-02	3.50E-01	7.90E-02	1.25E-01	0.05 (0.02)	0.07 (0.03)	0.09 (0.02)
43	heptanoic acid	3.08E-01	5.11E-01	1.29 (0.31)	1.29 (0.34)	1.48 (0.34)	0.99 (0.13)	6.65E-02	1.57E-01	3.22E-01	1.18E-01	1.78E-01	1.22 (0.74)	0.94 (0.43)	2.63 (0.5)
44	hexanoylcarnitine	8.48E-02	2.00E-01	0.06 (0.02)	0.07 (0.08)	0.05 (0.04)	0.02 (0)	2.80E-01	5.63E-02	1.56E-02	6.92E-01	7.68E-01	0.09 (0.04)	0.09 (0.16)	0.03 (0)
45	hippuric acid	1.60E-04	1.21E-03	7.11 (8.48)	2.2 (4.79)	3.85 (3.91)	4 (0.15)	1.01E-02	1.53E-05	2.87E-02	7.63E-04	2.45E-03	9.55 (9.68)	4.12 (7.41)	5.57 (0.91)
46	histidine	5.25E-06	9.18E-05	93.68 (19.99)	63.12 (15.15)	91.56 (12.15)	79.38 (3.27)	1.70E-01	1.37E-06	8.62E-05	3.95E-01	4.87E-01	95.28 (13.15)	92.7 (24.85)	172.19 (19.75)

47	homoserine	7.04E-02	1.70E-01	11.05 (2.85)	8.43 (3.25)	10.94 (3.36)	9.63 (1.29)	4.77E-01	2.08E-02	2.37E-02	5.48E-01	6.31E-01	8.82 (3.26)	8.51 (6.15)	11.97 (2.13)
48	indole-3-acetic acid	3.57E-03	1.35E-02	0.44 (0.14)	0.28 (0.46)	0.42 (0.19)	0.38 (0.09)	8.30E-02	4.11E-04	2.31E-02	9.95E-01	9.95E-01	0.52 (0.56)	0.7 (1.1)	0.64 (0.12)
49	indole-3-propionic acid	1.09E-05	1.45E-04	1.84 (1.38)	0.23 (17.33)	1.81 (1.68)	1.14 (0.14)	4.94E-01	1.46E-05	1.56E-05	1.96E-02	3.77E-02	1.67 (1.21)	0.98 (1.81)	1.44 (0.18)
50	indole-3-pyruvic acid	1.66E-06	4.41E-05	83.33 (22.64)	40.1 (14.28)	73.88 (23.17)	20.43 (1.78)	2.85E-01	1.01E-06	1.34E-05	8.99E-04	2.72E-03	146.58 (56.97)	101.7 (60.15)	2.94 (0.66)
51	isovaleric acid	2.81E-01	4.81E-01	1.47 (0.77)	1.1 (1)	1.03 (0.55)	0.59 (0.11)	5.95E-02	3.17E-01	1.48E-01	6.06E-03	1.36E-02	2.04 (0.93)	2.56 (1.42)	31.19 (5.82)
52	isovalerylcarnitine	1.55E-01	3.17E-01	0.09 (0.03)	0.1 (0.03)	0.08 (0.03)	0.08 (0.01)	7.94E-02	3.22E-01	3.30E-02	6.96E-01	7.68E-01	0.12 (0.04)	0.12 (0.1)	0.1 (0.02)
53	ketoleucine	1.86E-01	3.66E-01	109.99 (38.96)	88.08 (29.28)	102.56 (41.71)	71.65 (7.68)	1.79E-01	3.34E-02	1.75E-01	1.90E-02	3.73E-02	3487.89 (1283.53)	2781.92 (1103.8)	1117.9 (163.82)
54	kynurenine	8.79E-03	2.74E-02	7.44 (1.95)	10.31 (4.1)	7.69 (3.25)	3.38 (0.3)	2.91E-01	1.80E-03	8.81E-03	4.79E-01	5.77E-01	2.44 (2.58)	2.92 (4.01)	2.38 (0.53)
55	lactic acid	2.75E-05	2.92E-04	614.23 (136.68)	960.34 (422.92)	550.57 (166.95)	960.68 (100.36)	2.23E-01	1.76E-04	7.95E-06	1.20E-08	1.41E-07	817.58 (165.75)	1319.36 (504.51)	886.62 (105.83)
56	leucine	8.84E-01	9.54E-01	139.78 (51.46)	140.28 (35.07)	130.43 (47.64)	127.66 (3.98)	4.29E-01	3.75E-01	3.12E-01	6.98E-02	1.14E-01	147.91 (29.52)	166.89 (44.95)	309.3 (34.73)
57	linoleic acid	7.89E-01	8.99E-01	402.77 (216.87)	337.79 (199.34)	350.24 (218.49)	559.47 (52.99)	4.58E-01	2.94E-01	2.59E-01	6.47E-04	2.21E-03	8966.19 (3882.71)	12787.58 (7299.95)	19987.18 (3056.95)
58	linoleyl carnitine	8.85E-01	9.54E-01	0.08 (0.03)	0.09 (0.05)	0.08 (0.04)	0.13 (0.01)	3.65E-01	4.44E-01	3.16E-01	1.06E-02	2.12E-02	0.08 (0.04)	0.11 (0.07)	0.1 (0.01)
59	lysine	6.11E-01	7.75E-01	252.94 (62.83)	247.2 (52.69)	237.12 (45.89)	216.02 (7.05)	1.66E-01	2.57E-01	3.83E-01	6.47E-02	1.09E-01	207.83 (33.71)	231.88 (70.85)	342.73 (34.98)
60	malic acid	5.23E-03	1.76E-02	4.18 (1.52)	6.32 (3.74)	3.64 (2.5)	4.71 (0.23)	9.41E-02	2.60E-02	6.24E-04	8.83E-08	7.80E-07	3.22 (1.13)	5.75 (3.64)	4.3 (0.47)
61	malonylcarnitine	2.58E-01	4.48E-01	0.25 (0.09)	0.29 (0.39)	0.25 (0.11)	0.16 (0.02)	4.89E-01	7.35E-02	7.74E-02	5.18E-01	6.03E-01	0.5 (0.15)	0.43 (0.29)	0.32 (0.05)
62	methionine	5.05E-01	7.04E-01	27.6 (12.08)	25.98 (9.17)	28.23 (10.76)	41.71 (7.3)	2.38E-01	1.24E-01	3.22E-01	4.97E-01	5.85E-01	62.33 (11.74)	62.3 (28.68)	98.35 (9.09)
63	methylmalonic acid	5.48E-01	7.35E-01	6.89 (3.86)	7.19 (4.25)	7.36 (3.41)	2.94 (0.31)	1.42E-01	2.36E-01	3.72E-01	1.58E-10	5.59E-09	5.18 (2.11)	12.36 (4.66)	9.82 (1.87)
64	myristoleic acid	8.48E-01	9.36E-01	2.17 (2.17)	2.96 (4)	1.91 (2.82)	1.33 (0.13)	4.58E-01	3.29E-01	2.93E-01	3.85E-03	9.24E-03	3.18 (3.55)	7.3 (5.31)	4.78 (0.92)
65	n-acetylaspartic acid	3.23E-01	5.14E-01	0.44 (0.09)	0.45 (0.14)	0.41 (0.21)	0.41 (0.07)	8.73E-02	4.60E-01	1.10E-01	1.50E-03	4.19E-03	0.53 (0.12)	0.76 (0.45)	0.62 (0.07)
66	n-acetylneuraminic acid	1.24E-06	4.37E-05	1.1 (0.17)	1.58 (0.86)	1.1 (0.43)	1.05 (0.09)	4.97E-01	2.60E-06	2.70E-06	4.54E-10	9.63E-09	0.84 (0.22)	1.9 (0.91)	0.85 (0.13)
67	o-adipoylcarnitine	1.10E-06	4.37E-05	0.01 (0)	0.04 (0.05)	0.01 (0.01)	0.01 (0)	9.83E-02	2.08E-07	7.20E-05	9.45E-03	1.96E-02	0.02 (0.02)	0.03 (0.11)	0.01 (0)
68	octanoic acid	3.22E-01	5.14E-01	5.1 (2.92)	4.37 (1.42)	4.44 (1.81)	2.59 (0.14)	2.08E-01	6.64E-02	2.39E-01	7.17E-01	7.83E-01	38.63 (16.94)	38.96 (19.76)	31.75 (6.93)
69	octanoylcarnitine	9.78E-01	9.87E-01	0.14 (0.11)	0.13 (0.12)	0.14 (0.1)	0.07 (0.01)	4.17E-01	4.59E-01	4.59E-01	3.88E-01	4.87E-01	0.15 (0.08)	0.13 (0.2)	0.05 (0.01)
70	oleylcarnitine	1.21E-02	3.68E-02	0.21 (0.05)	0.27 (0.15)	0.23 (0.08)	0.13 (0.01)	2.40E-01	2.10E-03	1.48E-02	1.08E-04	4.96E-04	0.22 (0.11)	0.34 (0.18)	0.12 (0.03)
71	ornithine	9.90E-01	9.90E-01	83.29 (36.73)	86.98 (19.36)	91.62 (27.57)	82.2 (2.02)	4.52E-01	4.51E-01	4.98E-01	1.41E-08	1.50E-07	94.48 (20.89)	139.85 (34.22)	95.75 (10.22)
72	oxalic acid	1.20E-01	2.65E-01	36.4 (8.2)	47.74 (17.21)	38.55 (12.77)	83.38 (6.52)	1.30E-01	2.00E-02	1.70E-01	8.42E-03	1.78E-02	9.61 (10.86)	4.86 (5.7)	9.81 (2.12)

73	oxoglutaric acid	8.26E-07	4.37E-05	5.15 (2.38)	15.32 (4.85)	5.02 (9.7)	52.44 (4.09)	4.01E-01	1.08E-06	3.53E-06	5.69E-10	1.00E-08	22.61 (14.55)	52.38 (62.12)	18.88 (4.08)
74	palmitoylcarnitine	3.12E-02	8.49E-02	0.14 (0.03)	0.16 (0.06)	0.12 (0.04)	0.11 (0.01)	4.87E-01	1.03E-02	1.12E-02	1.40E-03	4.01E-03	0.08 (0.03)	0.12 (0.04)	0.07 (0.01)
75	phenylacetic acid	8.27E-01	9.33E-01	5.46 (3.5)	5.04 (5.01)	5.15 (3.06)	4.91 (0.48)	3.43E-01	2.74E-01	4.18E-01	2.20E-04	8.99E-04	6.62 (8.17)	19.13 (19.93)	27.03 (3.82)
76	phenylacetylglutamine	6.18E-01	7.75E-01	3.69 (2.29)	3.19 (9.85)	2.81 (3.69)	2.15 (0.13)	2.11E-01	4.59E-01	1.88E-01	3.92E-03	9.24E-03	3.67 (2.77)	8.23 (8.74)	2.41 (0.44)
77	phenylalanine	1.64E-03	7.24E-03	77.98 (21.38)	84.71 (30.37)	71.03 (20.98)	73.17 (10.16)	2.15E-02	5.58E-02	1.81E-04	3.88E-08	3.74E-07	74.98 (22.44)	121.23 (34.84)	154.78 (28.75)
78	phenylpyruvic acid	3.40E-01	5.23E-01	5.95 (1.85)	5.39 (5.35)	5.47 (1.63)	3.32 (0.17)	7.59E-02	1.64E-01	3.37E-01	3.21E-01	4.15E-01	10.84 (3.22)	12.04 (6.65)	3.11 (0.58)
79	pipecolic acid	8.97E-02	2.07E-01	1.55 (0.42)	1.91 (1.58)	1.47 (0.68)	1.09 (0.14)	4.66E-01	2.52E-02	3.05E-02	6.64E-02	1.10E-01	2.05 (1.31)	1.54 (0.83)	2.68 (0.34)
80	proline	3.29E-03	1.29E-02	268.33 (98.05)	232.74 (74.82)	214.04 (48.33)	263.69 (15.77)	3.67E-04	3.50E-02	6.90E-02	9.37E-01	9.74E-01	201.53 (84.03)	205.68 (71.76)	269.91 (36.06)
81	propionic acid	9.64E-01	9.87E-01	14.44 (2.55)	13.73 (2.47)	13.96 (3.81)	12.76 (1.66)	4.82E-01	4.16E-01	3.99E-01	8.86E-09	1.17E-07	6.49 (4.08)	18.12 (7.84)	11.19 (2.03)
82	propionylcarnitine	8.21E-04	4.33E-03	0.7 (0.35)	1.08 (0.68)	0.63 (0.41)	0.43 (0.02)	6.81E-02	1.09E-02	8.86E-05	9.77E-01	9.87E-01	1.35 (0.43)	1.15 (1.25)	0.94 (0.22)
83	pyroglutamic acid	1.87E-05	2.20E-04	16.87 (8.23)	30.82 (11.19)	19.88 (8.6)	38.48 (3.81)	9.35E-02	2.67E-06	5.52E-04	4.11E-10	9.63E-09	23.62 (7.7)	40.47 (15)	98.7 (15.4)
84	pyruvic acid	9.70E-05	8.57E-04	112.94 (46.59)	221.69 (93.44)	105.9 (42.89)	141.34 (8.33)	1.64E-01	7.47E-04	1.80E-05	2.43E-06	1.84E-05	51.91 (31.8)	118.32 (69.7)	9.34 (1.29)
85	sarcosine	1.83E-03	7.76E-03	5.62 (2)	6.46 (1.34)	5 (1.22)	5.35 (0.75)	4.67E-03	2.00E-01	3.63E-04	3.28E-04	1.29E-03	10.33 (2.16)	12.22 (3.82)	14.35 (2.1)
86	sebacic acid	7.15E-01	8.32E-01	0.04 (0.03)	0.04 (0.03)	0.04 (0.06)	0.05 (0.01)	4.70E-01	2.27E-01	2.49E-01	4.59E-02	8.11E-02	0.1 (0.02)	0.11 (0.04)	0.13 (0.02)
87	serine	2.12E-01	3.88E-01	121.62 (29.68)	106.07 (24.49)	109.46 (32.61)	106.18 (3.72)	1.58E-01	3.97E-02	2.19E-01	5.74E-05	3.04E-04	159.96 (22.36)	188.06 (27.61)	285.12 (39.81)
88	stearoylcarnitine	6.20E-01	7.75E-01	0.05 (0.02)	0.04 (0.02)	0.05 (0.02)	0.03 (0.01)	2.08E-01	1.92E-01	4.69E-01	6.31E-03	1.36E-02	0.06 (0.02)	0.08 (0.03)	0.04 (0.01)
89	succinic acid	9.00E-01	9.54E-01	9.57 (3.74)	10.03 (3.65)	10.3 (2.68)	8.68 (0.76)	3.29E-01	3.73E-01	4.57E-01	7.21E-11	3.82E-09	10.3 (3.54)	22.62 (9.98)	19.26 (2.16)
90	tetradecanoylcarnitine	1.44E-01	3.04E-01	0.04 (0.01)	0.04 (0.03)	0.04 (0.02)	0.02 (0)	4.04E-01	3.40E-02	5.61E-02	9.13E-02	1.42E-01	0.02 (0.01)	0.02 (0.01)	0.02 (0)
91	threonic acid	3.25E-01	5.14E-01	8.28 (2.35)	10.59 (5.21)	7.21 (4.37)	6.05 (0.37)	3.98E-01	1.22E-01	7.84E-02	8.90E-06	5.55E-05	10.86 (4.6)	5.45 (3.14)	4.53 (0.73)
92	threonine	3.07E-02	8.49E-02	102.66 (25.15)	79.11 (26.28)	106.66 (26.72)	96.61 (4.14)	2.85E-01	5.75E-03	2.42E-02	9.57E-02	1.47E-01	103.46 (36.9)	92.8 (34.12)	154.25 (22.84)
93	tryptophan	2.35E-04	1.56E-03	151.27 (35.11)	107.71 (24.65)	143.68 (33.57)	106.68 (10.1)	4.36E-01	2.45E-04	1.34E-04	6.47E-04	2.21E-03	162.99 (26.31)	128.91 (43.65)	181.81 (26.88)
94	tyrosine	9.77E-01	9.87E-01	73.78 (23.06)	76.93 (15.32)	75.1 (18.02)	71.43 (2.52)	4.97E-01	4.26E-01	4.23E-01	1.19E-01	1.78E-01	68.38 (13.34)	73.07 (21.17)	105.43 (13.97)
95	valeric acid	6.88E-01	8.19E-01	5.07 (1.01)	4.76 (1.11)	5.44 (1.07)	3.44 (0.34)	3.90E-01	2.82E-01	1.97E-01	1.32E-05	7.75E-05	3.26 (2.59)	7.14 (2.62)	3.96 (0.61)
96	valine	6.01E-01	7.75E-01	200.39 (48.27)	185.04 (34.01)	182.69 (52.37)	168.96 (7.98)	1.76E-01	2.13E-01	4.55E-01	2.43E-01	3.26E-01	241.72 (47.07)	218.84 (53.82)	308.32 (36.24)
116	chenodeoxycholic acid	4.77E-01	6.99E-01	21.42 (194.86)	28.8 (79.18)	11.62 (72.26)	67.57 (1.16)	1.19E-01	3.73E-01	2.03E-01	8.82E-05	4.45E-04	150.51 (295.93)	19.84 (144.13)	234.84 (1.76)
117	cholic acid	2.12E-01	3.88E-01	9.61 (166.89)	6.39 (56.49)	6.84 (61.09)	30.03 (0.19)	7.36E-02	5.71E-02	4.34E-01	1.40E-04	6.18E-04	62.62 (555.84)	11.25 (65.92)	175.38 (2.55)

118	glycocheno- deoxycholic acid	4.78E-01	6.99E-01	330.8 (310.52)	603 (597.06)	406.46 (400.43)	818.16 (14.27)	3.98E-01	1.22E-01	1.81E-01	2.13E-01	2.96E-01	275.29 (288.07)	335.63 (419.12)	1475.91 (49.66)
119	glycocholic acid	3.65E-02	9.43E-02	63.12 (81.07)	197.33 (209.57)	147.96 (135.02)	181.37 (2.09)	5.76E-02	5.47E-03	1.57E-01	6.31E-03	1.36E-02	0.23 (0.36)	0.57 (0.68)	1.67 (0.05)
120	glycodeoxycholic acid	4.23E-01	6.41E-01	323.08 (290.33)	537.67 (563.32)	381.85 (364.27)	789.48 (9.03)	3.58E-01	1.01E-01	1.78E-01	1.74E-01	2.52E-01	275.11 (297.62)	339.69 (430.43)	1482.2 (25.15)
121	glycourso- deoxycholic acid	4.81E-01	6.99E-01	342.9 (330.61)	613.54 (624.34)	429.64 (402.14)	869.11 (3.65)	4.10E-01	1.26E-01	1.77E-01	3.21E-03	8.11E-03	34.27 (41.88)	60.09 (182.22)	148.19 (2.42)
122	taurocheno-- deoxycholic acid	1.83E-02	5.40E-02	85.36 (144.78)	217.32 (371.2)	143.99 (238.09)	260.14 (3.46)	7.14E-02	2.35E-03	8.13E-02	2.10E-01	2.96E-01	37.44 (40.15)	50.86 (132.51)	236.67 (6.05)
123	taurocholic acid	8.58E-04	4.33E-03	7.82 (29.01)	50.48 (113)	25.77 (54.24)	49.95 (1.72)	2.32E-02	8.73E-05	3.52E-02	1.90E-03	5.17E-03	7.96 (26.19)	26.75 (115.29)	121.47 (3.33)
124	taurodeoxycholic acid	8.40E-01	9.36E-01	20.3 (36.71)	15.17 (82.14)	39.01 (32.53)	53.68 (0.72)	4.44E-01	2.85E-01	3.33E-01	3.03E-06	2.14E-05	1113.16 (1611.9)	3438.22 (8451.83)	7458.03 (97.73)
125	ursodeoxycholic acid	6.26E-01	7.75E-01	5.66 (40.92)	8.5 (54.38)	6.22 (7.13)	13.59 (0.44)	3.46E-01	2.82E-01	1.67E-01	2.95E-01	3.85E-01	16.74 (40.55)	9.46 (94.07)	34.02 (1.10)

Figure S1. Principal Component Analysis (PCA). Panel A and B present study samples (white) and replicate quality control (QC) samples (light blue), with clustering of QC samples indicating assay reproducibility. Panels C and D represent PCA of only study samples and are coloured by class: Healthy control (dark blue), SARS-CoV-2 positive (dark orange) and SARS-CoV-2 negative (white). SARS-CoV-2 negative were only available for the Australian cohort.

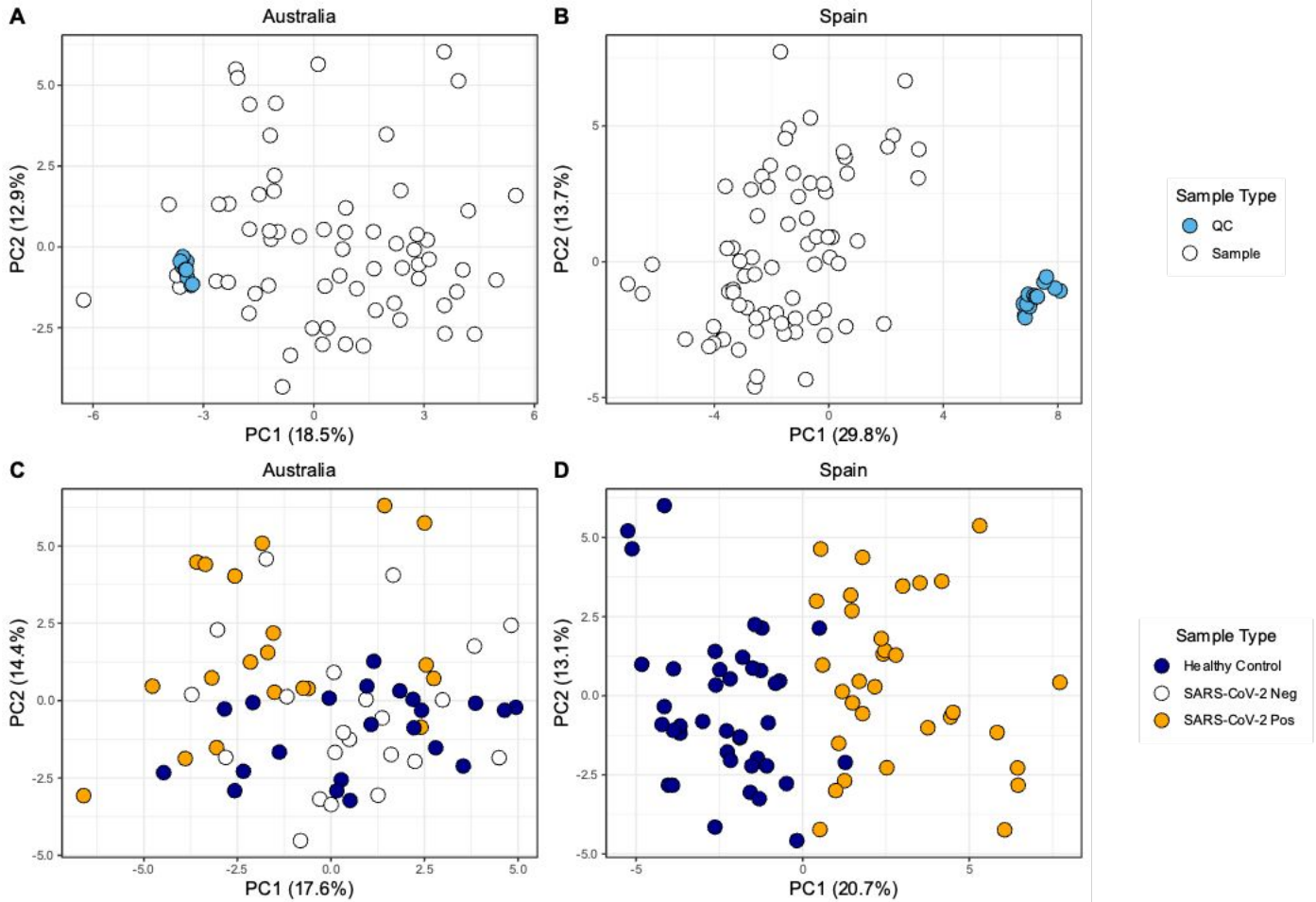


Figure S2. Boxplot visualizations of the metabolites (n = 23) that reported an agreement in univariate testing (Benjamini-Hochberg FDR $q < 0.1$) across both the Australian and Spanish cohorts.

