

Table S1. Definitions of clinical types of COVID-19 in adult patients

Mild	<ul style="list-style-type: none">• Upper respiratory symptoms (eg, pharyngeal congestion, sore throat, and fever) for a short duration or asymptomatic infection• Positive RT-PCR test for SARS-CoV-2• No abnormal radiographic and septic presentation
Moderate	<ul style="list-style-type: none">• Imaging shows pneumonia.• Symptoms such as fever, cough, fatigue, headache, and myalgia
Severe	Mild or moderate clinical features, plus any manifestations that suggest disease progression: <ul style="list-style-type: none">• Respiratory distress, breathing frequency ≥ 30 times/minute;• In the resting state, it means oxygen saturation $\leq 93\%$;• Arterial blood oxygen partial pressure (PaO_2)/oxygen concentration (FiO_2) ≤ 300 mmHg (1 mmHg = 0.133kPa).
Critical	Rapid disease progression, plus any other conditions: <ul style="list-style-type: none">• Respiratory failure with need for mechanical ventilation (eg, ARDS, persistent hypoxia that cannot be alleviated by inhalation through nasal catheters or masks)• Septic shock• Organ failure that needs monitoring in the ICU

COVID-19=coronavirus disease 2019. SARS-CoV-2=severe acute respiratory syndrome coronavirus 2. ARDS=acute respiratory distress syndrome. ICU=intensive care unit.

Table S2. Metabolites detected in the discovery cohort by untargeted metabolomics

Class	Name	HMDB_ID	KEGG_ID	Normal VS Mild				Normal VS Severe				Normal VS Recovery				Total	
				P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR
Others	1-methyladenosine	HMDB0003331	C02494	<0.001	<0.001	0.91	1.7671	<0.001	0.001	0.72	1.417	<0.001	<0.001	-1.29	1.5723	<0.001	<0.001
Amino acids	N-acetyl-l-leucine	HMDB0011756	C02710	<0.001	<0.001	2.482	2.1962	<0.001	<0.001	0.933	1.417	0.0049	0.009	-0.37	0.1649	<0.001	<0.001
Amino acids	N-acetyl-l-phenylalanine	HMDB0000512	C03519	<0.001	<0.001	3.14	2.1249	<0.001	0.002	1.87	1.4	<0.001	<0.001	-0.73	0.1835	<0.001	<0.001
Amino acids	N-acetylproline	HMDB0094701	-	<0.001	<0.001	2.223	1.8915	0.611	0.7068	0.277	0.916	0.0177	0.030	-0.16	0.2193	<0.001	<0.001
Amino acids	2-phenylglycine	HMDB0002210	-	<0.001	<0.001	2.68	0.6317	0.003	0.009	2.50	0.983	<0.001	<0.001	0.90	0.3909	<0.001	<0.001
Amino acids	Creatinine	HMDB0000562	C00791	0.6377	0.71101	0.06	0.1746	0.005	0.0138	-0.43	1.174	0.0025	0.005	0.27	0.6989	<0.001	<0.001
Amino acids	N-acetyl-l-alanine	HMDB0000766	-	0.417	0.518	0.06	0.5434	0.0114	0.025	0.18	1.18	<0.001	<0.001	0.50	0.7862	<0.001	<0.001
Amino acids	Nicotinic acid	HMDB0003269	C05380	0.65	0.71609	-0.08	0.1592	<0.001	0.0012	1.543	1.062	0.0016	0.003	0.65	0.8255	<0.001	<0.001
Amino acids	DL-tryptophan	HMDB0030396	C00806	0.045	0.089	-0.22	0.8762	0.0701	0.122	-0.30	0.73	0.0133	0.023	0.26	0.8387	<0.001	<0.001
Amino acids	Levothyroxine	HMDB0000248	C01829	0.0586	0.11279	0.228	0.7975	0.005	0.0137	-0.59	1.24	0.001	0.002	0.40	0.9823	<0.001	<0.001
Amino acids	L-allo-threonine	HMDB0004041	C05519	0.003	0.010	-0.54	1.2911	0.0298	0.056	-0.40	0.786	0.0033	0.006	0.41	0.9895	<0.001	<0.001
Amino acids	2-hydroxyphenylalanine	HMDB0006050	-	0.2258	0.31431	-0.96	0.1838	0.110	0.1715	-1.08	0.432	<0.001	<0.001	-2.15	1.1783	<0.001	<0.001
Amino acids	Leucyl proline	HMDB0011175	-	0.177	0.267	0.33	0.5544	<0.001	<0.001	1.17	1.32	<0.001	<0.001	-1.05	1.2378	<0.001	<0.001
Amino acids	S-lactoylglutathione	HMDB0001066	C03451	0.1827	0.26736	0.039	0.5327	0.011	0.0254	-0.24	1.068	<0.001	<0.001	0.15	1.1857	<0.001	<0.001
Amino acids	L-asparagine	HMDB0000168	C00152	0.170	0.258	0.14	0.7073	<0.001	<0.001	0.36	1.311	<0.001	<0.001	0.46	1.4447	<0.001	<0.001
Amino acids	5-aminovaleric acid	HMDB0003355	C00431	0.5277	0.63326	0.071	0.2779	0.406	0.5089	0.251	0.675	<0.001	0.002	0.52	1.107	0.01	0.0083
Amino acids	L-glutamine	HMDB0000641	C00064	0.006	0.018	-0.51	1.129	<0.001	0.001	-0.78	1.45	<0.001	<0.001	0.53	1.2554	<0.001	<0.001
Amino acids	L-kynurenine	HMDB0000684	C00328	0.1056	0.1811	0.033	0.5986	0.004	0.0106	0.895	1.352	<0.001	<0.001	0.56	1.1805	<0.001	<0.001
Amino acids	L-phenylalanine	HMDB0000159	C00079	<0.001	<0.001	0.76	2.0032	<0.001	<0.001	0.76	1.745	<0.001	<0.001	0.60	1.6617	<0.001	<0.001
Amino acids	Hexanoylglycine	HMDB0000701	-	0.9843	0.98427	-0.11	0.1943	0.216	0.3029	-0.2	0.48	<0.001	<0.001	0.65	1.4672	<0.001	<0.001
Amino acids	L-isoleucine	HMDB0000172	C00407	0.465	0.571	0.13	0.2977	0.2945	0.383	0.09	0.757	<0.001	<0.001	0.70	1.2506	0.001	0.0016
Amino acids	L-tyrosine	HMDB0000158	C00082	0.1348	0.21643	0.297	0.5804	0.302	0.3899	0.264	0.588	<0.001	<0.001	0.71	1.112	0.00	0.0063
Amino acids	L-norleucine	HMDB0001645	C01933	0.522	0.629	-0.10	0.2963	0.7689	0.835	-0.07	0.554	<0.001	0.002	0.75	1.1324	<0.001	0.0016
Amino acids	Beta-alanine	HMDB0000056	C00099	0.6217	0.70196	0.075	0.2938	0.910	0.9521	-0.03	0.03	<0.001	<0.001	0.76	1.1334	<0.001	<0.001
Amino acids	L-proline	HMDB0000162	C00148	0.115	0.192	-0.21	0.6577	0.8938	0.942	0.05	0.152	<0.001	<0.001	0.80	1.3218	<0.001	<0.001
Amino acids	DL-serine	HMDB0000187	C00716	0.7908	0.82013	0.029	0.1422	0.650	0.744	-0.21	0.346	<0.001	<0.001	0.87	1.6342	<0.001	<0.001
Amino acids	D-aspartate	HMDB0006483	C00402	<0.001	<0.001	1.46	1.936	<0.001	0.002	1.24	1.57	<0.001	<0.001	1.30	1.5896	<0.001	<0.001
Amino acids	L-histidine	HMDB0000177	C00135	0.7374	0.77753	0.128	0.2918	<0.001	<0.001	-0.93	1.636	<0.001	<0.001	1.36	1.6858	<0.001	<0.001
Amino acids	L-glutamic acid	HMDB0000148	C00025	<0.001	<0.001	0.74	1.7166	<0.001	<0.001	0.90	1.579	<0.001	<0.001	1.44	1.7968	<0.001	<0.001
Amino acids	L-lysine	HMDB0000182	C00047	0.2107	0.29826	0.622	0.6883	0.650	0.744	0.274	0.566	<0.001	<0.001	2.15	1.7559	<0.001	<0.001
Amino acids	N-acetylmethionine	HMDB0011745	C02712	0.258	0.352	0.25	0.5278	<0.001	<0.001	2.46	1.869	<0.001	<0.001	2.36	1.2883	<0.001	<0.001
Amino acids	D-ornithine	HMDB0003374	C00515	0.1827	0.26736	0.563	0.8691	0.005	0.0122	0.911	1.442	<0.001	<0.001	3.47	1.6865	<0.001	<0.001
Amino acids	N-acetylorithine	HMDB0003357	C00437	<0.001	<0.001	4.60	1.7166	<0.001	<0.001	4.01	1.631	<0.001	<0.001	5.04	1.3389	<0.001	<0.001
Amino acids	3-methoxytyrosine	HMDB0001434	-	0.5145	0.62333	-0.12	0.2264	0.087	0.1429	-0.38	0.583	0.036	0.058	-0.53	0.1469	0.16	0.1754
Amino acids	Betaine	HMDB0000043	C00719	0.038	0.078	0.47	0.9209	0.1053	0.168	-0.34	0.784	0.0413	0.065	0.32	0.7014	<0.001	0.0015
Amino acids	Creatine	HMDB0000064	C00300	0.6629	0.72636	0.052	0.1356	0.152	0.2238	0.256	0.901	0.0522	0.080	0.18	0.6083	0.12	0.1378
Amino acids	L-threonine	HMDB0000167	C00188	0.002	0.007	-0.58	1.2475	<0.001	<0.001	-1.08	1.713	0.0677	0.102	0.23	0.6784	<0.001	<0.001
Amino acids	N-acetyl-d-tryptophan	HMDB0013713	-	<0.001	<0.001	1.796	2.0075	<0.001	<0.001	1.642	0.862	0.1098	0.157	0.23	0.5085	<0.001	<0.001
Amino acids	L-threonic acid	HMDB0062620	C01620	0.011	0.027	-0.91	1.1489	0.0523	0.093	-0.82	0.721	0.1902	0.263	-0.25	0.4405	0.0414	0.0519
Amino acids	Cinnamoylglycine	HMDB00011621	-	0.0379	0.07764	-2.32	0.334	0.005	0.0138	-2.78	0.947	0.2497	0.331	-1.08	0.4048	0.02	0.021
Amino acids	1-methylhistidine	HMDB0000479	C01152	0.097	0.169	0.42	0.5338	0.2471	0.331	0.87	0.757	0.2497	0.331	0.61	0.4111	0.3989	0.4103
Amino acids	Capryloylglycine	HMDB0000832	-	0.0032	0.01018	0.668	0.383	0.087	0.1429	-0.18	0.775	0.2653	0.346	0.13	0.0884	<0.001	<0.001
Amino acids	Tyrosylalanine	HMDB0029098	-	0.006	0.017	-2.11	1.1888	0.4371	0.537	1.17	0.073	0.2815	0.362	0.87	0.0972	<0.001	<0.001
Amino acids	Valylproline	HMDB0029135	-	0.8792	0.89701	-0.02	0.1011	0.087	0.1429	0.424	0.757	0.3719	0.459	0.08	0.3003	0.22	0.2352
Amino acids	L-valine	HMDB0000883	C00183	0.540	0.639	-0.32	0.1266	0.2471	0.331	0.26	0.688	0.4022	0.487	-0.13	0.3295	0.1933	0.2081
Amino acids	L-tryptophan	HMDB0000929	C00078	0.0026	0.00898	-0.4	1.2159	0.004	0.0104	-0.57	1.181	0.4248	0.510	0.09	0.3291	<0.001	<0.001
Amino acids	N-acetylvaline	HMDB0011757	-	<0.001	<0.001	1.68	2.2194	<0.001	0.001	0.46	1.314	0.4337	0.518	-0.06	0.2726	<0.001	<0.001
Amino acids	Pyroglutamate	HMDB0000267	C01879	0.0032	0.01018	1.206	1.4344	0.002	0.006	0.402	1.317	0.5009	0.576	0.01	0.4296	0.00	0.0023

Amino acids	DL-2-aminocaprylic acid	HMDB0000991	-	0.046	0.091	-0.76	0.2538	0.0597	0.104	-1.17	0.458	0.5009	0.576	-0.18	0.0414	0.0632	0.0766
Amino acids	Glycyl-L-leucine	HMDB0000759	C02155	0.2107	0.29826	-0.67	0.0197	0.186	0.2679	-0.41	0.348	0.573	0.650	-0.35	0.1281	0.52	0.529
Amino acids	N-	HMDB0006344	C04148	0.708	0.756	0.52	0.3379	0.1095	0.171	1.12	0.693	0.5981	0.667	-0.63	0.1994	0.1812	0.196
Amino acids	L-arginine	HMDB0000517	C00062	0.5827	0.67983	-0.07	0.2749	<0.001	0.0015	-0.78	1.341	0.6093	0.676	-0.07	0.1231	<0.001	<0.001
Amino acids	N-methyl-L-glutamate	HMDB0062660	C01046	0.022	0.051	0.34	0.7411	0.0135	0.029	0.43	1.185	0.7029	0.757	0.12	0.2237	0.0083	0.0117
Benzenoids	3-hydroxybenzoate	HMDB0002466	C00587	0.3318	0.43551	4.07	1.1504	1.000	1	5.667	1.33	0.0037	0.007	-0.36	0.0483	0.10	0.1132
Benzenoids	Homogentisate	HMDB0000130	C00544	0.146	0.227	-0.44	0.6064	0.9362	0.958	0.36	0.583	0.0029	0.006	3.37	0.1422	<0.001	<0.001
Benzenoids	4-hydroxybenzoate	HMDB0000500	C00156	<0.001	<0.001	-0.58	0.3252	0.001	0.0041	-0.44	0.411	<0.001	0.002	-0.39	0.2614	<0.001	<0.001
Benzenoids	3,4-dihydroxyphenyl glycol	HMDB0000318	C05576	0.075	0.138	-0.17	0.5729	0.2254	0.307	-0.24	0.211	0.0055	0.010	-0.10	0.4837	0.1069	0.1214
Benzenoids	4-ethylphenol	HMDB0029306	C13637	0.0379	0.07764	-0.53	0.2892	0.030	0.0561	-0.46	0.463	<0.001	<0.001	-0.54	0.5119	0.01	0.0121
Benzenoids	4-methylcatechol	HMDB0000873	C06730	0.115	0.192	-1.53	0.1384	<0.001	<0.001	-3.94	1.167	<0.001	0.002	-2.94	0.5902	<0.001	0.0012
Benzenoids	Anthranilic acid	HMDB0001123	C00108	<0.001	<0.001	0.926	1.6657	<0.001	<0.001	0.983	1.209	0.0243	0.040	0.14	0.6255	<0.001	<0.001
Benzenoids	Dihydroxymandelic acid	HMDB0001866	C05580	0.275	0.369	-0.62	0.2896	0.0066	0.016	-2.50	0.921	0.0029	0.006	-1.73	0.6349	0.0067	0.0095
Benzenoids	Mandelate	HMDB0000703	C01984	0.1056	0.1811	-0.38	0.2688	0.769	0.8352	-0.02	0.287	<0.001	<0.001	-1.90	0.9602	<0.001	<0.001
Benzenoids	Monobutyl phthalate	HMDB0013247	-	<0.001	0.003	-1.55	0.2536	<0.001	<0.001	-2.10	0.973	<0.001	<0.001	-2.57	0.9983	<0.001	<0.001
Benzenoids	4-hydroxyphenylpyruvic acid	HMDB0000707	C01179	<0.001	<0.001	-1.76	1.8922	0.001	0.0039	-1.05	1.444	<0.001	<0.001	-6.71	1.831	<0.001	<0.001
Benzenoids	Mono(2-ethylhexyl) phthalate (mehp)	HMDB0013248	C03343	<0.001	<0.001	-2.55	2.0726	0.022	0.045	-2.04	0.417	<0.001	<0.001	-2.96	1.692	<0.001	<0.001
Benzenoids	2-methylhippuric acid	HMDB0011723	-	<0.001	<0.001	2.048	1.4231	<0.001	<0.001	1.176	1.737	<0.001	<0.001	-2.36	1.4519	<0.001	<0.001
Benzenoids	Isohomovanillic acid	HMDB0000333	-	<0.001	<0.001	-1.73	0.4035	<0.001	<0.001	-1.92	1.789	<0.001	<0.001	-2.19	1.6784	<0.001	<0.001
Benzenoids	3-hydroxyanthranilic acid	HMDB0001476	C00632	<0.001	<0.001	-1.43	0.0512	<0.001	<0.001	-1.4	1.772	<0.001	<0.001	-1.62	1.677	<0.001	<0.001
Benzenoids	4-hydroxybenzaldehyde	HMDB0011718	C00633	<0.001	<0.001	-0.63	1.7356	0.5743	0.676	-0.13	0.07	<0.001	<0.001	-1.54	1.8088	<0.001	<0.001
Benzenoids	Epinephrine	HMDB0000068	C00788	0.0122	0.03051	0.656	1.0316	0.852	0.9095	-0.04	0.64	<0.001	<0.001	-1.31	1.6769	<0.001	<0.001
Benzenoids	DL-metanephrine	HMDB0062493	C05588	0.002	0.008	1.20	1.0865	0.0768	0.131	0.38	0.972	<0.001	<0.001	-1.27	1.458	<0.001	<0.001
Benzenoids	Phenyl acetate	HMDB0040733	C00548	0.0056	0.01663	-0.34	0.2274	0.001	0.0041	-0.47	1.352	<0.001	0.002	-0.36	1.144	0.00	0.0031
Benzenoids	4-aminobenzoic acid	HMDB0001392	C00568	<0.001	0.001	0.86	0.9169	0.1105	0.172	0.16	0.771	<0.001	<0.001	0.38	1.2497	<0.001	<0.001
Benzenoids	4'-hydroxydiclofenac	HMDB0013974	-	0.5941	0.68671	0.037	0.3495	0.168	0.2452	0.176	0.635	0.0327	0.053	0.13	0.7607	0.16	0.174
Benzenoids	2-hydroxyhippuric acid	HMDB0000840	C07588	0.018	0.042	-1.32	0.3275	0.7283	0.819	-0.03	0.481	0.1474	0.209	0.51	0.2863	0.0134	0.018
Benzenoids	2-quinolinecarboxylic acid	HMDB0000842	C06325	0.0758	0.13946	-0.49	0.8929	0.035	0.063	0.727	0.652	0.1998	0.275	0.33	0.3889	0.00	0.0031
Benzenoids	2,4-dihydroxybenzoic acid	HMDB0029666	-	<0.001	<0.001	-1.51	1.5378	0.1095	0.171	-1.71	0.693	0.2815	0.362	0.27	0.5249	<0.001	<0.001
Benzenoids	Monomethyl phthalate	HMDB0002130	-	0.6045	0.69555	-0.04	0.2424	0.470	0.5717	0.123	0.678	0.2815	0.362	0.07	0.4408	0.33	0.3405
Benzenoids	Hippurate	HMDB0000714	C01586	0.025	0.055	-2.06	0.6406	0.7689	0.835	-0.06	0.349	0.3157	0.402	-0.55	0.2615	0.0855	0.1004
Benzenoids	Phenol	HMDB0013674	C00146	0.0307	0.06731	-0.74	0.1758	0.008	0.0192	-1.6	0.041	0.3919	0.477	-0.35	0.1255	0.01	0.0155
Benzenoids	4-toluic acid	HMDB0029635	C01454	0.046	0.091	0.38	0.4689	0.1519	0.224	0.50	0.566	0.5009	0.576	0.03	0.0434	0.065	0.078
Benzenoids	4-methylphenol	HMDB0001858	C01468	0.7374	0.77753	0.679	0.5414	0.347	0.44	-1.26	0.427	0.8989	0.917	0.12	0.3156	0.85	0.8603
Bile acids	Taurocholic acid	HMDB0000036	C05122	0.038	0.078	1.00	0.0116	0.0016	0.005	2.79	0.784	0.0297	0.048	0.51	0.0192	0.0018	0.0028
Bile acids	Deoxycholic acid	HMDB0000626	C04483	0.2416	0.33448	0.41	0.6297	0.205	0.2888	-0.63	0.668	<0.001	<0.001	0.95	1.0923	<0.001	<0.001
Bile acids	Glycocholic acid	HMDB0000331	C01921	0.798	0.820	0.35	0.0392	0.0257	0.051	2.00	0.614	0.2497	0.331	-0.23	0.2416	0.0132	0.0178
Bile acids	Glycoursodeoxycholic acid	HMDB0000708	-	0.1697	0.25761	0.781	0.5725	0.019	0.0388	2.16	1.044	0.3338	0.421	0.88	0.4162	0.06	0.0772
Bile acids	Cholate	HMDB0000619	C00695	0.373	0.477	-0.03	0.7301	0.5382	0.643	0.13	0.442	0.5981	0.667	0.08	0.343	0.2895	0.304
Bile acids	Glycocholate	HMDB0000138	C01921	0.6217	0.70196	0.231	0.1298	0.011	0.0254	2.247	0.69	0.6237	0.683	0.07	0.2939	0.02	0.0206
Bile acids	Taurolithocholic acid 3-sulfate	HMDB0002580	C03642	0.226	0.314	0.99	0.552	0.9362	0.958	-0.34	0.13	0.6237	0.683	-1.36	0.0171	0.3032	0.317
Bile acids	Taurochenodeoxycholic acid	HMDB0000951	C05465	0.1458	0.22681	1.202	0.478	<0.001	0.0028	2.331	1.225	0.73	0.776	-0.45	0.1752	<0.001	0.0013

Bile acids	Glycochenodeoxycholol	HMDB0000637	C05466	0.226	0.314	0.43	0.6022	0.0298	0.056	0.94	1.021	0.8989	0.917	-0.21	0.35	0.1312	0.1469
Biotin	Biotin	HMDB0000030	C00120	0.128	0.20815	-0.1	0.6879	0.936	0.9584	-0.01	0.706	<0.001	<0.001	0.35	1.3106	<0.001	<0.001
Carbohydrates	Alpha-d-glucose	HMDB0003345	C00267	0.010	0.024	0.67	0.9927	<0.001	0.003	-0.54	1.069	0.0219	0.037	-0.18	0.4208	<0.001	<0.001
Carbohydrates	D-lyxose	HMDB0003402	C00476	<0.001	<0.001	0.822	1.4656	0.005	0.0138	-0.48	1.21	0.0049	0.009	-0.29	0.7102	<0.001	<0.001
Carbohydrates	Muramic acid	HMDB0003254	-	0.708	0.756	0.12	0.1443	0.0257	0.051	-0.74	0.809	<0.001	<0.001	-5.13	1.8269	<0.001	<0.001
Carbohydrates	N-acetylneuraminic acid	HMDB0000773	C19909	<0.001	<0.001	1.963	1.113	<0.001	<0.001	2.308	1.694	<0.001	<0.001	-4.34	1.7562	<0.001	<0.001
Carbohydrates	D-glucosamine	HMDB0030091	C08349	0.737	0.778	0.08	0.3633	0.8517	0.909	0.03	0.05	<0.001	<0.001	-2.64	1.8273	<0.001	<0.001
Carbohydrates	N-acetylneuraminate	HMDB0000230	C00270	0.0564	0.10932	0.545	0.9743	0.002	0.006	0.893	0.963	<0.001	<0.001	-2.21	1.4997	<0.001	<0.001
Carbohydrates	Gluconic acid	HMDB0000625	C00257	<0.001	<0.001	0.49	1.2811	<0.001	<0.001	1.61	0.825	<0.001	<0.001	2.01	1.4428	<0.001	<0.001
Cinnamic acids	Caffeic acid	HMDB0001964	C01197	0.0816	0.14785	-1.02	0.9003	0.137	0.2049	-1.03	0.853	0.0396	0.063	-0.83	0.9795	0.18	0.1918
Cinnamic acids	Sinapinic acid	HMDB0032616	C00482	0.417	0.518	0.04	0.3123	0.0523	0.093	1.22	0.7	0.5244	0.598	0.02	0.3008	0.0555	0.0682
Cinnamic acids	Trans-cinnamate	HMDB0000930	C00423	<0.001	<0.001	2.163	1.5915	<0.001	0.0022	-1.54	0.059	<0.001	<0.001	-1.68	1.6046	<0.001	<0.001
Fatty acids	Lauric acid	HMDB0000638	C02679	0.183	0.267	-0.24	0.5214	<0.001	<0.001	-0.89	1.486	0.0177	0.030	-0.71	0.1695	<0.001	<0.001
Fatty acids	Glutaryl carnitine	HMDB0013130	-	<0.001	<0.001	2.293	1.5109	0.008	0.0192	1.095	1.122	<0.001	<0.001	-2.48	0.3866	<0.001	<0.001
Fatty acids	Gamma-linolenic acid	HMDB0003073	C06426	0.567	0.665	0.06	0.4361	<0.001	0.001	0.85	1.218	0.0243	0.040	0.43	0.5789	0.0011	0.0017
Fatty acids	Caprylic acid	HMDB0000482	C06423	0.0084	0.02288	-0.31	1.0097	0.769	0.8352	2.495	0.848	0.0127	0.022	0.32	0.6574	<0.001	<0.001
Fatty acids	Ethyl myristate	HMDB0034153	-	0.147	0.227	0.24	0.6608	0.144	0.215	-0.32	0.689	0.0297	0.048	-0.57	0.7535	0.0047	0.0067
Fatty acids	Sulcatol	HMDB0030030	C07288	0.0971	0.1687	0.063	0.697	<0.001	<0.001	1.381	0.807	0.0055	0.010	0.34	0.8195	<0.001	<0.001
Fatty acids	Dodecanedioic acid	HMDB0000623	C02678	<0.001	<0.001	-2.08	1.8519	<0.001	<0.001	-1.73	1.528	<0.001	<0.001	-2.01	1.0868	<0.001	<0.001
Fatty acids	Dethiobiotin	HMDB0003581	C01909	<0.001	<0.001	-2.24	1.898	<0.001	<0.001	1.1	1.281	<0.001	<0.001	-1.54	1.3269	<0.001	<0.001
Fatty acids	3-hydroxydecanoic acid	HMDB0002203	-	<0.001	<0.001	-0.76	1.4184	0.0298	0.056	-0.34	1.057	<0.001	<0.001	-1.34	1.0914	<0.001	<0.001
Fatty acids	16-hydroxyhexadecanoic	HMDB0006294	C18218	0.0095	0.02444	0.47	1.0618	0.574	0.6763	-0.25	0.508	<0.001	<0.001	-1.03	1.6345	<0.001	<0.001
Fatty acids	Arachidonic acid	HMDB0001043	C00219	0.344	0.449	0.14	0.4782	0.131	0.200	-0.25	0.631	<0.001	<0.001	-0.69	1.2291	<0.001	<0.001
Fatty acids	Isobutyric acid	HMDB0001873	C02632	0.0197	0.04598	0.176	0.8373	0.023	0.0463	-0.17	1.011	<0.001	<0.001	0.20	1.1638	<0.001	<0.001
Fatty acids	Adipate	HMDB0000448	C06104	<0.001	<0.001	0.97	0.8606	<0.001	<0.001	1.75	1.27	<0.001	<0.001	0.34	1.4453	<0.001	<0.001
Fatty acids	6-carboxyhexanoate	HMDB0000857	C02656	<0.001	<0.001	0.827	1.6822	<0.001	<0.001	2.908	1.251	<0.001	<0.001	0.41	1.3402	<0.001	<0.001
Fatty acids	Hexadecanamide	HMDB0012273	-	<0.001	<0.001	1.26	1.7976	0.0257	0.051	0.34	1.062	<0.001	<0.001	0.62	1.1851	<0.001	<0.001
Fatty acids	Sebacic acid	HMDB0000792	C08277	<0.001	<0.001	1.671	1.7722	<0.001	<0.001	3.5	0.628	<0.001	<0.001	2.27	1.2847	<0.001	<0.001
Fatty acids	Oleamide	HMDB0002117	C19670	<0.001	<0.001	2.33	1.6724	0.0976	0.158	-0.58	0.046	<0.001	0.002	2.31	1.2424	<0.001	<0.001
Fatty acids	Palmitoyl carnitine	HMDB0000222	C02990	0.3732	0.47744	0.321	0.3425	0.005	0.0122	0.937	1.21	<0.001	<0.001	2.62	1.6591	<0.001	<0.001
Fatty acids	Hexanoyl carnitine	HMDB0000705	-	0.679	0.740	0.29	0.3606	0.0345	0.063	1.71	0.89	<0.001	<0.001	2.78	1.2845	<0.001	<0.001
Fatty acids	Azelaic acid	HMDB0000784	C08261	<0.001	<0.001	3.717	1.5742	<0.001	<0.001	6.575	1.122	<0.001	<0.001	2.80	1.7577	<0.001	<0.001
Fatty acids	Propionyl carnitine	HMDB0000824	C03017	0.001	0.005	1.35	0.6504	<0.001	0.002	2.53	1.289	<0.001	<0.001	6.67	1.5714	<0.001	<0.001
Fatty acids	O-acetylcarnitine	HMDB0000201	C02571	0.0095	0.02444	0.5	0.5734	0.137	0.2049	0.328	0.833	<0.001	<0.001	10.15	1.3234	<0.001	<0.001
Fatty acids	Oleate	HMDB0000207	C00712	0.016	0.040	0.45	1.0761	0.5033	0.604	0.23	0.487	0.0531	0.081	0.35	0.654	0.0911	0.1057
Fatty acids	Lauroyl carnitine	HMDB0002250	-	0.1963	0.28269	-0.15	0.8379	0.503	0.604	-0.21	0.503	0.0737	0.109	1.01	0.5453	<0.001	0.001
Fatty acids	8z,11z,14z-eicosatrienoic acid	HMDB0002925	C03242	0.002	0.007	0.58	1.2425	0.0045	0.012	0.45	1.198	0.0868	0.127	0.41	0.5451	0.0136	0.0182
Fatty acids	Linoleic acid	HMDB0000673	C01595	0.1835	0.26736	0.3	0.6703	0.769	0.8352	-0.12	0.023	0.1001	0.145	-0.43	0.5959	0.01	0.0169
Fatty acids	Decanoic acid	HMDB0000511	C01571	0.008	0.023	-0.34	1.1473	0.4371	0.537	2.57	0.874	0.1098	0.157	-0.22	0.1429	0.07	0.0832
Fatty acids	L-carnitine	HMDB0000062	C00318	<0.001	0.00254	0.822	1.3897	<0.001	0.0012	2.076	1.311	0.1275	0.182	0.06	0.5486	<0.001	<0.001
Fatty acids	3-hydroxybutanoate	HMDB0000011	C01089	0.275	0.369	0.11	0.7747	0.2254	0.307	-0.53	0.315	0.1813	0.252	-0.24	0.1169	0.0406	0.0512
Fatty acids	DL-carnitine	HMDB0002095	-	0.2107	0.29826	0.054	0.4612	0.728	0.8194	0.033	0.065	0.2205	0.300	-0.18	0.384	0.18	0.196
Fatty acids	9-oxo-10(e),12(e)-octadecadienoic acid	HMDB0004669	C14766	0.312	0.416	0.33	0.2066	0.0345	0.063	0.88	0.791	0.3157	0.402	0.38	0.2903	0.148	0.1643
Fatty acids	4-hydroxybutyric acid (ghb)	HMDB0000710	C00989	<0.001	<0.001	1.431	1.5597	0.347	0.44	0.341	0.665	0.3526	0.438	0.30	0.4016	<0.001	<0.001
Fatty acids	Cis-5,8,11,14,17-eicosapentaenoic acid	HMDB0001999	C06428	0.146	0.227	0.30	0.5911	0.8938	0.942	-0.15	0.361	0.3526	0.438	-0.04	0.4888	0.4554	0.4665
Fatty acids	Decanoyl carnitine	HMDB0000651	-	0.0681	0.12878	-0.85	0.8955	0.979	0.9865	0.008	0.16	0.3526	0.438	1.17	0.3485	0.01	0.0107

	3-hydroxy-3-																
Fatty acids	methylbutanoic acid	HMDB0000754	C20827	0.183	0.267	0.15	0.8034	0.2701	0.356	-0.58	0.293	0.5244	0.598	-0.14	0.0665	0.0856	0.1004
Fatty acids	Palmitoleic acid	HMDB0003229	C08362	0.9533	0.96482	0.015	0.1129	0.755	0.8352	-0.11	0.154	0.675	0.730	0.10	0.1503	0.90	0.9062
Fatty acids	Hexadecanedioic acid	HMDB0000672	C19615	0.708	0.756	0.04	0.4163	0.2701	0.356	0.15	0.563	0.7575	0.802	-0.35	0.1767	0.5165	0.527
Fatty acids	Suberic acid	HMDB0000893	C08278	0.0379	0.07764	0.514	0.9295	<0.001	<0.001	1.645	0.896	0.7853	0.828	-0.06	0.1647	<0.001	<0.001
Fatty acids	Methyl jasmonate	HMDB0036583	C11512	0.125	0.204	0.42	0.7495	0.0016	0.005	-1.32	1.322	0.8134	0.851	-0.10	0.2372	<0.001	<0.001
Fatty acids	Tetradecanedioic acid	HMDB0000872	-	0.9215	0.93635	0.305	0.4043	0.769	0.8352	0.102	0.168	0.9566	0.960	0.35	0.3924	0.99	0.9947
Hydroxycinnamic acids	2-hydroxycinnamic acid	HMDB0002641	C01772	0.115	0.192	0.32	0.5918	0.2466	0.331	0.28	0.64	<0.001	<0.001	0.72	1.2773	0.0012	0.0019
Imidazoles	Imidazoleacetic acid	HMDB0002024	C02835	<0.001	<0.001	0.903	1.0188	0.002	0.005	0.412	1.343	0.0025	0.005	0.30	0.8189	<0.001	<0.001
Imidazoles	Urocanic acid	HMDB0000301	C00785	0.594	0.687	0.06	0.5268	0.2945	0.383	-0.23	0.378	<0.001	<0.001	0.92	1.0296	<0.001	<0.001
Imidazoles	Methylimidazoleacetic acid	HMDB0002820	C05828	0.4175	0.51822	0.093	0.0161	0.003	0.0088	1.09	0.919	0.0435	0.068	0.25	0.2705	0.00	0.0049
Indoles	Indole-3-methyl acetate	HMDB0029738	C20635	0.489	0.596	0.80	0.3416	0.4696	0.572	-0.36	0.558	0.0197	0.033	2.46	0.7348	0.0389	0.0493
Indoles	Indole-3-butyric acid	HMDB0002096	C11284	0.0036	0.0115	1.01	1.1482	0.002	0.0074	2.241	1.195	<0.001	<0.001	2.03	0.7928	<0.001	<0.001
Indoles	L-5-hydroxytryptophan	HMDB0000472	C01017	<0.001	0.003	0.78	1.208	<0.001	0.003	1.42	1.328	<0.001	<0.001	0.87	0.9032	<0.001	<0.001
Indoles	Indole-3-acetamide	HMDB0029739	C02693	<0.001	<0.001	-2.26	2.1848	0.085	0.1429	-0.38	0.729	<0.001	<0.001	-5.69	1.8601	<0.001	<0.001
Indoles	5-hydroxyindoleacetate	HMDB0000763	C05635	0.007	0.020	0.47	0.9899	<0.001	0.002	1.23	1.4	<0.001	<0.001	0.75	1.0693	<0.001	<0.001
Indoles	Indole-3-acetaldehyde	HMDB0001190	C00637	0.0056	0.01663	0.411	1.0309	<0.001	<0.001	1.744	1.378	<0.001	<0.001	0.88	1.328	<0.001	<0.001
Indoles	N-acetylserotonin	HMDB0001238	C00978	0.003	0.009	-0.26	1.3275	<0.001	<0.001	-0.49	1.547	<0.001	<0.001	3.07	1.0759	<0.001	<0.001
Indoles	Indole-3-pyruvic acid	HMDB0060484	C00331	0.0014	0.00536	-1.35	0.5906	<0.001	<0.001	-1.64	1.27	<0.001	<0.001	5.66	1.3306	<0.001	<0.001
Indoles	Indole	HMDB0000738	C00463	0.017	0.041	-0.26	1.0189	0.1225	0.189	-0.32	0.86	0.057	0.086	0.16	0.5501	<0.001	0.0011
Indoles	Indole-3-lactic acid	HMDB0000671	C02043	0.0415	0.08365	-0.32	0.927	0.002	0.0074	1.06	1.147	0.2653	0.346	0.17	0.4671	<0.001	<0.001
Indoles	Indole-3-acetic acid	HMDB0000197	C00954	<0.001	0.002	-0.60	1.2667	0.5743	0.676	0.12	0.267	0.8702	0.899	0.10	0.2476	0.0018	0.0027
Indoles	2-oxindole	HMDB0061918	C12312	0.3291	0.43422	-0.28	0.4543	0.503	0.604	-0.58	0.385	0.9277	0.939	-0.06	0.1884	0.64	0.6524
Lipids	Testosterone	HMDB0003193	C11134	<0.001	0.003	5.18	1.2285	0.0016	0.005	6.52	1.323	<0.001	<0.001	-0.40	0.2127	<0.001	<0.001
Lipids	Desoxycortone	HMDB0000016	C03205	<0.001	<0.001	1.461	1.6687	<0.001	<0.001	1.497	1.736	<0.001	<0.001	0.94	0.7677	<0.001	<0.001
Lipids	Perillic acid	HMDB0004586	C11924	0.441	0.544	0.29	0.2569	0.3475	0.440	-0.41	0.539	0.0127	0.022	-0.72	0.8404	0.0049	0.007
Lipids	Testosterone sulfate	HMDB0002833	-	0.6507	0.71609	-0.14	0.1226	<0.001	0.0022	-1.09	1.489	0.0093	0.017	-0.77	0.8735	0.01	0.0121
Lipids	Coenzyme q2	HMDB0006709	C00399	0.021	0.048	0.56	0.9541	<0.001	<0.001	1.75	1.262	<0.001	<0.001	-1.74	0.9403	<0.001	<0.001
Lipids	1-oleoyl-rac-glycerol	HMDB0011567	-	<0.001	<0.001	4.417	1.7869	<0.001	<0.001	5.912	0.905	<0.001	<0.001	4.47	0.9459	<0.001	<0.001
Lipids	Palmitoyl sphingomyelin	HMDB0061712	-	<0.001	<0.001	0.97	1.6054	0.1683	0.245	0.11	0.672	<0.001	<0.001	0.52	1.1082	<0.001	<0.001
Lipids	Alpha-tocopherol	HMDB0001893	C02477	0.0052	0.01604	0.544	1.2201	0.295	0.3826	0.358	0.636	<0.001	<0.001	0.58	1.156	0.01	0.0184
Lipids	D-erythro-sphingosine 1-phosphate	HMDB0000277	C06124	<0.001	0.001	-0.45	1.3921	0.1861	0.268	0.18	0.787	<0.001	<0.001	0.61	1.3743	<0.001	<0.001
Lipids	Tetrahydrocortisone	HMDB0000903	C05470	0.0816	0.14785	0.563	0.9128	0.010	0.0233	0.55	1.119	<0.001	<0.001	1.36	1.275	<0.001	<0.001
Lipids	Cortisol	HMDB0000063	C00735	<0.001	<0.001	1.23	1.5382	<0.001	<0.001	1.07	1.742	<0.001	<0.001	1.66	1.532	<0.001	<0.001
Lipids	Cortisone	HMDB0002802	C00762	<0.001	<0.001	0.938	1.4806	0.376	0.4738	0.254	0.563	<0.001	<0.001	1.99	1.6781	<0.001	<0.001
Lipids	Epitestosterone	HMDB0000628	-	0.006	0.017	1.07	1.0573	<0.001	<0.001	3.11	0.82	<0.001	<0.001	2.01	1.3094	<0.001	<0.001
Lipids	Medroxyprogesterone 5-alpha-pregnan-3,20-dione	HMDB0001939	C07119	0.089	0.15803	-0.85	0.2758	<0.001	<0.001	4.322	1.933	<0.001	<0.001	4.80	1.2956	<0.001	<0.001
Lipids	Androsterone glucuronide	HMDB0002829	C11135	0.001	0.00396	-0.94	1.422	0.137	0.2049	0.715	0.725	0.3823	0.470	-0.21	0.3158	<0.001	0.001
Lipids	19-nortestosterone	HMDB0002725	C07254	0.650	0.716	0.40	0.147	0.0298	0.056	1.46	0.509	0.4555	0.534	0.45	0.0124	0.0345	0.0439
Lipids	Progesterone	HMDB0001830	C00410	0.0383	0.07778	0.58	0.8772	0.225	0.307	-0.64	0.222	0.5981	0.667	-0.25	0.0893	0.03	0.037
Lipids	Coenzyme q1	HMDB0002012	-	0.622	0.702	0.15	0.4405	0.9787	0.987	-0.13	0.749	0.6237	0.683	-0.22	0.8291	0.3427	0.354
Lipids	2,6-di-tert-butyl-1,4-benzoquinone	HMDB0013817	-	0.1245	0.20373	-0.4	0.3541	0.016	0.0341	-0.54	0.874	0.73	0.776	0.36	0.2441	0.03	0.037
Lipids	Corticosterone	HMDB0001547	C02140	0.708	0.756	-0.03	0.4355	0.003	0.009	0.69	0.784	0.8417	0.873	-0.16	0.2766	0.0461	0.0575
Nucleosides	Adenosine	HMDB0000050	C00212	<0.001	<0.001	-1.67	0.7191	0.098	0.1577	-0.52	0.549	0.0033	0.006	-1.22	0.5375	<0.001	<0.001

Nucleosides	Pseudouridine	HMDB0000767	C02067	0.417	0.518	-0.13	0.2493	0.0096	0.023	0.71	1.355	<0.001	<0.001	0.45	0.728	<0.001	<0.001
Nucleosides	Xanthosine	HMDB0000299	C01762	0.0247	0.05509	0.473	0.8854	<0.001	<0.001	3.638	1.246	<0.001	<0.001	2.36	0.8664	<0.001	<0.001
Nucleosides	Angiotensin iv	HMDB0001038	C15849	0.125	0.204	-0.98	0.9206	<0.001	<0.001	-1.42	2.064	<0.001	<0.001	-1.86	1.8993	<0.001	<0.001
Nucleosides	5'-methylthioadenosine	HMDB0001173	C00170	0.0027	0.00924	-0.63	1.2093	0.005	0.0138	0.743	0.518	<0.001	<0.001	-0.56	1.2378	<0.001	<0.001
Nucleosides	Uridine	HMDB0000296	C00299	0.146	0.227	-0.52	0.6057	0.9394	0.958	-0.02	0.099	0.0057	0.011	-0.55	1.011	0.0655	0.0782
Nucleosides	Inosine	HMDB0000195	C00294	<0.001	<0.001	-3.29	1.5318	0.022	0.0447	-3.58	0.263	0.0868	0.127	0.53	0.5281	<0.001	<0.001
Organic acids	4-acetamidobutanoate	HMDB0003681	C02946	0.146	0.227	-0.28	0.3438	<0.001	0.001	0.88	1.307	<0.001	<0.001	0.76	0.5725	<0.001	<0.001
Organic acids	Acrylic acid	HMDB0031647	C00511	<0.001	0.00294	0.672	1.2054	0.032	0.06	-0.46	0.987	0.0159	0.027	-0.56	0.6465	<0.001	<0.001
Organic acids	Trans-aconitic acid	HMDB0000958	C02341	0.417	0.518	-0.24	0.3072	0.6885	0.782	-0.02	0.668	0.0071	0.013	0.48	0.6884	0.0126	0.017
Organic acids	12-hydroxydodecanoic acid	HMDB0002059	C08317	0.5404	0.63935	-0.22	0.4397	0.007	0.0162	-1.77	0.952	0.0063	0.011	-1.29	0.8575	0.00	0.002
Organic acids	Citrate	HMDB0000094	C00158	0.089	0.158	0.24	0.8585	0.9362	0.958	-0.14	0.787	0.009	0.016	0.60	0.8977	0.1329	0.1481
Organic acids	Oxoglutaric acid	HMDB0000208	C00026	0.089	0.15803	0.27	0.8682	0.936	0.9584	-0.11	0.786	0.0063	0.011	0.62	0.9258	0.11	0.124
Organic acids	Pipecolate	HMDB0000716	C00408	0.046	0.091	0.46	0.8223	0.218	0.304	-0.30	0.529	0.0022	0.004	0.55	0.9869	0.0014	0.0023
Organic acids	Alanyltyrosine	HMDB0028699	-	0.1348	0.21643	-0.58	0.1538	0.005	0.0138	-2.44	1.024	<0.001	<0.001	-2.06	1.1496	<0.001	0.0016
Organic acids	Acetoacetate	HMDB0000060	C00164	0.036	0.077	0.15	0.8947	0.1278	0.196	-0.12	0.718	<0.001	<0.001	0.31	1.2648	<0.001	<0.001
Organic acids	3-ureidopropionic acid	HMDB0000026	C02642	0.7674	0.79989	0.004	0.2378	0.611	0.7068	0.104	0.37	<0.001	<0.001	0.76	1.4771	<0.001	<0.001
Organic acids	L-(+)-lactic acid	HMDB0000190	C00186	0.010	0.024	0.23	0.9414	0.0066	0.016	0.38	1.273	<0.001	<0.001	0.94	1.4703	<0.001	<0.001
Organic acids	Taurine	HMDB0000251	C00245	0.0901	0.15875	-0.48	0.7193	0.902	0.9475	0.036	0.162	<0.001	<0.001	1.87	1.4882	<0.001	<0.001
Organic acids	3-indoxyl sulphate	HMDB0000682	-	0.009	0.024	-0.70	1.211	0.2051	0.289	-0.54	0.24	0.0737	0.109	-0.44	0.4108	0.0794	0.0939
Organic acids	Oxalic acid	HMDB0002329	C00209	0.6258	0.70196	0.025	0.213	0.005	0.0138	-0.28	1.175	0.1778	0.249	0.07	0.4808	0.00	0.0035
Organic acids	2-oxobutyric acid	HMDB0000005	C00109	0.016	0.038	0.48	0.9308	0.0114	0.025	-0.51	0.752	0.233	0.316	-0.17	0.4368	<0.001	<0.001
Organic acids	Pyruvic acid	HMDB0000243	C00022	0.1827	0.26736	0.262	0.5671	0.101	0.1616	-0.36	0.694	0.5957	0.667	0.08	0.2039	0.03	0.0365
Organic acids	Levulinic acid	HMDB0000720	-	0.627	0.702	0.09	0.2947	0.0538	0.095	-0.43	0.879	0.6699	0.729	0.07	0.1994	0.0552	0.0682
Organic acids	6-hydroxycaproic acid	HMDB0012843	C06103	0.2754	0.36918	-0.12	0.495	0.347	0.44	0.147	0.777	0.6716	0.729	0.03	0.1389	0.23	0.2478
Organonitrogen compounds	Choline	HMDB0000097	C00114	<0.001	<0.001	0.63	1.8628	<0.001	<0.001	1.02	1.94	<0.001	<0.001	0.79	1.735	<0.001	<0.001
Organonitrogen compounds	D-sphingosine	HMDB0000252	C00319	<0.001	<0.001	1.846	1.5341	<0.001	<0.001	2.113	1.647	<0.001	<0.001	2.24	1.516	<0.001	<0.001
Organonitrogen compounds	Spermidine	HMDB0001257	C00315	0.006	0.019	1.36	1.1196	<0.001	<0.001	2.65	1.185	<0.001	<0.001	3.14	1.3326	<0.001	<0.001
Organonitrogen compounds	Acetylcholine	HMDB0000895	C01996	0.7674	0.79989	0.053	0.287	0.011	0.0254	-0.52	1.035	0.73	0.776	0.03	0.2396	0.03	0.037
Organooxygen compounds	Pantothenic acid	HMDB0000210	C00864	0.020	0.046	0.52	0.9206	<0.001	<0.001	1.68	1.225	0.0159	0.027	-0.50	0.0008	<0.001	<0.001
Organooxygen compounds	Diacetyl	HMDB0003407	C00741	0.0084	0.02288	-0.51	0.9885	0.437	0.5373	1.438	1.092	0.0522	0.080	-0.23	0.5616	0.00	0.0054
Others	4-oxoproline	-	C01877	0.008	0.023	1.14	1.355	0.2051	0.289	-0.18	0.582	0.0063	0.011	-0.46	0.4335	<0.001	<0.001
Others	N-oleoyl dopamine	-	C12272	<0.001	<0.001	-1.81	2.0595	0.005	0.0122	-2.71	0.263	<0.001	<0.001	-2.69	1.9338	<0.001	<0.001
Others	4-hydroxy-l-phenylglycine	-	C12323	<0.001	<0.001	0.93	1.4212	<0.001	<0.001	1.38	1.279	<0.001	<0.001	0.87	1.0854	<0.001	<0.001
Others	11,12-epoxy-(5z,8z,11z)-icosatrienoic acid	-	C14770	<0.001	<0.001	-3.27	1.0576	<0.001	<0.001	2.905	1.659	<0.001	<0.001	2.65	1.2377	<0.001	<0.001
Others	2-phenylpropanoic acid	HMDB0030524	C14437	<0.001	<0.001	-0.49	1.6841	0.0135	0.029	-0.59	1.39	<0.001	<0.001	3.83	1.2863	<0.001	<0.001
Phenylpropanoic acids	DL-4-hydroxyphenyllactic acid	HMDB0000755	C03672	0.9843	0.98427	-0.17	0.0125	0.583	0.6803	0.163	0.323	0.0553	0.084	0.40	0.6595	0.17	0.1885
Phenylpropanoic acids	3-phenyllactic acid	HMDB0000748	C05607	0.062	0.118	0.60	0.7215	0.2051	0.289	0.49	0.921	0.3919	0.477	0.22	0.3841	0.2892	0.304
Phospholipids	2-amino-1,3,4-octadecanetriol	HMDB0004610	C12144	<0.001	<0.001	-2.15	2.1547	<0.001	<0.001	-2.53	2.019	<0.001	<0.001	-2.90	1.8376	<0.001	<0.001
Purines	1-methylxanthine	HMDB0010738	C16358	0.859	0.880	-0.39	0.4509	0.0135	0.029	-2.52	0.207	0.0029	0.006	-2.01	0.5731	<0.001	<0.001

Purines	1,3-dimethyluric acid	HMDB0001857	-	0.2581	0.35161	-1.58	0.2478	0.077	0.1308	-4.55	0.552	0.0033	0.006	-4.46	0.7327	0.02	0.023
Purines	Guanine	HMDB0000132	C00242	<0.001	<0.001	-2.37	1.6194	<0.001	0.002	-2.73	0.489	<0.001	<0.001	-2.11	1.235	<0.001	<0.001
Purines	Adenine	HMDB0000034	C00147	0.0147	0.03644	-0.27	1.0969	0.098	0.1577	-0.38	0.509	<0.001	<0.001	-1.05	1.6859	<0.001	<0.001
Purines	Xanthine	HMDB0000292	C00385	0.069	0.129	0.49	0.7945	0.0273	0.053	0.68	1.134	<0.001	<0.001	1.65	1.5564	<0.001	<0.001
Purines	Hypoxanthine	HMDB0000157	C00262	0.1963	0.28269	0.35	0.7281	<0.001	<0.001	1.541	1.521	<0.001	<0.001	2.13	1.8049	<0.001	<0.001
Purines	7-methylxanthine	HMDB0001991	C16353	0.489	0.596	-1.73	0.0221	0.0768	0.131	-3.72	0.442	0.0435	0.068	-3.04	0.0538	0.0062	0.0089
Purines	7-methylguanine	HMDB0000897	C02242	0.9843	0.98427	0.02	0.0777	0.019	0.0388	0.462	0.847	0.2497	0.331	0.24	0.5149	0.10	0.1123
Purines	1-methyluric acid	HMDB0003099	C16359	0.258	0.352	-0.17	0.4852	0.2701	0.356	1.07	0.628	0.4555	0.534	-0.26	0.4341	0.1069	0.1214
Purines	Uric acid	HMDB0000289	C00366	<0.001	0.00125	-0.55	1.4295	<0.001	0.0034	-0.89	1.408	0.8771	0.902	0.02	0.0026	<0.001	<0.001
Pyridines	3-hydroxypicolinic acid	HMDB0013188	C18620	<0.001	<0.001	-1.00	0.3146	0.994	0.998	0.00	0.045	<0.001	<0.001	-1.09	1.7924	<0.001	<0.001
Pyridines	Pyridoxamine	HMDB0001431	C00534	0.5404	0.63935	-0.01	0.2831	0.689	0.7816	0.18	0.186	<0.001	<0.001	1.58	1.3447	<0.001	<0.001
Pyridines	Nicotinamide	HMDB0001406	C00153	0.038	0.078	0.90	0.9976	<0.001	<0.001	1.96	1.75	<0.001	<0.001	2.48	1.6519	<0.001	<0.001
Pyridines	Pyridoxal	HMDB0001545	C00250	0.0108	0.0272	0.733	0.5748	0.581	0.6803	-0.1	0.281	0.094	0.137	0.20	0.5012	0.00	0.0047
Pyridines	6-methylnicotinamide	HMDB0013704	-	0.322	0.427	-0.13	0.3975	0.4288	0.535	0.08	0.347	0.4555	0.534	0.02	0.295	0.3168	0.3299
Pyridines	4-pyridoxic acid	HMDB0000017	C00847	0.5486	0.64607	0.145	0.2229	<0.001	<0.001	2.655	1.208	0.9566	0.960	-0.19	0.3254	<0.001	<0.001
Pyridines	Cotinine	HMDB0001046	-	<0.001	<0.001	-0.52	1.3511	<0.001	<0.001	-1.10	1.66	<0.001	0.002	-0.56	1.1065	<0.001	<0.001
Pyrimidines	Dihydrothymine	HMDB0000079	C00906	0.0032	0.01018	-0.51	0.7256	0.046	0.0829	-0.45	0.62	<0.001	<0.001	0.66	1.0555	<0.001	<0.001
Pyrimidines	Thymine	HMDB0000262	C00178	0.004	0.011	-0.40	1.1869	0.0188	0.039	-0.35	1.009	0.2653	0.346	0.19	0.5139	<0.001	<0.001
Pyrrolines	Bilirubin	HMDB0000054	C00486	0.0095	0.02444	-0.37	0.9187	0.016	0.0341	-0.96	0.71	0.1702	0.240	0.27	0.5101	<0.001	<0.001
Quinolines and derivatives	Kynurenic acid	HMDB0000715	C01717	0.708	0.756	0.20	0.0612	0.0096	0.023	0.74	1.12	0.8417	0.873	0.09	0.1905	0.0115	0.0158
Tetrahydroisoquinolines	Salsolinol	HMDB0042012	C09642	<0.001	<0.001	3.624	2.1251	<0.001	<0.001	4.464	1.977	<0.001	<0.001	2.69	1.742	<0.001	<0.001

Table S3. Metabolites quantified in the discovery cohort by targeted metabolomics (related to figure S3)

Class	Name	HMDB_ID	KEGG_ID	Cluster number	Normal VS Mild				Normal VS Severe				Normal VS Recovery				Total	
					P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR
Amino Acids	Lysine	HMDB0000	C00047	2	0.9992	1	0	0.1996	0.655	0.7759	0.085	0.213	0.5208	0.8034	0.011	0.51	0.8406	0.862297531
Amino Acids	Histidine	0177	C00135	13	0.3844	0.59691	-0.17	0.4865	0.3529	0.498	-0.17	0.585	0.5595	0.813	0.083	0.3946	0.3009	0.396500222
Amino Acids	Arginine	HMDB0000	C00062	6	0.9143	0.94804	0.016	0.0469	0.0019	0.0113	-0.48	1.643	0.0089	0.0603	-0.37	1.3098	0.0025	0.009752072
Amino Acids	Ornithine	HMDB000	C00077	4	0.0311	0.18193	0.371	1.5216	<0.001	0.0035	0.981	1.794	<0.001	<0.001	1.557	2.3139	9E-08	<0.001
Amino Acids	Glutamine	HMDB0000	C00064	8	0.0373	0.18541	-0.36	1.4032	0.0019	0.0113	-0.62	1.791	0.0043	0.0346	-0.48	1.8552	0.0019	0.008166109
Amino Acids	Glutamic acid	HMDB000	C00025	2	<0.001	0.00256	0.82	1.8495	<0.001	<0.001	1.482	2.015	<0.001	<0.001	1.454	2.6133	3E-07	<0.001
Amino Acids	beta-Alanine	HMDB0000	C00099	1	0.8807	0.92245	-0.01	0.3399	0.0439	0.1105	0.544	1.32	0.0311	0.157	0.128	0.8346	0.0063	0.020427551
Amino Acids	Alanine	0161	C00041	14	0.9472	0.97157	-0.04	0.2593	0.7221	0.8312	-0.06	0.256	0.2497	0.5287	0.17	0.7592	0.7447	0.779998678
Amino Acids	Dimethylglycine	HMDB0000	C01026	3	0.007	0.077	0.643	1.2967	0.007	0.0273	0.508	1.14	0.1115	0.2883	0.303	0.7737	0.0262	0.061379059
Amino Acids	GABA	0112	C00334	5	<0.001	0.01124	-0.59	2.402	0.0188	0.0594	-0.53	1.12	0.0094	0.0603	-0.39	1.6741	0.0018	0.008130636
Amino Acids	Serine	HMDB0000	C00065	14	0.2662	0.52973	0.168	0.6391	0.6796	0.7982	-0.08	0.224	0.0922	0.2883	0.153	1.0318	0.0932	0.162657087
Amino Acids	Threonine	0167	C00188	13	0.0506	0.22879	-0.5	1.3725	0.3944	0.5489	-0.2	0.493	0.6746	0.8462	0.08	0.4134	0.0312	0.06974413
Amino Acids	Homoserine	HMDB0000	C00263	13	0.0164	0.12118	-0.8	1.5409	0.3513	0.498	-0.19	0.531	0.7181	0.8621	-0.06	0.0236	0.0516	0.109342478
Amino Acids	Creatine	0064	C00300	16	0.2917	0.5432	0.341	0.6911	0.0036	0.0165	1.969	1.569	0.2758	0.5435	-0.26	0.5015	0.0002	0.001896725
Carbohydrates	Threonic acid	HMDB0000	C01620	3	0.5801	0.72152	0.129	0.545	0.2852	0.4368	0.22	0.678	0.4604	0.7545	0.188	0.2305	0.9099	0.914540271
Organic Acids	Hydroxypropionic acid	HMDB0000	C01013	12	0.8771	0.92245	-0.13	0.1221	0.0156	0.0509	0.484	0.877	0.4369	0.7322	-0.12	0.5262	0.0089	0.026848137
Amino Acids	Homocitrulline	HMDB0000	C02427	12	0.3175	0.54459	-0.16	1.1381	0.0036	0.0165	1.153	1.487	0.7739	0.8902	0.164	0.4166	0.0004	0.002455499
Organic Acids	Lactic acid	HMDB000	C00186	2	0.4647	0.64663	0.105	0.5539	<0.001	<0.001	1.238	2.229	<0.001	<0.001	1.158	2.7261	3E-08	<0.001
Organic Acids	Nicotinic acid	HMDB0001	C00253	9	0.3352	0.5559	0.002	1.0209	0.9221	0.9607	0	0.48	0.8321	0.9261	0	0.5128	0.5303	0.631915816
Amino Acids	Methylcysteine	2108	-	14	0.1546	0.38936	0.392	1.0025	0.347	0.4968	-0.82	0.399	0.1626	0.3763	0.308	0.825	0.1563	0.246843247
Benzoic acids	m-	HMDB0001	-	11	0.0922	0.29123	-0.13	0.7543	0.8886	0.9357	0.01	0.033	0.8639	0.9384	0.009	0.1152	0.1743	0.26429579
Amino Acids	2-Phenylglycine	2210	-	2	0.0756	0.26378	0.087	0.8204	<0.001	0.003	0.456	1.398	0.0311	0.157	0.083	0.5041	0.0012	0.006010721
Amino Acids	Tyrosine	HMDB0000	C00082	9	0.5501	0.70505	0.029	0.3511	0.6819	0.7982	0.066	0.302	0.412	0.7067	-0.27	0.3591	0.8629	0.880599077
Phenylpropanoid	Dihydroxyhydrocinnamic acid	HMDB0000	C10447	2	0.3175	0.54459	-0.5	0.2193	<0.001	0.0019	1.653	1.775	<0.001	<0.001	2.003	2.5133	1E-06	<0.001
Amino Acids	Asparagine	HMDB0000	C00152	4	0.0108	0.09813	-0.34	1.2909	0.8328	0.891	0.075	0.333	0.0094	0.0603	0.199	1.3742	0.0001	0.001460997
Benzoic acids	Protocatechuic acid	HMDB0000	C00230	9	0.4581	0.64653	-0.05	0.2115	0.4601	0.6063	0.238	0.153	0.3227	0.5891	-0.07	0.9878	0.1559	0.246843247
Phenylpropanoic Acids	Hydroxyphenyllactic acid	HMDB0000	C03672	16	0.3622	0.58704	0.113	0.4488	0.1693	0.3149	0.116	0.98	0.8424	0.9261	-0.05	0.1466	0.624	0.682266767
Amino Acids	Kynurenine	0684	C00328	16	0.0358	0.18259	0.426	1.133	0.0036	0.0165	1.05	1.398	0.9472	0.9666	-0.03	0.3139	0.0055	0.018589645
Amino Acids	Aspartic acid	HMDB0000	C00049	3	<0.001	0.00192	1.403	2.4534	<0.001	0.0035	1.162	1.623	<0.001	<0.001	1.122	2.2054	0.0001	0.001335961
Amino Acids	Amino adipic acid	HMDB0000	C00956	3	0.1834	0.43026	0.296	0.6988	0.2776	0.4316	0.35	0.729	0.4292	0.7299	0.195	0.4944	0.5817	0.667115721
Carbohydrates	Glucaric acid	HMDB0000	C00818	12	0.486	0.65341	-0.22	0.4936	0.0908	0.2009	0.769	1.123	0.8771	0.9384	5E-04	0.31	0.0643	0.123058223

Fatty Acids	2-Hydroxy-3-methylbutyric	HMDB0000407	-	4	0.9821	0.99235	-0.01	0.0716	0.9508	0.9766	0.07	0.042	0.132	0.3164	0.888	0.7095	0.3659	0.460850622
Pyridines	Picolinic acid ortho-Hydroxyphenyla	HMDB00002	C10164	16	0.4379	0.63142	0.226	0.6754	0.0374	0.0993	0.93	0.933	0.3175	0.5891	0.256	0.947	0.1662	0.258444795
Benzenoids	cetic acid	HMDB0000669	C05852	12	0.588	0.72678	-0.02	0.3463	<0.001	0.0037	1.614	1.344	0.6888	0.8462	-0.04	0.3361	4E-05	<0.001
Amino Acids	Hippuric acid	HMDB00000	C01586	12	0.0188	0.12455	-2.53	1.3265	0.7859	0.8547	-0.82	0.498	0.0836	0.2867	-1.52	1.4563	0.0605	0.118118137
Organic Acids	Malic acid	HMDB0000156	C00149	1	0.4258	0.63142	0.163	0.3095	<0.001	0.0037	0.711	1.387	<0.001	0.0066	0.765	1.6304	7E-05	0.001022042
Amino Acids	N-Acetyaspartic	HMDB00000	C01042	12	0.275	0.53291	-0.56	0.9152	0.0438	0.1105	0.917	0.922	0.6832	0.8462	0.179	0.0024	0.0026	0.010231941
SCFAs	Ethylmethylacet	HMDB00002176	C18319	14	0.0551	0.23247	0.496	1.1753	0.5095	0.6418	0.302	0.28	0.0442	0.2043	0.56	1.2436	0.0864	0.154840858
Benzenoids	Phenylacetic	HMDB00000	C07086	1	0.2085	0.45106	0.5	0.8852	0.5254	0.6576	0.311	0.479	0.4379	0.7322	-0.58	0.4238	0.697	0.737827049
Indoles	Indole-3-	HMDB00000	C19837	8	0.0536	0.23247	-0.49	1.2611	0.2069	0.3613	-0.49	0.721	0.049	0.2166	-0.5	1.0488	0.1221	0.204112785
Indoles	Indoleacetic	HMDB00000	C00954	11	0.0081	0.08483	-0.9	1.2431	0.7859	0.8547	0.111	0.248	0.6423	0.83	0.007	0.3086	0.0168	0.042779448
Organic Acids	Fumaric acid	HMDB0000134	C00122	11	0.0108	0.09813	-0.77	1.9912	0.171	0.3151	0.461	0.744	0.55	0.8109	0.149	0.1311	0.0004	0.002455499
Organic Acids	Glutaric acid	HMDB00000	C00489	12	0.1593	0.39621	-0.77	0.6319	0.7859	0.8547	-0.01	0.544	0.0614	0.2304	-0.8	0.004	0.1678	0.258882255
Organic Acids	Aconitic acid	HMDB0000958	C02341	12	0.1643	0.39943	-0.27	0.7983	0.6505	0.7752	-0.3	0.668	0.8594	0.9384	-0.03	0.3304	0.61	0.678205771
Phenylpropanoids	Cinnamic acid	HMDB00000	C10438	16	0.5733	0.72152	0.057	0.6623	0.0525	0.1274	0.314	1.308	0.7696	0.8902	0.082	0.1137	0.0886	0.157384982
Phenylpropanoic Acids	2-Phenylpropiona	HMDB0001743	-	15	0.6744	0.78943	-0.17	0.2313	0.0086	0.0324	-0.91	0.246	0.1015	0.2883	-0.45	0.8772	0.0441	0.096395696
Phenylpropanoic Acids	Hydrocinnamic	HMDB00000	C05629	15	0.707	0.79211	0.368	0.4902	0.4134	0.5531	-0.6	0.256	0.1105	0.2883	-0.53	1.0868	0.0788	0.147983398
Indoles	3-Indolepropionic	HMDB0002302	-	7	0.0686	0.26242	-1.1	0.9673	0.007	0.0273	-2.06	0.116	0.2204	0.482	-0.76	1.0969	0.0814	0.148643527
Organic Acids	Azelaic acid	HMDB00000	C08261	12	0.0043	0.06646	1.061	1.3719	<0.001	0.0026	4.285	1.413	0.1223	0.3005	0.604	1.0539	0.0004	0.002455499
Fatty Acids	Sebacic acid	HMDB0000792	C08277	12	0.0756	0.26378	0.421	1.2193	<0.001	0.0037	2.926	0.773	0.0013	0.013	0.688	1.4755	0.0001	0.001460997
Organic Acids	alpha-Ketoisovaleric	HMDB00000	C00141	12	0.4855	0.65341	0.116	0.8576	0.0028	0.0144	1.792	1.206	0.9459	0.9666	-0.17	0.5712	0.0044	0.016156797
Organic Acids	Ketoleucine	HMDB0000695	C00233	8	0.3152	0.54459	-0.17	0.3886	0.1507	0.2856	-0.45	0.469	0.088	0.2883	-0.25	0.924	0.62	0.681611159
Organic Acids	3-Methy2-oxo	HMDB00000	C03465	5	0.0546	0.23247	-0.38	0.9724	0.0982	0.2148	-0.4	0.943	0.1015	0.2883	-0.42	0.8101	0.1734	0.26429579
Benzenoids	Phenylpyruvic	HMDB0000205	C00166	10	0.0614	0.24425	0.62	1.3036	0.0136	0.0459	0.572	1.38	0.6678	0.8462	-0.07	0.3372	0.0087	0.026675754
Fatty Acids	Methylmalonic	HMDB00000	C02170	11	0.1004	0.30609	-0.32	1.1855	0.6075	0.7372	0.051	0.426	0.9824	0.9873	0.033	0.1772	0.0812	0.148643527
Amino Acids	2-Hydroxyglutaric	HMDB0000606	C01087	1	0.1223	0.3428	0.449	0.3595	0.0022	0.0114	0.98	1.403	0.0094	0.0603	0.863	1.3835	0.0013	0.00612856
Amino Acids	Glycine	HMDB00000	C00037	14	0.1223	0.3428	0.372	1.0326	0.4141	0.5531	0.132	0.507	0.0186	0.1086	0.298	1.1063	0.105	0.181412743
Organic Acids	Guanidoacetic	HMDB0000128	C00581	8	0.0015	0.03043	-0.75	1.742	<0.001	0.0037	-0.67	1.629	0.0013	0.013	-0.79	1.9507	0.0022	0.009123449
Amino Acids	Citrulline	HMDB00000	C00327	13	0.0067	0.077	-0.59	1.7025	0.0233	0.0672	-0.49	1.342	0.2564	0.5316	-0.28	0.3809	0.026	0.061379059
Carbohydrates	Galactonic acid	HMDB0000565	C00880	4	0.2733	0.53291	0	0.5973	1	1	0	0.203	0.5398	0.8109	0.017	0.914	0.3973	0.492960325
Carbohydrates	Gluconolactone	HMDB00000	C00198	12	0.0125	0.10419	0.269	1.2912	<0.001	0.0018	0.935	0.846	0.007	0.0533	0.138	1.1524	0.0001	0.001248639

		HMDB000																	
Organic Acids	Glycolic acid	0115	C00160	9	0.5321	0.69793	0.102	0.4281	0.7345	0.8319	-0.06	0.401	0.3114	0.5891	-0.17	0.9779	0.2111	0.297870491	
Amino Acids	alpha-	HMDB00000	C02356	14	0.5208	0.69093	-0.04	0.4167	0.1037	0.2219	-0.42	1.033	0.2564	0.5316	-0.13	0.2412	0.0649	0.123058223	
		HMDB000																	
Carbohydrates	Glyceric acid	0139	C00258	3	0.0015	0.03043	0.784	2.0707	<0.001	<0.001	0.886	2.061	<0.001	<0.001	0.786	2.1064	0.0004	0.002455499	
Amino Acids	Proline	HMDB00000	C00148	4	0.0349	0.18259	-0.35	1.3856	0.7825	0.8547	-0.05	0.285	0.0527	0.2194	0.318	1.084	0.0016	0.007348811	
		HMDB000																	
Amino Acids	N-Acetylglycine	0532	-	16	0.2204	0.46666	0.171	0.8397	0.2115	0.3628	0.196	0.986	0.6109	0.8214	-0.09	0.1057	0.1552	0.246843247	
Amino Acids	Pipecolic acid	HMDB00000	C00408	15	0.7402	0.81835	0.027	0.5135	0.0512	0.1258	0.326	1.352	0.1015	0.2883	-0.37	0.6057	0.015	0.039769314	
		HMDB000																	
Organic Acids	Erythronic acid	0613	-	3	0.2564	0.51545	0.223	0.8471	0.4042	0.5531	0.095	0.469	0.8771	0.9384	-0.08	0.1394	0.6925	0.736906462	
Amino Acids	N-Acetylserine	HMDB00002	-	1	0.3775	0.59691	0.043	0.6044	<0.001	0.0037	0.386	1.621	0.0551	0.2194	0.071	0.7795	0.0009	0.004525869	
		HMDB000																	
Organic Acids	Shikimic acid	3070	C00493	1	0.4572	0.64653	0.006	1.062	<0.001	<0.001	0.03	1.443	0.6527	0.838	0.002	0.8312	0.0046	0.016483381	
Amino Acids	N-	HMDB00006	-	11	0.3333	0.5559	0	0.8695	0.6005	0.7372	0.003	0.32	0.982	0.9873	8E-04	0.3624	0.5862	0.667115721	
		HMDB000																	
Organic Acids	Quinic acid	3072	C00296	11	0.6109	0.73675	0.002	0.9231	0.2953	0.4452	0.017	0.035	0.0504	0.2182	0.03	0.1009	0.1319	0.218740682	
Carbohydrates	N-	HMDB00000	C19910	12	0.0173	0.1231	0.185	1.2763	<0.001	<0.001	1.108	1.938	<0.001	0.0026	0.339	1.5079	3E-07	<0.001	
		HMDB000																	
SCFAs	Acetic acid	0042	C00033	9	0.0756	0.26378	0.384	1.2805	0.7399	0.8319	-0.13	0.288	0.1115	0.2883	-0.41	0.9916	0.0056	0.018589645	
Amino Acids	Valine	HMDB00000	C00183	12	0.558	0.70728	-0.08	0.3557	0.9759	0.9809	-0.05	0.312	0.7081	0.8592	-0.04	0.3937	0.8852	0.898727628	
Amino Acids	Pyroglutamic	HMDB00000	C01879	1	<0.001	0.00156	1.01	2.1727	<0.001	<0.001	1.386	1.881	<0.001	<0.001	1.134	2.3065	6E-06	<0.001	
Amino Acids	5-	HMDB00001	C00430	1	0.2758	0.53291	0.099	0.4984	0.0045	0.0203	0.383	1.413	0.0682	0.2467	0.239	0.8973	0.0135	0.037174896	
		HMDB000																	
Carbohydrates	Glucose	0122	C00221	9	0.035	0.18259	0.407	1.4496	0.6505	0.7752	-0.07	0.282	0.001	0.0115	-0.79	1.8431	8E-05	0.001022042	
Carbohydrates	Maltose/Lactos	-	-	12	0.1015	0.30609	0.675	1.235	<0.001	<0.001	2.31	0.511	0.0043	0.0346	1.303	1.9046	3E-06	<0.001	
		HMDB000																	
Carbohydrates	Maltotriose	1262	C01835	1	0.2851	0.54041	0	0.4261	0.0032	0.0159	0.61	1.214	0.0281	0.1514	0.296	1.2114	8E-05	0.001022042	
Organic Acids	3-	HMDB00000	C01089	9	0.3628	0.58704	0.019	0.9704	0.4134	0.5531	-1.15	0.367	0.1223	0.3005	-1.19	0.7464	0.0556	0.114158789	
		HMDB000																	
Amino Acids	Methionine	0696	C00073	5	0.5527	0.70505	-0.09	0.461	0.6333	0.7638	-0.09	0.348	0.5208	0.8034	-0.08	0.179	0.8363	0.862263386	
Benzoic acids	4-	HMDB00001	D06890	10	0.4184	0.63082	0.015	1.0061	0.0575	0.1378	0.027	0.961	0.7191	0.8621	0.007	0.3967	0.3988	0.492960325	
	alpha-	HMDB000																	
Organic Acids	Hydroxyisobutyr	0729	-	16	0.4005	0.61311	0.307	0.6835	0.0162	0.052	0.962	1.453	0.5879	0.8182	0.231	0.4005	0.0226	0.055453445	
Organic Acids	2-	HMDB00000	C05984	10	<0.001	0.00156	0.927	1.8588	0.0056	0.0243	0.836	1.476	0.0144	0.0866	0.496	1.1065	0.0002	0.001896725	
SCFAs	3-	HMDB00000	-	16	0.0108	0.09813	0.152	1.1381	0.0022	0.0114	0.412	1.481	0.8079	0.9084	-0.08	0.119	0.0007	0.003514111	
Carbohydrates	Glutaconic acid	HMDB00000	C02214	12	0.6573	0.7833	-0.17	0.4907	0.0022	0.0114	0.656	1.181	0.1841	0.4117	0.439	0.679	0.0004	0.002455499	
		HMDB000																	
Amino Acids	Isoleucine	0172	C00407	11	0.2921	0.5432	-0.23	0.6572	0.6075	0.7372	0.04	0.415	0.3281	0.5936	0.174	0.4879	0.15	0.242747664	
Amino Acids	Leucine	HMDB00000	C00123	1	0.2231	0.46728	0.219	0.7753	0.1896	0.3369	0.294	0.908	0.0909	0.2883	0.278	0.929	0.4235	0.520239055	
		HMDB000																	
Carbohydrates	Xylose	0098	C00181	3	0.0051	0.07249	1.02	1.8583	<0.001	0.0037	0.838	1.316	0.0037	0.0319	0.599	1.2375	0.0037	0.013861781	
Carbohydrates	Ribulose	HMDB00000	C00309	1	0.1402	0.38217	0.163	0.7683	<0.001	<0.001	0.722	1.514	<0.001	<0.001	0.534	1.9111	2E-06	<0.001	
Carbohydrates	Xylulose	HMDB00000	C00310	1	0.058	0.23552	0.215	0.9864	<0.001	0.0035	1.033	1.383	<0.001	<0.001	0.496	1.644	4E-06	<0.001	
Carbohydrates	Rhamnose	HMDB00000	C00507	10	0.0126	0.10419	0.599	1.3382	0.022	0.0666	0.564	1.268	0.5801	0.813	-0.21	0.117	0.029	0.066152981	
		HMDB000																	
Carbohydrates	beta-Fucose	3081	C02095	12	0.4246	0.63142	-0.02	0.3349	0.5532	0.6838	0.003	0.802	0.2297	0.4967	-0.02	0.3279	0.2631	0.358553093	
Carbohydrates	Fructose	HMDB00000	C02336	16	0.0188	0.12455	0.718	0.362	<0.001	0.0019	2.252	1.201	0.0022	0.0208	1.418	0.4771	8E-05	0.001022042	

Carbohydrates	N-Acetylglucosamine	HMDB0000215	C00140	12	0.8741	0.92245	-0.07	0.6856	<0.001	0.0035	0.519	1.562	0.1208	0.3005	0.176	0.7617	0.0013	0.00612856
SCFAs	Propanoic acid	HMDB000000	C00163	10	0.0069	0.077	0.683	1.5451	0.0268	0.0751	0.548	0.985	0.2654	0.5389	-0.34	0.7249	0.0004	0.002455499
Amino Acids	Norleucine	HMDB00001645	C01933	1	0.1646	0.39943	0.257	0.8904	0.1179	0.247	0.198	0.923	0.0587	0.2251	0.315	1.0363	0.3431	0.443400159
Phenols	Homovanillic acid	HMDB000000	C05582	12	0.6744	0.78943	-0.04	0.2518	0.2604	0.4081	0.077	0.9	0.6744	0.8462	0.011	0.0455	0.3395	0.441526714
Amino Acids	Tryptophan	HMDB00000929	C00078	5	0.0327	0.18259	-0.38	1.4182	0.0372	0.0993	-0.39	1.069	0.4663	0.7545	-0.1	0.4088	0.0201	0.04991134
SCFAs	Butyric acid	HMDB000000	C00246	9	0.1223	0.3428	0.205	0.9242	0.4134	0.5531	0.109	0.399	0.3993	0.691	-0.25	0.7767	0.0535	0.110860503
SCFAs	Isobutyric acid	HMDB00001873	C02632	12	0.9472	0.97157	-0.13	0.2896	0.0225	0.0666	2.549	1.208	0.9472	0.9666	-0.2	0.2364	0.0131	0.036691375
Benzenoids	Mandelic acid	HMDB000000	C01984	12	0.3175	0.54459	0.022	1.015	<0.001	0.0013	0.797	0.934	0.1115	0.2883	0.044	0.6183	0.0006	0.003120262
Organic Acids	Malonic acid	HMDB00000691	C00383	14	0.3869	0.59691	-0.35	0.0219	0.2351	0.3835	-0.26	0.366	0.7402	0.8716	0.122	0.1794	0.7401	0.779270562
Amino Acids	N-Tartaric acid	HMDB000006	C04148	1	0.8424	0.90125	0.044	0.2511	0.2875	0.4368	0.821	0.618	0.2962	0.5722	-1.07	0.3927	0.2149	0.301198836
Carbohydrates	Tartaric acid	HMDB00000956	C00898	1	0.3175	0.54459	2.328	0.5763	0.007	0.0273	4.743	1.141	0.0922	0.2883	2.684	0.6213	0.0293	0.066152981
SCFAs	Isovaleric acid	HMDB000000	C08262	14	0.0682	0.26242	0.483	1.181	0.5468	0.6801	0.194	0.234	0.0551	0.2194	0.521	1.2594	0.0807	0.148643527
SCFAs	Pentanoic acid	HMDB00000892	C00803	15	0.412	0.62579	0.133	0.7092	0.2604	0.4081	0.351	0.599	0.2631	0.5389	-0.42	1.0609	0.0246	0.059511486
Pyridines	N-Phenylpropanoic acid	HMDB000003	-	3	0.4647	0.64663	0.896	0.9049	0.7399	0.8319	0.312	0.42	0.5801	0.813	-0.27	0.4694	0.6136	0.678389706
Phenylpropanoic Acids	Phenyllactic acid	HMDB00000779	C01479	2	0.2062	0.45106	1.336	0.7125	0.0012	0.0076	2.147	1.738	0.2875	0.5609	1.192	0.6793	0.0071	0.022838158
Organic Acids	Oxalic acid	HMDB000002	C00209	9	0.0311	0.18193	0.928	1.5695	0.8534	0.9082	-0.03	0.203	0.3568	0.6339	-0.35	0.3714	0.0248	0.059511486
Organic Acids	Maleic acid	HMDB000000	C01384	11	<0.001	0.01741	-0.88	2.3177	0.0872	0.1973	0.428	0.934	0.912	0.9502	-0.05	0.0033	7E-06	<0.001
Fatty Acids	Itaconic acid	HMDB000002	C00490	12	0.6043	0.73675	0.074	0.071	0.8271	0.891	-0.09	0.723	0.9092	0.9502	-0.03	0.822	0.9672	0.967235285
Organic Acids	Citraconic acid	HMDB00000634	C02226	7	0.0897	0.28775	-0.08	0.9995	0.9279	0.9617	0	0.306	0.1005	0.2883	-0.08	0.6193	0.0599	0.118107903
Organic Acids	Methylsuccinic acid	HMDB000001	-	12	0.8424	0.90125	-0.08	0.0082	0.347	0.4968	0.168	0.65	0.3175	0.5891	-0.18	0.1733	0.2194	0.305319709
Organic Acids	Adipic acid	HMDB00000448	C06104	12	0.3327	0.5559	0.201	0.0736	0.0329	0.0896	1.917	0.711	0.1201	0.3005	0.883	0.1561	0.0503	0.107711735
Fatty Acids	Methylglutaric acid	HMDB000000	-	10	0.088	0.28775	0.205	1.1655	0.1796	0.3249	0.174	0.76	0.841	0.9261	0.03	0.1309	0.269	0.364179211
Benzoic acids	Phthalic acid	HMDB00002107	C01606	16	0.615	0.73723	0.01	0.4245	0.0512	0.1258	0.037	0.61	0.9984	0.9984	5E-05	0.1007	0.2792	0.372872578
Organic Acids	Pimelic acid	HMDB000000	C02656	12	0.207	0.45106	14.13	0.344	0.0096	0.0353	17.53	1.073	0.1242	0.3015	15.41	0.754	0.02	0.04991134
Fatty Acids	3-Methyladipic acid	HMDB00000555	-	1	0.3138	0.54459	0.431	0.3207	0.1693	0.3149	0.687	0.863	0.5801	0.813	0.091	0.4686	0.5188	0.629509226
SCFAs	2-Methyladipic acid	HMDB000031	-	16	0.0754	0.26378	0.365	0.889	<0.001	0.0019	0.981	1.757	0.1099	0.2883	0.311	1.0539	6E-06	<0.001
SCFAs	3-Methyladipic acid	HMDB000003	-	8	0.1461	0.38268	-0.69	0.8143	0.2115	0.3628	-0.89	0.663	0.0922	0.2883	-0.95	0.8911	0.2402	0.329714158
SCFAs	Isocaproic acid	HMDB000000	-	13	0.2564	0.51545	-0.19	0.6802	0.2875	0.4368	-0.29	0.247	0.9824	0.9873	0	0.0362	0.3552	0.456038704
SCFAs	Caproic acid	HMDB00000535	C01585	9	0.3096	0.54459	0.183	0.7203	0.8302	0.891	0.038	0.079	0.882	0.9386	-0.03	0.4599	0.5259	0.630450514
Organic Acids	Suberic acid	HMDB000000	C08278	12	0.3338	0.5559	0.027	0.141	0.0246	0.0701	1.986	1.264	0.1105	0.2883	0.497	0.7625	0.0582	0.116892422
Organic Acids	Citric acid	HMDB00000094	C00158	12	0.1957	0.44265	-0.26	0.7875	0.6947	0.8085	-0.3	0.66	0.5501	0.8109	-0.33	0.4163	0.6723	0.723200219
Organic Acids	Isocitric acid	HMDB000000	C00311	12	0.7085	0.79211	-0.05	0.4303	0.3164	0.4664	0.025	0.684	0.3397	0.609	-0.26	0.4352	0.272	0.365671548
Fatty Acids	Heptanoic acid	HMDB00000666	C17714	6	0.1733	0.4154	-0.34	0.2424	0.2257	0.3807	-0.33	0.81	0.0454	0.2055	-0.5	1.3645	0.2012	0.286060167

Organic Acids	Pyruvic acid	HMDB0000	C00022	6	0.1881	0.43524	-0.48	0.2487	0.1783	0.3249	-0.37	0.768	<0.001	<0.001	-1.57	2.3614	0.0002	0.001460997
Bile Acids	TCDC	0951	C05465	16	0.1184	0.3428	2.22	0.3909	<0.001	0.005	3.623	1.258	0.9092	0.9502	0.45	0.0952	0.0004	0.002455499
Bile Acids	aMCA	HMDB0000	C17647	4	0.1461	0.38268	-0.05	0.8295	0.4769	0.6203	-0.03	0.752	0.5998	0.8214	-0.05	0.515	0.6028	0.673879841
Bile Acids	bMCA	0865	-	4	0.1461	0.38268	-0.05	0.8295	0.4769	0.6203	-0.03	0.752	0.5998	0.8214	-0.05	0.515	0.6028	0.673879841
Bile Acids	HCA	HMDB0000	-	4	0.6686	0.78943	0	0.5618	0.78	0.8547	0.021	0.168	0.3959	0.691	-0.18	0.614	0.5258	0.630450514
Bile Acids	CA	0619	C00695	4	0.0144	0.10987	-0.87	1.8791	0.1896	0.3369	-0.74	0.795	0.3628	0.639	-0.61	0.4379	0.1753	0.26429579
Organic Acids	Oxoglutaric acid	HMDB0000	C00026	10	0.0442	0.20434	0.891	1.5354	<0.001	<0.001	0.879	1.487	0.3175	0.5891	0.106	0.7912	0.0008	0.004246796
Bile Acids	GCA	0138	C01921	12	0.7696	0.8415	0.166	0.2691	0.0209	0.0649	1.556	0.728	0.7357	0.8715	-0.16	0.5175	0.0162	0.041832276
Fatty Acids	Octanoic acid	HMDB0000	C06423	12	0.2786	0.53311	-0.17	0.5476	0.0688	0.1592	2.131	1.02	0.0977	0.2883	-0.25	1.2516	0.0093	0.02776942
Bile Acids	bUDCA	0686	C17662	4	0.4304	0.63142	-0.33	0.9242	0.2172	0.3695	-0.51	0.392	0.6858	0.8462	0.558	0.4808	0.2832	0.375735466
Bile Acids	bHDCA	HMDB0000	-	6	0.9816	0.99235	-0.06	0.0858	0.386	0.5409	-0.12	0.723	0.5291	0.81	-0.01	1.0778	0.6375	0.693274003
Bile Acids	UDCA	0946	C07880	2	0.2164	0.46303	-0.61	1.0712	0.9754	0.9809	-0.09	0.559	0.8396	0.9261	0.141	0.5293	0.59	0.667115721
Bile Acids	bDCA	-	-	8	0.4849	0.65341	0.008	0.8571	0.1262	0.2563	-0.09	1.01	0.0735	0.2612	-0.06	1.4472	0.1057	0.181412743
Bile Acids	CDCA	0518	C02528	13	0.0037	0.0642	-0.97	1.9874	0.0439	0.1105	-1.33	0.75	0.5801	0.813	-0.2	0.0776	0.0098	0.028794967
Bile Acids	DCA	HMDB0000	C04483	8	0.0442	0.20434	-0.7	1.4687	0.0129	0.045	-1.57	1.445	0.0081	0.0597	-0.94	2.0178	0.008	0.025358738
Bile Acids	isoDCA	2536	C17661	14	0.7639	0.83983	0.091	0.2942	0.2319	0.3835	-0.04	1.047	0.6796	0.8462	0.081	0.2817	0.1603	0.251163974
Fatty Acids	Nonanoic acid	HMDB0000	C01601	16	0.7049	0.79211	0.099	0.3487	0.0228	0.0666	0.768	1.153	0.8017	0.9084	-0.07	0.4145	0.0049	0.017390693
Fatty Acids	Decanoic acid	0511	C01571	12	0.4379	0.63142	-0.31	0.5643	0.0225	0.0666	3.266	1.14	0.2758	0.5435	-0.57	0.0595	0.005	0.017390693
Fatty Acids	Undecylenic	HMDB0033	C13910	6	0.5435	0.70505	-0.13	0.0302	<0.001	0.0027	-2.76	1.819	0.0032	0.0292	-1.6	1.9347	0.0005	0.003085233
Bile Acids	GCDCA	0637	C05466	1	0.3869	0.59691	0.242	0.5814	0.007	0.0273	0.897	1.137	0.6109	0.8214	0.106	0.7113	0.0649	0.123058223
Bile Acids	GDCA	HMDB0000	C05464	6	1	1	-0.02	0.2832	0.2059	0.3613	-0.53	0.692	0.1101	0.2883	-0.49	1.4866	0.3591	0.458136424
Fatty Acids	Undecanoic acid	0947	C17715	16	0.5331	0.69793	0.232	0.6776	0.0768	0.1756	0.722	0.902	0.7258	0.8648	-0.15	0.3722	0.0452	0.097810062
Fatty Acids	5-Dodecenoic	HMDB0000	-	8	0.0442	0.20434	-0.98	1.0462	0.0022	0.0114	-1.6	0.837	<0.001	0.0112	-1.51	1.8089	0.0083	0.025661803
Fatty Acids	Dodecanoic acid	0638	C02679	11	0.0275	0.17109	-0.73	1.3143	0.1335	0.2606	-0.79	0.22	0.1115	0.2883	-0.86	0.0644	0.1841	0.269434721
Fatty Acids	12-Tridecenoic	-	-	12	0.5208	0.69093	0.169	0.1695	0.347	0.4968	0.21	0.37	0.6423	0.83	0.081	0.4835	0.8164	0.846208063
Fatty Acids	Tridecanoic acid	0910	C17076	12	0.4751	0.65341	0.235	0.6537	0.9754	0.9809	0.023	0.472	0.4583	0.7545	0.185	0.2829	0.587	0.667115721
Fatty Acids	Myristoleic acid	HMDB0002	C08322	5	0.0846	0.2854	-0.79	1.0513	0.0688	0.1592	-1.06	0.723	0.2181	0.482	-0.51	1.1699	0.1922	0.279234018
Fatty Acids	Myristelaidic acid	HMDB006	2248	12	0.3107	0.54459	-1.17	0.5432	0.1012	0.2189	-2	0.459	0.0339	0.1644	-1.14	1.3806	0.1796	0.268676669
Fatty Acids	Ricinoleic acid	HMDB0034	C08365	7	0.1518	0.38936	-0.33	0.9298	0.9543	0.9766	-0.02	0.027	0.1115	0.2883	-0.42	1.2999	0.305	0.399256464
Fatty Acids	12-Myristic acid	HMDB006	-	9	0.2564	0.51545	0.171	1.0626	0.3164	0.4664	0.084	0.921	0.5196	0.8034	0.134	0.3776	0.4933	0.602242014
Fatty Acids	Myristic acid	HMDB0000	C06424	12	0.9824	0.99235	-0.14	0.2086	0.4865	0.6205	0.322	0.57	0.8079	0.9084	-0.11	0.0301	0.7881	0.821085916
Fatty Acids	Pentadecanoic acid	HMDB0000	0826	12	0.5801	0.72152	0.132	0.5753	0.2351	0.3835	0.346	0.593	0.912	0.9502	-0.07	0.6092	0.5715	0.665242357
Fatty Acids	Palmitoleic acid	HMDB0003	C08362	15	0.733	0.81488	0.116	0.4068	0.4895	0.6205	0.28	0.504	0.568	0.813	-0.19	0.576	0.5724	0.665242357

Fatty Acids	10Z-	HMDB006	-	16	0.6792	0.79037	0.175	0.5127	0.4134	0.5531	0.645	0.704	0.5438	0.8109	-0.14	0.2084	0.5401	0.636034564
Fatty Acids	alpha-Linolenic	HMDB0001	C06427	15	0.7739	0.84154	0.075	0.2695	0.4865	0.6205	0.314	0.478	0.1593	0.3729	-0.74	1.1444	0.1363	0.224197294
	gamma-	HMDB000																
Fatty Acids	Linolenic acid	3073	C06426	16	0.3397	0.55864	0.918	0.7207	0.0439	0.1105	1.29	1.133	0.707	0.8592	0.101	0.638	0.0288	0.066152981
Fatty Acids	Linoleic acid	HMDB0000	C01595	10	0.1539	0.38936	0.422	1.1452	0.1198	0.2483	0.6	0.865	0.3215	0.5891	-0.32	0.8895	0.0535	0.110860503
		HMDB000																
Fatty Acids	Linoelaidic acid	6270	-	15	0.697	0.79211	0.183	0.5299	0.125	0.2563	0.923	0.872	0.2404	0.5143	-0.66	1.1165	0.0563	0.114407548
Fatty Acids	EPA	HMDB0001	C06428	3	0.0895	0.28775	4.617	1.4092	0.0625	0.1481	3.958	0.833	0.0316	0.157	4.138	1.0327	0.1475	0.240539662
		HMDB000																
Fatty Acids	Arachidonic acid	1043	C00219	10	0.2038	0.45106	0.359	1.2004	0.1161	0.2458	0.369	1.095	0.6158	0.8224	0.102	0.4564	0.3734	0.467356495
	8,11,14-																	
Fatty Acids	Eicosatrienoic	HMDB0002	C03242	10	0.0344	0.18259	0.936	1.5072	0.0051	0.0227	1.284	1.578	0.1815	0.4105	0.535	0.7195	0.0141	0.038524316
		HMDB000																
Fatty Acids	DHA	2183	C06429	14	0.1115	0.3313	0.768	1.4623	0.957	0.9766	-0.02	0.143	0.1699	0.3886	0.428	0.7454	0.1821	0.269434721
Fatty Acids	DPA	HMDB0006	C16513	10	0.3869	0.59691	0.889	0.9398	0.2351	0.3835	0.484	0.681	0.4647	0.7545	0.2	0.2561	0.6817	0.729349363
		HMDB000																
Fatty Acids	DPAn-6	1976	-	14	0.4779	0.65341	0.362	0.7475	0.7226	0.8312	0.177	0.364	0.5501	0.8109	-0.01	0.515	0.9029	0.912098904
Fatty Acids	Adrenic acid	HMDB0002	C16527	16	0.238	0.49329	0.725	0.8888	0.0106	0.0376	1.268	1.392	0.2758	0.5435	0.326	0.5394	0.0597	0.118107903
		HMDB000																
Organic Acids	Succinic acid	0254	C00042	11	0.0988	0.30609	-0.5	1.1445	0.7399	0.8319	-0.15	0.555	0.631	0.83	0.118	0.0972	0.0379	0.08387254
Organic Acids	Citramalic acid	HMDB0000	C00815	12	0.4379	0.63142	-0.2	0.1546	0.8801	0.9316	-0.01	0.611	0.4869	0.7751	0.145	0.4847	0.575	0.665242357
	Heptadecanoic	HMDB000																
Fatty Acids	acid	2259	-	16	0.707	0.79211	0.514	0.6317	0.0908	0.2009	1.279	1.196	0.8771	0.9384	-0.14	0.097	0.1828	0.269434721
Fatty Acids	Oleic acid	HMDB0000	C00712	10	0.1338	0.36983	0.345	1.1887	0.1507	0.2856	0.338	0.995	0.7965	0.9084	-0.06	0.1768	0.0854	0.154481889
Fatty Acids	10Z-	HMDB0001	-	12	0.6109	0.73675	-0.38	0.3217	0.4865	0.6205	0.208	0.772	0.6109	0.8214	-0.24	0.0924	0.5401	0.636034564
Carnitines	Carnitine	HMDB0000	C00318	15	0.9147	0.94804	0.029	0.15	0.3004	0.4494	0.282	0.73	0.4855	0.7751	-0.16	0.4413	0.3648	0.460850622
		HMDB000																
Carnitines	Acetylcarnitine	0201	C02571	15	0.8783	0.92245	-0.03	0.1384	0.4491	0.5959	0.106	0.799	0.0756	0.2638	-0.53	0.7293	0.0898	0.158226749
Carnitines	Propionylcarniti	HMDB0000	C03017	16	0.3696	0.59308	0.3	0.3817	0.0059	0.0248	0.907	1.494	0.7572	0.8863	-0.08	0.343	0.0051	0.017486838
	Malonylcarnitin	HMDB000																
Carnitines	e	2095	-	12	0.1921	0.43933	-0.06	1.0785	0.0319	0.0882	0.168	1.16	0.7739	0.8902	-0.02	0.0695	0.0101	0.029087
Carnitines	Butyrylcarnitine	HMDB0002	C02862	15	0.6109	0.73675	-0.04	0.5046	0.1335	0.2606	0.463	0.842	0.0275	0.1514	-0.3	0.6959	0.0159	0.041619728
	2-	HMDB000																
Carnitines	Methylbutyroylc	0378	-	7	0.0243	0.15591	-0.17	1.4797	0.347	0.4968	0.023	0.027	0.1461	0.3462	-0.16	1.2195	0.0031	0.011844061
Carnitines	Valeryl carnitine	HMDB0013	-	15	0.707	0.79211	-0.12	0.097	0.1335	0.2606	0.5	0.678	0.6423	0.83	-0.05	0.6749	0.1989	0.28471129
	Isovelarylcarniti	HMDB000																
Carnitines	ne	0688	-	15	0.707	0.79211	-0.12	0.097	0.1335	0.2606	0.5	0.678	0.6423	0.83	-0.05	0.6749	0.1989	0.28471129
	3-																	
	Hydroxylisovale																	
Carnitines	rylcarnitine	-	-	12	0.0756	0.26378	0.176	0.7897	<0.001	0.0019	0.624	1.551	0.0549	0.2194	0.177	1.0826	0.0004	0.002455499
	Glutaryl carnitin	HMDB001																
Carnitines	e	3130	-	13	0.007	0.077	-1.1	1.9659	0.2514	0.4068	-0.35	0.618	0.4923	0.7775	-0.47	0.4844	0.0102	0.029087
Carnitines	Hexanylcarnitin	HMDB0000	-	7	0.0144	0.10987	-0.36	1.5109	0.2604	0.4081	-0.22	0.255	<0.001	<0.001	-0.61	2.1799	0.0003	0.002455499
		HMDB006																
Carnitines	Adipoylcarnitine	1677	-	15	0.5501	0.70505	-0.09	0.3823	0.7859	0.8547	-0.07	0.779	0.0125	0.0777	-0.31	0.7721	0.1076	0.182961667
Carnitines	Octanoylcarniti	HMDB0000	C02838	8	<0.001	0.01308	-1.19	1.8693	0.0156	0.0509	-1.55	0.994	<0.001	0.0011	-2.25	2.3595	0.0002	0.001896725
	Decanoylcarniti	HMDB000																
Carnitines	ne C10	0651	-	8	<0.001	0.01124	-1.04	1.929	0.0106	0.0376	-1.31	1.309	<0.001	<0.001	-1.41	2.4164	0.0003	0.002266751
Carnitines	Lauroyl carnitine	HMDB0002	-	8	0.0561	0.23247	-0.32	1.5984	<0.001	0.003	-1.73	1.583	<0.001	0.0069	-2.31	2.0478	0.0012	0.005766773

Carnitines	Palmitoylcarnitine	HMDB0000222	C02990	11	0.0808	0.2774	-0.64	1.219	0.9005	0.9431	-0.05	0.111	0.9382	0.9666	0.026	0.0232	0.2399	0.329714158
Carnitines	Oleylcarnitine	HMDB00005	-	1	0.441	0.63143	0.275	0.4818	0.0086	0.0324	1.18	1.505	0.035	0.166	0.599	1.3856	0.0143	0.038552004
Carnitines	Linoleylcarnitine	HMDB0006469	-	1	0.1838	0.43026	-0.81	0.5237	0.0132	0.0452	1.029	1.236	0.0588	0.2251	0.669	0.8809	0.0024	0.009752072
Carnitines	Stearylarnitine	HMDB00000	-	2	0.8424	0.90125	-0.27	0.3862	0.1507	0.2856	0.181	1.181	0.0682	0.2467	0.458	1.286	0.1149	0.193855084
Bile Acids	NorCA	-	-	1	0.0039	0.0642	0.011	1.2554	<0.001	0.0041	0.152	1.089	0.0229	0.1303	0	0.5068	0.002	0.008598336
Fatty Acids	2,2-	-	-	6	0.3175	0.54459	-0.02	0.3565	0.2604	0.4081	-0.03	0.602	0.5801	0.813	0.004	0.7027	0.6648	0.718999439

Table S4. Characteristics of validation cohort patients infected with COVID-19 at admission according to disease severity

Characteristics	Mild (n=46)	Recovery (n=22)	Severe (n=22)	P
Age, years	49.85(45.85-53.85)	51.14(45.00-57.27)	65.73(60.55-70.90)	<0.001
Gender				
Male	22(47.8%)	11(50.0%)	13(59.1%)	0.874
Female	24(52.2%)	11(50.0%)	9(40.9%)	
Coexisting disorder ^a	27(58.7%)	10(45.5%)	9(40.9%)	0.324
Clinical signs and symptoms				
Fever	38(82.6%)	15(68.2%)	18(81.8%)	0.366
Cough	36(78.3%)	13(59.1%)	12(54.5%)	0.089
Chilly	10(21.7%)	6(27.3%)	0(0.0%)	0.037
Myalgia	14(30.4%)	2(9.1%)	0(0.0%)	0.004
Fatigue	22(47.8%)	1(4.5%)	4(18.2%)	<0.001
Rhinorrhoea	10(21.7%)	0(0.0%)	0(0.0%)	0.005
Shortness of breath	4(8.7%)	1(4.5%)	19(86.4%)	<0.001
Sore throat	10(21.7%)	0(0.0%)	2(9.1%)	0.038
Diarrhea	0(0.0%)	1(4.5%)	0(0.0%)	0.210
Chest CT findings				
Ground-glass opacity	24(52.2%)	17(77.3%)	21(95.5%)	0.001
Local mottling shadow	4(8.7%)	2(9.1%)	0(0.0%)	0.353
Bilateral mottling shadow	19(41.3%)	7(31.8%)	4(18.2%)	0.164
Laboratory parameters				
Leucocytes($\times 10^9$ /L; NR:3.5-9.5)	6.41(5.78-7.07)	4.91(4.07-5.76)	6.60(5.01-8.21)	0.050
Lymphocytes($\times 10^9$ /L; NR:1.1-3.2)	1.38(1.15-1.61)	1.48(1.04-1.93)	0.77(0.61-0.94)	0.006
Neutrophils($\times 10^9$ /L; NR:1.8-6.3)	3.60(3.06-4.15)	3.16(2.74-3.59)	3.54(2.81-4.27)	0.570
Platelets($\times 10^9$ /L; NR:125.0-350.0)	183.92(165.24-202.60)	175.27(150.12-200.42)	180.32(151.46-209.17)	0.864
HGB(g/L; NR:130.0-175.0)	126.44(119.35-133.54)	124.63(108.37-140.89)	126.68(118.66-134.70)	0.958
APTT(s; NR:21.0-37.0) ^b	39.10(37.81-40.39)	40.04(38.07-42.02)	40.35(38.57-42.12)	0.523
PT(s; NR:10.5-13.5) ^b	13.87(13.57-14.18)	14.30(13.49-15.10)	13.93(13.25-14.61)	0.447
D-dimer(mg/L; NR:0-500) ^b	2063.9(1189.3-2938.6)	1867.4(1175.4-2559.5)	1600.7(1365.4-1835.9)	0.816
Albumin (g/L; NR:40.0-55.0)	38.79(36.85-40.73)	38.47(36.26-40.68)	35.41(33.44-37.39)	0.071
ALT (U/L; NR:9.0-50.0)	37.41(22.91-51.92)	37.32(26.02-48.62)	50.70(22.08-79.31)	0.543
AST (U/L; NR:15.0-40.0)	26.77(22.34-31.20)	37.02(18.77-35.27)	23.95(22.08-25.82)	0.707
TB (μ mol/L; NR:0.0-21.0)	15.32(11.53-19.12)	13.35(6.96-19.73)	16.22(12.15-20.29)	0.732
BUN (mmol/L; NR:3.6-9.5)	4.72(3.98-5.46)	4.30(3.31-5.29)	4.35(4.10-4.59)	0.672
Scr (μ mol/L; NR:57.0-111.0)	69.78(61.11-78.46)	68.41(49.99-86.83)	69.26(66.07-72.45)	0.984
CK (U/L; NR:50.0-310.0)	79.03(64.33-93.73)	71.12(47.24-95.00)	85.68(67.52-103.84)	0.612
LDH (U/L; NR:120.0-250.0)	218.71(189.48-247.94)	199.36(165.60-233.12)	217.89(195.28-240.50)	0.651
CRP (mg/L; NR:0.0-5.0)	20.13(15.42-24.84)	15.79(10.81-20.76)	16.25(11.07-21.44)	0.377

Abbreviation: HGB, hemoglobin; APTT, activated partial thromboplastin time; PT, prothrombin time; ALT, alanine aminotransferase; AST, aspartate aminotransferase; TB, total bilirubin; BUN, blood urea nitrogen; Scr, serum creatinine; CK, creatine kinase; LDH, lactate dehydrogenase; CRP, C-reactive protein; NR, normal reference. ^a Including hypertension, type 2 diabetes mellitus, cancer, hyperlipidemia, liver disease and other chronic diseases, ^b missing for 9 severe group.

Table S5. Metabolites quantified in the discovery cohort by targeted metabolomics with FDR<0.05 (related to figure 2-A)

Class	Name	HMDB_ID	KEGG_ID	Normal VS Mild				Normal VS Severe				Normal VS Recovery				Total	
				P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR
Amino Acids	Arginine	HMDB0000517	C00062	0.914	0.948	0.02	0.0469	0.0019	0.011	-0.48	1.643	0.0089	0.060	-0.37	1.3098	0.0025	0.0098
Amino Acids	Ornithine	HMDB0000214	C00077	0.0311	0.18193	0.371	1.5216	<0.001	0.0035	0.981	1.794	<0.001	<0.001	1.56	2.3139	0.00	<0.001
Amino Acids	Glutamine	HMDB0000641	C00064	0.037	0.185	-0.36	1.4032	0.0019	0.011	-0.62	1.791	0.0043	0.035	-0.48	1.8552	0.0019	0.0082
Amino Acids	Glutamic acid	HMDB0000148	C00025	<0.001	0.00256	0.82	1.8495	<0.001	<0.001	1.482	2.015	<0.001	<0.001	1.45	2.6133	0.00	<0.001
Amino Acids	beta-Alanine	HMDB0000056	C00099	0.881	0.922	-0.01	0.3399	0.0439	0.111	0.54	1.32	0.0311	0.157	0.13	0.8346	0.0063	0.0204
Amino Acids	GABA	HMDB0000112	C00334	<0.001	0.01124	-0.59	2.402	0.019	0.0594	-0.53	1.12	0.0094	0.060	-0.39	1.6741	0.00	0.0081
Amino Acids	Creatine	HMDB0000064	C00300	0.292	0.543	0.34	0.6911	0.0036	0.016	1.97	1.569	0.2758	0.543	-0.26	0.5015	0.0002	0.0019
Organic Acids	Hydroxypropionic acid	HMDB0000700	C01013	0.8771	0.92245	-0.13	0.1221	0.016	0.0509	0.484	0.877	0.4369	0.732	-0.12	0.5262	0.01	0.0268
Amino Acids	Homocitrulline	HMDB0000679	C02427	0.317	0.545	-0.16	1.1381	0.0036	0.016	1.15	1.487	0.7739	0.890	0.16	0.4166	0.0004	0.0025
Organic Acids	Lactic acid	HMDB0000190	C00186	0.4647	0.64663	0.105	0.5539	<0.001	<0.001	1.238	2.229	<0.001	<0.001	1.16	2.7261	0.00	<0.001
Amino Acids	2-Phenylglycine	HMDB0002210	-	0.076	0.264	0.09	0.8204	<0.001	0.003	0.46	1.398	0.0311	0.157	0.08	0.5041	0.0012	0.006
Phenylpropanoid	Dihydroxyhydrocinnamic acid	HMDB0000423	C10447	0.3175	0.54459	-0.5	0.2193	<0.001	0.0019	1.653	1.775	<0.001	<0.001	2.00	2.5133	0.00	<0.001
Amino Acids	Asparagine	HMDB0000168	C00152	0.011	0.098	-0.34	1.2909	0.8328	0.891	0.08	0.333	0.0094	0.060	0.20	1.3742	0.0001	0.0015
Amino Acids	Kynurenine	HMDB0000684	C00328	0.0358	0.18259	0.426	1.133	0.004	0.0165	1.05	1.398	0.9472	0.967	-0.03	0.3139	0.01	0.0186
Amino Acids	Aspartic acid	HMDB0000191	C00049	<0.001	0.002	1.40	2.4534	<0.001	0.003	1.16	1.623	<0.001	<0.001	1.12	2.2054	0.0001	0.0013
Benzenoids	ortho-Hydroxyphenylacetic acid	HMDB0000669	C05852	0.588	0.72678	-0.02	0.3463	<0.001	0.0037	1.614	1.344	0.6888	0.846	-0.04	0.3361	0.00	<0.001
Organic Acids	Malic acid	HMDB0000156	C00149	0.426	0.631	0.16	0.3095	<0.001	0.004	0.71	1.387	<0.001	0.007	0.76	1.6304	7E-05	0.001
Amino Acids	N-Acetylaspartic acid	HMDB0000812	C01042	0.275	0.53291	-0.56	0.9152	0.044	0.1105	0.917	0.922	0.6832	0.846	0.18	0.0024	0.00	0.0102
Indoles	Indoleacetic acid	HMDB0000197	C00954	0.008	0.085	-0.90	1.2431	0.7859	0.855	0.11	0.248	0.6423	0.830	0.01	0.3086	0.0168	0.0428
Organic Acids	Fumaric acid	HMDB0000134	C00122	0.0108	0.09813	-0.77	1.9912	0.171	0.3151	0.461	0.744	0.55	0.811	0.15	0.1311	0.00	0.0025
Organic Acids	Azelaic acid	HMDB0000784	C08261	0.004	0.066	1.06	1.3719	<0.001	0.003	4.29	1.413	0.1223	0.300	0.60	1.0539	0.0004	0.0025
Fatty Acids	Sebacic acid	HMDB0000792	C08277	0.0756	0.26378	0.421	1.2193	<0.001	0.0037	2.926	0.773	0.0013	0.013	0.69	1.4755	0.00	0.0015
Organic Acids	alpha-Ketoisovaleric acid	HMDB0000019	C00141	0.485	0.653	0.12	0.8576	0.0028	0.014	1.79	1.206	0.9459	0.967	-0.17	0.5712	0.0044	0.0162
Benzenoids	Phenylpyruvic acid	HMDB0000205	C00166	0.0614	0.24425	0.62	1.3036	0.014	0.0459	0.572	1.38	0.6678	0.846	-0.07	0.3372	0.01	0.0267
Amino Acids	2-Hydroxyglutaric acid	HMDB0000606	C01087	0.122	0.343	0.45	0.3595	0.0022	0.011	0.98	1.403	0.0094	0.060	0.86	1.3835	0.0013	0.0061
Organic Acids	Guanidoacetic acid	HMDB0000128	C00581	0.0015	0.03043	-0.75	1.742	<0.001	0.0037	-0.67	1.629	0.0013	0.013	-0.79	1.9507	0.00	0.0091
Carbohydrates	Gluconolactone	HMDB0000150	C00198	0.012	0.104	0.27	1.2912	<0.001	0.002	0.94	0.846	0.007	0.053	0.14	1.1524	0.0001	0.0012
Carbohydrates	Glyceric acid	HMDB0000139	C00258	0.0015	0.03043	0.784	2.0707	<0.001	<0.001	0.886	2.061	<0.001	<0.001	0.79	2.1064	0.00	0.0025
Amino Acids	Proline	HMDB0000162	C00148	0.035	0.183	-0.35	1.3856	0.7825	0.855	-0.05	0.285	0.0527	0.219	0.32	1.084	0.0016	0.0073
Amino Acids	Pipecolic acid	HMDB0000716	C00408	0.7402	0.81835	0.027	0.5135	0.051	0.1258	0.326	1.352	0.1015	0.288	-0.37	0.6057	0.01	0.0398
Amino Acids	N-Acetylserine	HMDB0002931	-	0.377	0.597	0.04	0.6044	<0.001	0.004	0.39	1.621	0.0551	0.219	0.07	0.7795	0.0009	0.0045
Organic Acids	Shikimic acid	HMDB0003070	C00493	0.4572	0.64653	0.006	1.062	<0.001	<0.001	0.03	1.443	0.6527	0.838	0.00	0.8312	0.00	0.0165
Carbohydrates	N-Acetylneuraminic acid	HMDB0000230	C19910	0.017	0.123	0.18	1.2763	<0.001	<0.001	1.11	1.938	<0.001	0.003	0.34	1.5079	3E-07	<0.001
SCFAs	Acetic acid	HMDB0000042	C00033	0.0756	0.26378	0.384	1.2805	0.740	0.8319	-0.13	0.288	0.1115	0.288	-0.41	0.9916	0.01	0.0186
Amino Acids	Pyroglutamic acid	HMDB0000267	C01879	<0.001	0.002	1.01	2.1727	<0.001	<0.001	1.39	1.881	<0.001	<0.001	1.13	2.3065	6E-06	<0.001
Amino Acids	5-Aminolevulinic acid	HMDB0001149	C00430	0.2758	0.53291	0.099	0.4984	0.004	0.0203	0.383	1.413	0.0682	0.247	0.24	0.8973	0.01	0.0372
Carbohydrates	Glucose	HMDB0000122	C00221	0.035	0.183	0.41	1.4496	0.6505	0.775	-0.07	0.282	0.001	0.012	-0.79	1.8431	8E-05	0.001
Carbohydrates	Maltose/Lactose	-	-	0.1015	0.30609	0.675	1.235	<0.001	<0.001	2.31	0.511	0.0043	0.035	1.30	1.9046	0.00	<0.001
Carbohydrates	Maltotriose	HMDB0001262	C01835	0.285	0.540	0.00	0.4261	0.0032	0.016	0.61	1.214	0.0281	0.151	0.30	1.2114	8E-05	0.001
Organic Acids	2-Hydroxybutyric acid	HMDB0000008	C05984	<0.001	0.00156	0.927	1.8588	0.006	0.0243	0.836	1.476	0.0144	0.087	0.50	1.1065	0.00	0.0019
SCFAs	3-Hydroxyisovaleric acid	HMDB0000754	-	0.011	0.098	0.15	1.1381	0.0022	0.011	0.41	1.481	0.8079	0.908	-0.08	0.119	0.0007	0.0035
Carbohydrates	Glutaconic acid	HMDB0000620	C02214	0.6573	0.7833	-0.17	0.4907	0.002	0.0114	0.656	1.181	0.1841	0.412	0.44	0.679	0.00	0.0025
Carbohydrates	Xylose	HMDB0000098	C00181	0.005	0.072	1.02	1.8583	<0.001	0.004	0.84	1.316	0.0037	0.032	0.60	1.2375	0.0037	0.0139

Carbohydrates	Ribulose	HMDB0000621	C00309	0.1402	0.38217	0.163	0.7683	<0.001	<0.001	0.722	1.514	<0.001	<0.001	0.53	1.9111	0.00	<0.001
Carbohydrates	Xylulose	HMDB0001644	C00310	0.058	0.236	0.22	0.9864	<0.001	0.003	1.03	1.383	<0.001	<0.001	0.50	1.644	4E-06	<0.001
Carbohydrates	Fructose	HMDB0000660	C02336	0.0188	0.12455	0.718	0.362	<0.001	0.0019	2.252	1.201	0.0022	0.021	1.42	0.4771	0.00	0.001
Carbohydrates	N-Acetylglucosamine	HMDB0000215	C00140	0.874	0.922	-0.07	0.6856	<0.001	0.003	0.52	1.562	0.1208	0.300	0.18	0.7617	0.0013	0.0061
SCFAs	Propanoic acid	HMDB0000237	C00163	0.0069	0.077	0.683	1.5451	0.027	0.0751	0.548	0.985	0.2654	0.539	-0.34	0.7249	0.00	0.0025
Amino Acids	Tryptophan	HMDB0000929	C00078	0.033	0.183	-0.38	1.4182	0.0372	0.099	-0.39	1.069	0.4663	0.754	-0.10	0.4088	0.0201	0.0499
SCFAs	Isobutyric acid	HMDB0001873	C02632	0.9472	0.97157	-0.13	0.2896	0.023	0.0666	2.549	1.208	0.9472	0.967	-0.20	0.2364	0.01	0.0367
Benzenoids	Mandelic acid	HMDB0000703	C01984	0.317	0.545	0.02	1.015	<0.001	0.001	0.80	0.934	0.1115	0.288	0.04	0.6183	0.0006	0.0031
Phenylpropanoic Acids	Phenyllactic acid	HMDB0000779	C01479	0.2062	0.45106	1.336	0.7125	0.001	0.0076	2.147	1.738	0.2875	0.561	1.19	0.6793	0.01	0.0228
Organic Acids	Maleic acid	HMDB0000176	C01384	<0.001	0.017	-0.88	2.3177	0.0872	0.197	0.43	0.934	0.912	0.950	-0.05	0.0033	7E-06	<0.001
Organic Acids	Pimelic acid	HMDB0000857	C02656	0.207	0.45106	14.13	0.344	0.010	0.0353	17.53	1.073	0.1242	0.301	15.41	0.754	0.02	0.0499
SCFAs	2-Methylpentanoic acid	HMDB0031580	-	0.075	0.264	0.36	0.889	<0.001	0.002	0.98	1.757	0.1099	0.288	0.31	1.0539	6E-06	<0.001
Organic Acids	Pyruvic acid	HMDB0000243	C00022	0.1881	0.43524	-0.48	0.2487	0.178	0.3249	-0.37	0.768	<0.001	<0.001	-1.57	2.3614	0.00	0.0015
Bile Acids	TCDCa	HMDB0000951	C05465	0.118	0.343	2.22	0.3909	<0.001	0.005	3.62	1.258	0.9092	0.950	0.45	0.0952	0.0004	0.0025
Organic Acids	Oxoglutaric acid	HMDB0000208	C00026	0.0442	0.20434	0.891	1.5354	<0.001	<0.001	0.879	1.487	0.3175	0.589	0.11	0.7912	0.00	0.0042
Bile Acids	GCA	HMDB0000138	C01921	0.770	0.842	0.17	0.2691	0.0209	0.065	1.56	0.728	0.7357	0.871	-0.16	0.5175	0.0162	0.0418
Fatty Acids	Octanoic acid	HMDB0000482	C06423	0.2786	0.53311	-0.17	0.5476	0.069	0.1592	2.131	1.02	0.0977	0.288	-0.25	1.2516	0.01	0.0278
Bile Acids	CDCA	HMDB0000518	C02528	0.004	0.064	-0.97	1.9874	0.0439	0.111	-1.33	0.75	0.5801	0.813	-0.20	0.0776	0.0098	0.0288
Bile Acids	DCA	HMDB0000626	C04483	0.0442	0.20434	-0.7	1.4687	0.013	0.045	-1.57	1.445	0.0081	0.060	-0.94	2.0178	0.01	0.0254
Fatty Acids	Nonanoic acid	HMDB0000847	C01601	0.705	0.792	0.10	0.3487	0.0228	0.067	0.77	1.153	0.8017	0.908	-0.07	0.4145	0.0049	0.0174
Fatty Acids	Decanoic acid	HMDB0000511	C01571	0.4379	0.63142	-0.31	0.5643	0.023	0.0666	3.266	1.14	0.2758	0.543	-0.57	0.0595	0.00	0.0174
Fatty Acids	Undecylenic acid	HMDB0033724	C13910	0.544	0.705	-0.13	0.0302	<0.001	0.003	-2.76	1.819	0.0032	0.029	-1.60	1.9347	0.0005	0.0031
Fatty Acids	5-Dodecenoic acid	HMDB0000529	-	0.0442	0.20434	-0.98	1.0462	0.002	0.0114	-1.6	0.837	<0.001	0.011	-1.51	1.8089	0.01	0.0257
Fatty Acids	8,11,14-Eicosatrienoic acid	HMDB0002925	C03242	0.034	0.183	0.94	1.5072	0.0051	0.023	1.28	1.578	0.1815	0.410	0.53	0.7195	0.0141	0.0385
Carnitines	Propionylcarnitine	HMDB0000824	C03017	0.3696	0.59308	0.3	0.3817	0.006	0.0248	0.907	1.494	0.7572	0.886	-0.08	0.343	0.01	0.0175
Carnitines	Malonylcarnitine	HMDB0002095	-	0.192	0.439	-0.06	1.0785	0.0319	0.088	0.17	1.16	0.7739	0.890	-0.02	0.0695	0.0101	0.0291
Carnitines	Butyrylcarnitine	HMDB0002013	C02862	0.6109	0.73675	-0.04	0.5046	0.134	0.2606	0.463	0.842	0.0275	0.151	-0.30	0.6959	0.02	0.0416
Carnitines	2-Methylbutyrylcarnitine	HMDB0000378	-	0.024	0.156	-0.17	1.4797	0.347	0.497	0.02	0.027	0.1461	0.346	-0.16	1.2195	0.0031	0.0118
Carnitines	3-Hydroxyisovalerylcarnitine	-	-	0.0756	0.26378	0.176	0.7897	<0.001	0.0019	0.624	1.551	0.0549	0.219	0.18	1.0826	0.00	0.0025
Carnitines	Glutaryl carnitine	HMDB0013130	-	0.007	0.077	-1.10	1.9659	0.2514	0.407	-0.35	0.618	0.4923	0.778	-0.47	0.4844	0.0102	0.0291
Carnitines	Hexanoylcarnitine	HMDB0000705	-	0.0144	0.10987	-0.36	1.5109	0.260	0.4081	-0.22	0.255	<0.001	<0.001	-0.61	2.1799	0.00	0.0025
Carnitines	Octanoylcarnitine	HMDB0000791	C02838	<0.001	0.013	-1.19	1.8693	0.0156	0.051	-1.55	0.994	<0.001	0.001	-2.25	2.3595	0.0002	0.0019
Carnitines	Decanoylcarnitine C10	HMDB0000651	-	<0.001	0.01124	-1.04	1.929	0.011	0.0376	-1.31	1.309	<0.001	<0.001	-1.41	2.4164	0.00	0.0023
Carnitines	Lauroyl carnitine	HMDB0002250	-	0.056	0.232	-0.32	1.5984	<0.001	0.003	-1.73	1.583	<0.001	0.007	-2.31	2.0478	0.0012	0.0058
Carnitines	Oleylcarnitine C18 1	HMDB0005065	-	0.441	0.63143	0.275	0.4818	0.009	0.0324	1.18	1.505	0.035	0.166	0.60	1.3856	0.01	0.0386
Carnitines	Linoleyl carnitine	HMDB0006469	-	0.184	0.430	-0.81	0.5237	0.0132	0.045	1.03	1.236	0.0588	0.225	0.67	0.8809	0.0024	0.0098
Bile Acids	NorCA	-	-	0.0039	0.0642	0.011	1.2554	<0.001	0.0041	0.152	1.089	0.0229	0.130	0.00	0.5068	0.00	0.0086

Table S6. 11 mtabolites of urea cycle and TCA cycle presented marked difference across stages in the discovery cohort by targeted metabolomics analysis (related to figure 3)

Class	Name	HMDB ID	KEGG ID	Normal VS Mild				Normal VS Severe				Normal VS Recovery				Total	
				P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR
Amino Acids	Proline	HMDB0000162	C00148	0.035	0.183	-0.35	1.3856	0.7825	0.8547	-0.05	0.285	0.0527	0.2194	0.318	1.084	0.002	0.007
Amino Acids	Creatine	HMDB0000064	C00300	0.2917	0.5432	0.341	0.6911	0.0036	0.0165	1.969	1.569	0.2758	0.5435	-0.26	0.5015	0.0002	0.0019
Amino Acids	Aspartic acid	HMDB0000191	C00049	<0.001	0.002	1.403	2.4534	<0.001	0.0035	1.162	1.623	<0.001	<0.001	1.122	2.205	0.000	0.001
Amino Acids	Arginine	HMDB0000517	C00062	0.9143	0.94804	0.016	0.0469	0.0019	0.0113	-0.48	1.643	0.0089	0.0603	-0.37	1.3098	0.0025	0.00975
Amino Acids	Ornithine	HMDB0000214	C00077	0.031	0.182	0.371	1.5216	<0.001	0.0035	0.981	1.794	<0.001	<0.001	1.557	2.314	0.000	<0.001
Amino Acids	Glutamine	HMDB0000641	C00064	0.0373	0.18541	-0.36	1.4032	0.0019	0.0113	-0.62	1.791	0.0043	0.0346	-0.48	1.8552	0.0019	0.00817
Amino Acids	Citrulline	HMDB0000904	C00327	0.007	0.077	-0.59	1.7025	0.0233	0.0672	-0.49	1.342	0.2564	0.5316	-0.28	0.381	0.026	0.061
Organic Acids	Pyruvic acid	HMDB0000243	C00022	0.1881	0.43524	-0.48	0.2487	0.1783	0.3249	-0.37	0.768	<0.001	<0.001	-1.57	2.3614	0.0002	0.00146
Organic Acids	Malic acid	HMDB0000156	C00149	0.426	0.631	0.163	0.3095	<0.001	0.0037	0.711	1.387	<0.001	0.0066	0.765	1.630	0.000	0.00102
Organic Acids	Oxoglutaric acid	HMDB0000208	C00026	0.0442	0.20434	0.891	1.5354	<0.001	<0.001	0.879	1.487	0.3175	0.5891	0.106	0.7912	0.0008	0.00425
Organic Acids	Fumaric acid	HMDB0000134	C00122	0.011	0.098	-0.77	1.9912	0.171	0.3151	0.461	0.744	0.55	0.8109	0.149	0.131	0.000	0.00246

Table S7. 11 mtabolites in table S6 verified with marked difference across stages in the validation cohort by targeted metabolomics analysis (related to figure 3)

Class	Name	HMDB_ID	KEGG_ID	Normal VS Mild				Normal VS Severe				Normal VS Recovery				Total	
				P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR	log2FC	VIP	P	FDR
Amino Acids	Proline	HMDB0000162	C00148	0.723	0.88364	-0.04	0.1954	0.7449	0.7449	-0.05	0.28	0.508	0.6985	0.087	0.387	0.674	0.674
Amino Acids	Creatine	HMDB0000064	C00300	1	1	0.055	0.74	0.0179	0.0543	0.621	0.8	0.1413	0.3108	-0.47	1.1978	0.0011	0.0039
Amino Acids	Aspartic acid	HMDB0000191	C00049	0.000	0.00075	0.552	1.9226	0.0046	0.0256	0.602	1.198	0.0008	0.0086	0.487	1.673	0.0005	0.0027
Amino Acids	Arginine	HMDB0000517	C00062	0.5058	0.88364	-0.11	0.2043	0.0221	0.0543	-0.38	0.659	0.8748	0.8748	0.021	0.0217	0.1035	0.1423
Amino Acids	Ornithine	HMDB0000214	C00077	0.978	1	-0.2	0.2909	0.0582	0.08	0.408	0.829	0.2403	0.4406	0.318	0.8414	0.215	0.263
Amino Acids	Glutamine	HMDB0000641	C00064	0.056	0.15388	-0.21	1.3017	0.0247	0.0543	-0.32	1.508	0.0491	0.1799	-0.22	1.3212	0.0771	0.1212
Amino Acids	Citrulline	HMDB0000904	C00327	0.0098	0.03592	-0.28	2.0044	0.046	0.0723	-0.36	0.923	0.0793	0.218	-0.28	1.0479	0.0734	0.1212
Organic Acids	Pyruvic acid	HMDB0000243	C00022	0.6381	0.88364	-0.14	0.2986	0.0721	0.0881	-0.72	0.98	0.0017	0.0095	-0.93	1.6329	0.0044	0.0121
Organic Acids	Malic acid	HMDB0000156	C00149	0.7172	0.88364	-0.27	0.1704	0.0315	0.0578	0.398	0.753	0.5817	0.711	0.045	0.4834	0.0707	0.1212
Organic Acids	Oxoglutaric acid	HMDB0000208	C00026	0.0015	0.00817	0.787	0.8295	<0.001	0.0009	1.013	1.598	0.428	0.6726	-0.28	0.3292	<0.001	<0.001
Organic Acids	Fumaric acid	HMDB0000134	C00122	0.42	0.88364	-0.48	0.2704	0.2221	0.2443	0.116	0.72	0.6796	0.7476	-0.05	0.2367	0.2749	0.3024