

Table S1: Metabolic changes following ε-toxin treatment

Heat map of statistically significant biochemicals profiled in this study. For paired comparisons, shaded cells indicate $p < 0.05$ red indicates that the mean values are significantly higher for that comparison; green values significantly lower). The q-value gives the false discovery rate for the selected list (i.e., an estimate of the proportion of false discoveries for the list of compounds whose p-value is below the cutoff for significance). HI: heat-inactivated; TT:ε-toxin treated; C: untreated control.

SUPER PATHWAY	SUB PATHWAY	BIOCHEMICAL NAME	PLATFORM
Amino acid	Glycine, serine and threonine metabolism	glycine	GC/MS
		serine	GC/MS
		threonine	GC/MS
		betaine	LC/MS pos
	Alanine and aspartate metabolism	aspartate	GC/MS
		asparagine	GC/MS
		beta-alanine	GC/MS
		alanine	GC/MS
		N-acetylaspargate (NAA)	LC/MS pos
	Glutamate metabolism	glutamate	LC/MS pos
		glutamate, gamma-methyl ester	LC/MS pos
		glutamine	LC/MS pos
		gamma-aminobutyrate (GABA)	GC/MS
		N-acetyl-aspartyl-glutamate (NAAG)	LC/MS pos
	Histidine metabolism	histidine	LC/MS neg
	Lysine metabolism	lysine	GC/MS
	Phenylalanine & tyrosine metabolism	phenylalanine	LC/MS pos
		tyrosine	LC/MS pos
		3-(4-hydroxyphenyl)lactate	LC/MS neg
		4-hydroxyphenylpyruvate	LC/MS neg
	Tryptophan metabolism	tryptophan	LC/MS pos
		C-glycosyltryptophan*	LC/MS pos
	Valine, leucine and isoleucine metabolism	3-methyl-2-oxobutyrate	LC/MS neg
		3-methyl-2-oxovalerate	LC/MS neg
		isoleucine	LC/MS pos
		leucine	LC/MS pos
		valine	LC/MS pos
		4-methyl-2-oxopentanoate	LC/MS neg
		isobutyrylcarnitine	LC/MS pos
		2-methylbutyrylcarnitine	LC/MS pos
		isovalerylcarnitine	LC/MS pos
		cysteine	GC/MS
	Cysteine, methionine, SAM, taurine metabolism	hypotaaurine	GC/MS
		S-adenosylhomocysteine (SAH)	LC/MS pos
		methionine	LC/MS pos
		N-acetylmethionine	LC/MS neg
	Urea cycle; arginine-, proline-, metabolism	arginine	LC/MS neg
		ornithine	GC/MS
		proline	GC/MS
	Creatine metabolism	creatine	LC/MS pos
	Polyamine metabolism	5-methylthioadenosine (MTA)	LC/MS pos
		putrescine	GC/MS
		spermidine	LC/MS pos
	Guanidino and acetamido metabolism	4-guanidinobutanoate	LC/MS pos
		glutathione, reduced (GSH)	LC/MS pos
	Glutathione metabolism	5-oxoproline	LC/MS pos
		glutathione, oxidized (GSSG)	LC/MS pos
		ophthalmate	LC/MS pos
		glycylvaline	LC/MS pos
		glycylproline	LC/MS pos

Fold Change									
HI C		TT C		TT HI		60 min 30 min			
30 min	60 min	30 min	60 min	30 min	60 min	C	MT	TT	
1.51	1.03	0.90	0.91	0.59	0.50	1.74	1.19	1.00	
1.78	1.08	1.35	0.77	0.76	0.71	1.86	1.13	1.07	
1.89	1.09	1.48	0.81	0.78	0.74	1.92	1.10	1.05	
0.46	1.06	0.75	0.92	0.83	0.87	0.61	0.98	1.00	
1.12	0.99	0.02	0.01	0.01	0.01	1.69	1.51	1.00	
2.40	1.26	0.85	0.38	0.35	0.30	1.95	1.03	0.88	
0.87	0.84	0.26	0.27	0.32	0.32	1.03	1.00	1.00	
1.86	1.08	1.44	0.86	0.77	0.80	1.79	1.04	1.07	
0.92	1.07	0.16	0.11	0.17	0.10	0.87	1.02	0.60	
0.55	1.20	0.10	0.19	0.17	0.16	0.47	0.96	0.94	
1.19	1.56	0.54	0.74	0.45	0.47	0.73	0.97	1.00	
1.82	2.03	2.02	2.37	1.11	1.17	0.60	0.67	0.71	
0.76	0.91	0.39	0.45	0.51	0.54	0.79	0.95	1.00	
1.07	1.11	0.53	0.31	0.49	0.28	1.04	1.09	0.62	
1.78	1.18	2.16	1.60	1.21	1.35	1.45	0.96	1.07	
2.08	1.30	2.66	1.60	1.28	1.23	1.35	0.84	0.81	
1.90	1.25	2.21	1.48	1.16	1.18	1.53	1.00	1.02	
1.88	1.27	2.14	1.46	1.14	1.15	1.51	1.02	1.03	
1.25	1.66	2.26	0.71	1.82	0.43	1.20	1.60	0.38	
2.03	0.72	3.45	2.88	1.70	3.99	1.75	0.52	1.46	
1.73	1.16	2.00	1.32	1.16	1.14	1.54	1.03	1.02	
1.00	1.05	0.48	0.38	0.48	0.36	0.97	1.02	0.76	
2.66	0.42	5.75	2.14	2.16	5.15	2.80	0.44	1.04	
3.48	0.42	6.62	2.19	1.90	5.18	2.44	0.30	0.81	
2.00	1.25	2.20	1.53	1.10	1.23	1.62	1.01	1.13	
1.93	1.27	2.13	1.44	1.10	1.14	1.59	1.04	1.08	
1.83	1.27	2.11	1.60	1.15	1.26	1.41	0.97	1.07	
2.72	0.53	5.28	2.49	1.94	4.73	1.96	0.38	0.93	
0.86	0.93	1.46	0.84	1.70	0.90	1.28	1.39	0.73	
0.94	0.90	1.00	0.33	1.07	0.35	1.69	1.62	0.55	
0.91	1.05	1.08	0.60	1.19	0.57	1.17	1.35	0.65	
1.00	1.06	0.32	0.07	0.32	0.06	1.32	1.40	0.27	
0.90	1.02	0.40	0.38	0.44	0.37	1.06	1.19	1.00	
1.43	1.33	0.94	0.56	0.88	0.42	1.19	1.11	0.71	
1.68	1.20	2.05	1.70	1.22	1.42	1.34	0.96	1.12	
0.99	1.12	1.02	0.99	1.03	0.88	1.00	1.14	0.97	
1.76	1.20	2.49	2.15	1.42	1.79	1.30	0.89	1.12	
1.60	1.21	1.41	1.02	0.88	0.85	1.31	0.99	0.96	
1.43	1.06	0.73	0.51	0.51	0.49	1.30	0.96	0.91	
1.01	1.11	0.23	0.17	0.22	0.15	0.90	0.99	0.65	
1.24	1.13	0.68	0.44	0.55	0.39	1.26	1.14	0.81	
1.05	1.05	0.31	0.15	0.30	0.14	1.02	1.01	0.47	
1.09	0.96	0.58	0.58	0.60	0.60	1.08	0.95	0.95	
1.14	0.93	1.00	0.60	0.88	0.65	1.28	1.05	0.77	
1.09	1.11	0.88	0.90	0.81	0.82	0.97	0.99	1.00	
1.94	1.23	2.36	1.61	1.22	1.32	1.43	0.90	0.98	
1.11	1.07	0.66	0.55	0.59	0.52	1.19	1.14	1.00	
1.20	1.00	0.82	0.86	0.68	0.86	0.95	0.79	1.00	
1.46	1.55	1.63	1.29	1.12	0.83	1.08	1.14	0.85	
0.96	1.16	0.75	1.02	0.78	0.88	0.80	0.96	1.09	

Peptide	Dipeptide	glycylisoleucine	LC/MS pos	0.86	1.14	0.78	0.95	0.91	0.83	0.81	1.08	0.98
		glycylleucine	LC/MS pos	1.09	1.10	0.76	0.85	0.70	0.49	0.98	0.99	0.71
		glycyltyrosine	LC/MS pos	1.05	1.35	1.09	0.67	1.03	0.50	0.86	1.10	0.53
		alanylvaline	LC/MS pos	1.10	0.97	1.42	0.62	1.29	0.64	0.90	0.79	0.39
		alanylleucine	LC/MS pos	1.20	1.21	0.78	0.84	0.65	0.70	1.05	1.06	1.14
		alanylisoleucine	LC/MS pos	1.16	1.07	0.64	0.95	0.95	0.88	1.14	1.05	0.92
		alanylphenylalanine	LC/MS pos	1.18	1.21	1.05	0.86	0.88	0.71	1.14	1.17	0.94
		leucylleucine	LC/MS pos	1.42	1.27	1.69	1.33	1.20	1.05	1.07	0.96	0.84
		threonylphenylalanine	LC/MS pos	1.15	1.30	1.03	1.20	0.90	0.93	0.95	1.07	1.10
		valylglutamate	LC/MS pos	1.26	1.16	1.12	1.20	0.89	1.03	1.03	0.96	1.11
		cysteinylglycine	LC/MS pos	0.96	1.31	0.64	0.87	0.66	0.67	0.73	0.99	1.00
		valylleucine	LC/MS pos	1.11	1.13	0.82	0.87	0.74	0.58	1.04	1.06	0.84
		arginylisoleucine	LC/MS pos	1.48	1.18	1.60	1.53	1.08	1.30	1.04	0.83	0.99
		arginylleucine	LC/MS pos	1.29	1.26	0.89	0.78	0.69	0.62	0.96	0.93	0.84
		isoleucylalanine	LC/MS pos	1.08	1.16	1.42	1.24	1.31	1.07	1.01	1.08	0.88
		isoleucylglycine	LC/MS pos	1.24	1.10	1.34	1.04	1.08	0.95	1.12	1.00	0.88
		isoleucylserine	LC/MS pos	0.60	1.35	0.96	1.18	1.60	0.88	0.58	1.31	0.72
		leucylalanine	LC/MS pos	1.14	1.09	2.07	1.75	1.81	1.60	1.25	1.19	1.05
		leucylaspartate	LC/MS pos	0.87	1.29	0.61	1.26	0.71	0.98	0.74	1.10	1.53
		leucylglutamate	LC/MS pos	1.26	1.14	1.28	0.90	1.02	0.79	1.36	1.22	0.94
		leucylglycine	LC/MS pos	1.04	0.97	1.50	0.83	1.43	0.86	1.15	1.07	0.64
		leucylphenylalanine	LC/MS pos	1.22	1.63	1.56	1.65	1.28	1.01	0.79	1.05	0.83
		leucylserine	LC/MS pos	0.91	1.44	1.42	1.31	1.56	0.91	0.91	1.43	0.84
		lysylisoleucine	LC/MS pos	1.33	1.15	1.43	1.53	1.08	1.33	1.05	0.91	1.12
		lysylleucine	LC/MS pos	1.23	1.22	0.78	0.82	0.63	0.66	0.99	0.97	1.04
		phenylalanylleucine*	LC/MS pos	0.95	1.30	1.34	0.96	1.40	0.74	0.86	1.17	0.67
		phenylalanylserine	LC/MS pos	1.21	1.14	1.30	1.03	1.07	0.91	1.04	0.98	0.83
		serylleucine	LC/MS pos	1.39	1.16	1.10	0.83	0.79	0.71	1.17	0.98	0.88
		serylphenylalanine	LC/MS pos	1.03	1.01	0.76	1.00	0.74	0.98	1.03	1.02	1.36
		threonylleucine	LC/MS pos	1.24	1.19	1.30	0.99	1.05	0.83	1.17	1.13	0.90
		tryptophyllleucine	LC/MS pos	1.15	1.35	1.27	1.75	1.10	1.30	0.78	0.91	1.08
		tyrosylalanine	LC/MS pos	0.95	1.30	1.95	2.34	2.04	1.79	1.07	1.46	1.28
		tyrosylleucine	LC/MS pos	1.02	1.34	0.83	0.68	0.81	0.51	0.85	1.12	0.70
		valylisoleucine	LC/MS pos	1.21	0.99	1.18	0.89	0.97	0.89	1.17	0.96	0.88
		serylisoleucine*	LC/MS pos	1.32	1.07	1.39	0.93	1.05	0.86	1.23	1.00	0.82
	gamma-glutamyl	gamma-glutamylvaline	LC/MS pos	1.28	1.07	0.37	0.20	0.29	0.19	1.15	0.96	0.64
		gamma-glutamylleucine	LC/MS pos	1.39	1.22	0.48	0.35	0.35	0.28	1.18	1.03	0.84
		gamma-glutamylisoleucine*	LC/MS pos	1.31	1.15	0.44	0.29	0.34	0.25	1.21	1.06	0.75
		gamma-glutamylcysteine	LC/MS pos	0.95	1.10	0.68	0.85	0.61	0.78	0.68	0.76	1.00
		gamma-glutamylmethionine	LC/MS pos	1.67	1.48	0.96	0.71	0.58	0.48	1.18	1.04	0.86
		gamma-glutamylglutamate	LC/MS pos	0.81	1.10	0.03	0.03	0.03	0.03	0.72	0.97	0.82
		gamma-glutamyltyrosine	LC/MS pos	1.24	0.76	0.80	0.63	0.65	0.82	1.18	0.73	0.92
		gamma-glutamylthreonine*	LC/MS pos	0.98	1.09	0.25	0.26	0.25	0.24	0.97	1.07	1.01
		gamma-glutamylalanine	LC/MS pos	1.12	1.14	0.75	0.70	0.67	0.62	1.08	1.09	1.00
		erythronate*	GC/MS	0.98	0.87	0.59	0.70	0.60	0.80	0.85	0.75	1.00
Carbohydrate	Aminosugars metabolism	galactitol (dulcitol)	GC/MS	0.70	0.65	0.03	0.05	0.04	0.02	2.05	1.92	1.22
		galactose	GC/MS	2.23	1.06	1.90	1.17	0.85	1.10	1.66	0.79	1.02
		lactose	GC/MS	2.28	1.07	3.49	2.27	1.53	2.12	1.53	0.72	1.00
		6'-sialyllactose	GC/MS	1.52	1.25	1.14	0.36	0.75	0.44	1.47	1.21	0.71
		mannitol	GC/MS	5.84	4.42	7.15	7.17	1.22	1.62	0.98	0.74	0.98
		maltotetraose	LC/MS neg	0.76	1.69	1.48	4.60	1.94	2.73	0.44	0.99	1.38
		maltopentaose	LC/MS neg	0.67	1.93	1.32	6.14	1.96	3.19	0.34	0.97	1.57
		glycerate	GC/MS	0.95	0.79	0.80	0.74	0.85	0.93	1.07	0.90	0.99
		glucose-6-phosphate (G6P)	GC/MS	0.57	0.75	0.15	0.41	0.26	0.54	0.37	0.49	1.00
		glucose 1-phosphate	GC/MS	1.05	1.06	1.07	0.92	1.02	0.87	1.08	1.10	0.94
	Glycolysis, gluconeogenesis, pyruvate metabolism	glucose	GC/MS	2.53	3.53	4.48	2.44	1.78	0.69	0.87	1.22	0.47
		Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate	LC/MS neg	0.79	1.24	0.27	0.33	0.34	0.27	0.67	1.04	0.81
		2-phosphoglycerate	GC/MS	1.39	1.62	1.28	0.68	0.92	0.42	1.31	1.53	0.70
		3-phosphoglycerate	GC/MS	3.56	2.08	4.85	0.99	1.30	0.48	2.44	1.42	0.52
		pyruvate	GC/MS	0.98	1.94	1.38	10.80	1.41	5.55	0.54	1.08	4.25
		lactate	GC/MS	1.34	1.01	0.94	0.72	0.70	0.72	1.29	0.97	0.99
		6-phosphogluconate	GC/MS	0.64	0.79	0.19	0.25	0.30	0.37	0.65	0.80	1.00
		arabitol	GC/MS	0.89	1.20	0.50	0.65	0.57	0.54	0.77	1.04	1.00

0.4209	0.2386	0.4142	0.3145	0.1620	0.0224	0.7335	0.0984	0.5385	0.1251	0.2513	0.0244	0.2342	0.3608	0.6712	0.9875	0.9041	1.0000	0.3581	0.0121	0.6033	0.5983	0.5038	0.4338
0.3229	0.1987	0.2218	0.2401	0.0014	0.0003	< 0.001	0.0000	< 0.001	0.0001	< 0.001	0.0000	0.8358	0.6963	0.9718	0.9875	< 0.001	0.0009	< 0.001	0.0000	0.0121	0.0398	0.0052	0.0140
0.6549	0.3153	0.3539	0.2926	0.9758	0.1079	0.2017	0.0317	0.6768	0.1484	0.0333	0.0040	0.7500	0.6673	0.8662	0.9875	0.1088	0.3546	0.1875	0.0066	0.3044	0.4034	0.4187	0.3863
0.6037	0.3009	0.9329	0.4710	0.1924	0.0256	0.1293	0.0214	0.4231	0.1049	0.1107	0.0118	0.8778	0.6963	0.5565	0.9875	0.0053	0.0246	0.8290	0.0265	0.0373	0.0898	0.1064	0.1499
0.2437	0.1618	0.2991	0.2690	0.2016	0.0265	0.1474	0.0241	0.0193	0.0076	0.0172	0.0022	0.6938	0.6350	0.7935	0.9875	0.8320	1.0000	0.0058	0.0003	0.6170	0.5983	0.9910	0.6145
0.4970	0.2668	0.7227	0.4064	0.0575	0.0084	0.0071	0.0015	0.0129	0.0054	0.0030	0.0005	0.5685	0.5759	0.8065	0.9875	0.7165	0.9721	< 0.001	0.0000	0.7935	0.6243	0.7960	0.5533
0.2802	0.1801	0.2055	0.2326	0.8049	0.0909	0.5025	0.0718	0.4010	0.1015	0.0590	0.0066	0.5449	0.5759	0.4255	0.9875	0.7544	0.9862	0.1182	0.0044	0.5283	0.5648	0.6997	0.5317
0.0456	0.0494	0.2244	0.2401	0.0061	0.0011	0.1695	0.0276	0.3780	0.0961	0.8671	0.0708	0.6204	0.5985	0.7219	0.9875	0.2869	0.6372	0.0122	0.0005	0.5894	0.5966	0.5389	0.4516
0.1992	0.1446	0.0367	0.1698	0.6928	0.0803	0.1150	0.0193	0.3665	0.0939	0.5692	0.0505	0.6762	0.6276	0.6427	0.9875	0.4242	0.8005	0.0612	0.0023	0.6240	0.5983	0.6702	0.5169
0.0629	0.0617	0.2316	0.2408	0.3939	0.0480	0.2704	0.0412	0.2898	0.0760	0.9220	0.0744	0.7666	0.6692	0.6760	0.9875	0.5805	0.8939	0.0966	0.0036	0.8028	0.6243	0.7735	0.5500
0.6083	0.3009	< 0.001	0.0322	< 0.001	0.0000	0.0803	0.0140	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0018	0.8339	0.9875	1.0000	1.0000	< 0.001	0.0000	0.0116	0.0388	0.0055	0.0144
0.3971	0.2303	0.3057	0.2697	0.1755	0.0239	0.0031	0.0007	0.0333	0.0121	< 0.001	0.0000	0.7789	0.6746	0.6438	0.9875	0.1220	0.3561	< 0.001	0.0000	0.6278	0.5983	0.2873	0.3093
0.1369	0.1079	0.4540	0.3228	0.0625	0.0091	0.0409	0.0077	0.6825	0.1484	0.1745	0.0178	0.8413	0.6963	0.3367	0.9875	0.9962	1.0000	0.0263	0.0011	0.5030	0.5515	0.7658	0.5500
0.1096	0.0929	0.0987	0.1829	0.2925	0.0371	0.1712	0.0278	0.0115	0.0049	0.0046	0.0007	0.6147	0.5973	0.6539	0.9875	0.4068	0.7834	0.0015	0.0001	0.3069	0.4034	0.9565	0.6079
0.8058	0.3507	0.3149	0.2697	0.0425	0.0064	0.2242	0.0348	0.0704	0.0232	0.8267	0.0678	0.9578	0.7153	0.4140	0.9875	0.4087	0.7834	0.0726	0.0027	0.9800	0.6769	0.5063	0.4338
0.2184	0.1535	0.6780	0.3972	0.1085	0.0153	0.9992	0.1298	0.6904	0.1495	0.6787	0.0573	0.4522	0.5110	0.9373	0.9875	0.3760	0.7534	0.4058	0.0136	0.9012	0.6554	0.5093	0.4338
0.0018	0.0057	0.0643	0.1730	0.7994	0.0909	0.2902	0.0440	0.0035	0.0017	0.3995	0.0371	0.0013	0.0101	0.0855	0.5745	0.0301	0.1179	0.2508	0.0087	0.0245	0.0636	0.0021	0.0069
0.5136	0.2710	0.5358	0.3506	0.0056	0.0010	0.0408	0.0077	0.0255	0.0098	0.1381	0.0145	0.3940	0.4932	0.4130	0.9875	0.9885	1.0000	0.0032	0.0001	0.3399	0.4189	0.7810	0.5503
0.5384	0.2786	0.3118	0.2697	0.0364	0.0055	0.8211	0.1088	0.1243	0.0374	0.4289	0.0391	0.2334	0.3608	0.6675	0.9875	0.2332	0.5471	0.2141	0.0075	0.8037	0.6243	0.2311	0.2596
0.0740	0.0712	0.2978	0.2690	0.0728	0.0105	0.5139	0.0728	0.9934	0.2023	0.0970	0.0105	0.0386	0.1105	0.1787	0.8628	0.7293	0.9789	0.1360	0.0050	0.0750	0.1425	0.2069	0.2416
0.7057	0.3242	0.8504	0.4452	0.0384	0.0058	0.3000	0.0453	0.0830	0.0267	0.3936	0.0367	0.2996	0.4061	0.6304	0.9875	0.0384	0.1410	0.6966	0.0227	0.7137	0.6131	0.0681	0.1067
0.3800	0.2243	0.1274	0.1968	0.1183	0.0165	0.4641	0.0672	0.4750	0.1135	0.4119	0.0381	0.5045	0.5537	0.9943	0.9945	0.1333	0.3678	0.1637	0.0059	0.2114	0.3144	0.5504	0.4587
0.7015	0.3242	0.0875	0.1767	0.0318	0.0049	0.1756	0.0282	0.0135	0.0056	0.7033	0.0586	0.9374	0.7120	0.0474	0.4577	0.3452	0.7281	0.0485	0.0019	0.5510	0.5818	0.1060	0.1499
0.0135	0.0192	0.2422	0.2462	0.0036	0.0007	0.0011	0.0003	0.5764	0.1309	0.0191	0.0024	0.6159	0.5973	0.3474	0.9875	0.3333	0.7089	< 0.001	0.0000	0.7591	0.6172	0.3730	0.3659
0.0405	0.0449	0.0649	0.1730	0.0123	0.0020	0.0597	0.0109	< 0.001	0.0000	< 0.001	0.0001	0.8889	0.6963	0.7130	0.9875	0.5606	0.8795	< 0.001	0.0000	0.9650	0.6718	0.7790	0.5503
0.7879	0.3457	0.3567	0.2926	0.1136	0.0159	0.5973	0.0836	0.1834	0.0512	0.1532	0.0158	0.7975	0.6831	0.9875	0.0226	0.0930	0.6425	0.0211	0.1990	0.3012	0.1312	0.1738	
0.2184	0.1535	0.5269	0.3468	0.1680	0.0231	0.9238	0.1209	0.8761	0.1843	0.5904	0.0515	0.6660	0.6257	0.8549	0.9875	0.3834	0.7578	0.3775	0.0127	0.7168	0.6131	0.6495	0.5060
0.0021	0.0062	0.1301	0.1968	0.4179	0.0507	0.0581	0.0106	0.0152	0.0062	0.0016	0.0003	0.1071	0.2180	0.8447	0.9875	0.2656	0.6116	< 0.001	0.0000	0.8477	0.6379	0.1504	0.1896
0.8858	0.3717	0.8070	0.4409	0.1015	0.0144	0.9508	0.1240	0.0769	0.0250	0.7598	0.0628	0.9717	0.7153	0.9480	0.9875	0.1216	0.3561	0.2856	0.0099	0.3546	0.4299	0.4419	0.3959
0.4058	0.2314	0.6546	0.3891	0.7051	0.0812	0.7272	0.0980	0.6473	0.1432	0.4282	0.0391	0.5616	0.5759	0.8467	0.9875	0.8842	1.0000	0.5841	0.0193	0.7164	0.6131	0.8739	0.5814
0.5294	0.2768	0.0816	0.1730	0.1776	0.0241	0.0034	0.0008	0.4601	0.1109	0.1653	0.0169	0.1329	0.2564	0.7102	0.9875	0.7634	0.9928	0.0117	0.0005	0.3568	0.4299	0.4254	0.3879
0.7718	0.3431	0.1179	0.1934	< 0.001	0.0002	< 0.001	0.0000	< 0.001	0.0002	0.0058	0.0008	0.8268	0.6963	0.0430	0.4322	0.2770	0.6310	< 0.001	0.0000	0.0566	0.1240	0.4127	0.3863
0.7665	0.3431	0.0538	0.1730	0.1819	0.0244	0.0146	0.0029	0.1069	0.0329	< 0.001	0.0000	0.3618	0.4631	0.4328	0.9875	0.0388	0.1410	< 0.001	0.0000	0.1933	0.2952	0.1277	0.1708
0.2200	0.1535	0.8357	0.4416	0.3555	0.0442	0.4029	0.0600	0.7538	0.1612	0.5271	0.0470	0.2997	0.4061	0.6860	0.9875	0.4702	0.8253	0.7163	0.0232	0.9622	0.6718	0.4146	0.3863
0.1513	0.1166	0.7928	0.4374	0.1802	0.0243	0.6697	0.0921	0.9199	0.1904	0.4922	0.0447	0.2931	0.4058	0.8887	0.9875	0.4681	0.8253	0.4761	0.0158	0.9108	0.6554	0.4386	0.3953
0.0391	0.0438	0.4858	0.3320	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.2456	0.3663	0.7784	0.9875	< 0.001	0.0054	< 0.001	0.0000	0.1120	0.1975	0.0057	0.0144
0.0072	0.0124	0.0971	0.1829	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.1531	0.2724	0.7925	0.9875	0.1190	0.3561	< 0.001	0.0000	0.9433	0.6696	0.1095	0.1530
0.0129	0.0189	0.1630	0.2107	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.0689	0.1636	0.5175	0.9875	0.0263	0.1049	< 0.001	0.0000	0.9119	0.6554	0.0173	0.0368
0.5775	0.2974	0.3654	0.2977	< 0.001	0.0000	0.1010	0.0171	< 0.001	0.0000	0.0147	0.0019	< 0.001	0.0031	0.0118	0.2119	1.0000	1.0000	< 0.001	0.0000	< 0.001	0.0042	0.0209	0.0432
< 0.001	0.0021	0.0039	0.0615	0.7217	0.0828	0.0140	0.0028	< 0.001	0.0001	< 0.001	0.0000	0.2324	0.3608	0.7975	0.9875	0.2979	0.6503	< 0.001	0.0000	0.8102	0.6243	0.2857	0.3093
0.0863	0.0771	0.3689	0.2985	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.0072	0.0364	0.8157	0.9875	0.1193	0.3561	< 0.001	0.0000	0.0107	0.0372	0.1823	0.2208
0.1491	0.1158	0.1452	0.2023	0.2112	0.0274	0.0102	0.0021	0.0105	0.0046	0.2118	0.0212	0.3208	0.4230	0.0590	0.4935	0.6285	0.9390	0.0107	0.0005	0.4080	0.4684	0.1278	0.1708
0.8098	0.3507	0.3220	0.2713	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.6959	0.6350	0.3988	0.9875	0.7695	0.9950	< 0.001	0.0000	0.6648	0.5983	0.6781	0.5178
0.2357	0.1584	0.2236	0.2401	0.0135	0.0022	0.0019	0.0005	< 0.001	0.0004	< 0.001	0.0000	0.4224	0.4932	0.4042	0.9875	1.0000	1.0000	< 0.001	0.0000	0.3459	0.4226	0.7952	0.5533
0.9399	0.3887	0.1960	0.2318	< 0.001	0.0000	0.0020	0.0005	< 0.001	0.0000	0.0431	0.0050	0.1053	0.2169	0.0072	0.1898	1.0000	1.0000	< 0.001	0.0000	0.0135	0.0419	0.1358	0.1777
0.2246	0.1542	0.1039	0.1829	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	<													

Energy	Nucleotide sugars, pentose metabolism	sedoheptulose-7-phosphate	GC/MS	2.28	1.15	15.14	14.74	6.65	12.82	1.31	0.66	1.28
		ribose 5-phosphate	GC/MS	1.41	2.15	2.89	4.41	2.05	2.05	1.10	1.67	1.68
		Isobar: ribulose 5-phosphate, xylulose 5-phosphate	GC/MS	2.28	2.76	4.42	3.41	1.94	1.23	1.41	1.71	1.09
		UDP-glucose	GC/MS	0.93	0.90	0.55	0.52	0.60	0.58	1.06	1.03	1.00
	Nucleotide sugars	UDP-galactose	GC/MS	1.22	1.31	0.59	0.74	0.48	0.57	0.79	0.85	1.00
		citrate	GC/MS	1.37	1.10	0.53	0.45	0.39	0.42	1.35	1.08	1.16
	Krebs cycle	alpha-ketoglutarate	LC/MS neg	1.17	0.57	0.31	0.69	0.26	1.21	0.70	0.34	1.57
		succinate	GC/MS	2.16	1.21	1.77	0.75	0.82	0.62	2.06	1.16	0.88
		fumarate	GC/MS	0.94	0.97	0.17	0.29	0.18	0.36	0.99	1.02	1.72
		malate	GC/MS	1.18	1.00	0.10	0.03	0.09	0.03	1.56	1.33	0.51
	Oxidative phosphorylation	phosphate	GC/MS	1.51	1.07	1.97	1.67	1.30	1.57	1.32	0.93	1.12
		linoleate (18:2n6)	LC/MS neg	1.04	1.08	1.50	1.51	1.44	1.40	0.98	1.02	0.98
Lipid	Essential fatty acid	linolenate [alpha or gamma, (18:3n3 or 6)]	LC/MS neg	1.04	1.11	1.60	1.77	1.54	1.59	0.93	0.99	1.02
		dihomo-linolenate (20:3n3 or n6)	LC/MS neg	0.99	1.05	2.06	1.87	2.08	1.79	1.00	1.06	0.91
		docosapentaenoate (n3 DPA; 22:5n3)	LC/MS neg	1.03	1.03	1.74	1.97	1.69	1.92	1.01	1.00	1.14
		docosahexaenoate (DHA; 22:6n3)	LC/MS neg	1.10	1.01	1.50	1.67	1.36	1.65	1.06	0.97	1.18
	Medium chain fatty acid	laurate (12:0)	LC/MS neg	1.26	1.18	1.68	1.71	1.34	1.45	1.05	0.98	1.06
		myristate (14:0)	LC/MS neg	1.24	1.13	1.71	1.71	1.38	1.52	1.07	0.97	1.07
	Long chain fatty acid	myristoleate (14:1n5)	LC/MS neg	1.32	0.97	1.74	1.66	1.31	1.70	1.32	0.97	1.26
		pentadecanoate (15:0)	LC/MS neg	1.25	1.09	1.94	1.82	1.56	1.67	1.06	0.93	0.99
		palmitate (16:0)	LC/MS neg	1.17	1.16	1.78	1.74	1.52	1.50	0.99	0.98	0.96
		palmitoleate (16:1n7)	LC/MS neg	1.16	1.13	1.77	1.72	1.53	1.52	1.06	1.04	1.03
		margarate (17:0)	LC/MS neg	1.15	1.21	2.15	2.41	1.86	1.99	0.97	1.03	1.09
		10-heptadecenoate (17:1n7)	LC/MS neg	1.24	1.10	1.99	1.93	1.61	1.76	1.07	0.95	1.03
		stearate (18:0)	LC/MS neg	1.15	1.29	1.91	2.30	1.66	1.79	0.89	0.99	1.07
		oleate (18:1n9)	GC/MS	1.25	1.16	1.51	1.57	1.21	1.36	0.94	0.87	0.98
		cis-vaccenate (18:1n7)	GC/MS	1.20	1.39	1.33	1.67	1.11	1.21	0.86	1.00	1.08
		nonadecanoate (19:0)	LC/MS neg	1.40	1.05	2.37	2.51	1.70	2.39	0.99	0.75	1.05
		10-nonadecenoate (19:1n9)	LC/MS neg	1.02	1.16	1.88	2.29	1.83	1.96	0.88	1.00	1.07
		arachidate (20:0)	GC/MS	1.14	1.32	1.43	1.97	1.26	1.49	0.77	0.90	1.07
		eicosenoate (20:1n9 or 11)	LC/MS neg	1.01	1.28	1.93	2.80	1.91	2.19	0.81	1.03	1.18
		dihomo-linoleate (20:2n6)	LC/MS neg	0.95	1.13	1.98	2.27	2.09	2.00	0.91	1.09	1.05
		arachidonate (20:4n6)	LC/MS neg	1.04	1.08	1.69	2.00	1.63	1.85	1.01	1.05	1.20
		behenate (22:0)	GC/MS	1.43	1.46	1.75	2.53	1.22	1.73	0.92	0.94	1.33
		docosadienoate (22:2n6)	LC/MS neg	1.18	1.19	2.26	2.66	1.93	2.23	0.96	0.98	1.13
		adrenate (22:4n6)	LC/MS neg	1.52	0.80	2.55	2.55	1.68	3.20	1.08	0.57	1.08
		lignocerate (24:0)	GC/MS	0.96	1.01	1.02	1.16	1.06	1.15	0.90	0.95	1.03
	Fatty acid, ester	n-Butyl Oleate	GC/MS	1.38	1.50	1.09	1.74	0.79	1.17	0.86	0.93	1.37
	Fatty acid, dicarboxylate	2-hydroxyglutarate	GC/MS	0.84	0.70	0.12	0.19	0.15	0.27	0.72	0.40	1.10
		azelate (nonanedioate)	LC/MS neg	1.27	1.03	2.36	1.99	1.87	1.94	1.10	0.90	0.93
	Fatty acid, branched	13-methylmyristic acid	LC/MS neg	1.42	1.21	1.65	1.64	1.16	1.36	1.18	1.00	1.18
		15-methylpalmitate (isobar with 2-methylpalmitate)	LC/MS neg	1.13	1.20	1.67	1.85	1.47	1.54	0.92	0.97	1.02
	Fatty acid metabolism (also BCAA metabolism)	propionylcarnitine	LC/MS pos	0.98	1.03	0.18	0.04	0.18	0.04	1.22	1.29	0.29
		butyrylcarnitine	LC/MS pos	0.87	0.97	0.16	0.14	0.18	0.14	0.92	1.02	0.80
	Carnitine metabolism	deoxycarnitine	LC/MS pos	1.16	1.04	0.96	0.88	0.83	0.84	1.09	0.98	1.00
		carnitine	LC/MS pos	0.71	1.11	0.07	0.06	0.09	0.05	0.62	0.97	0.55
		3-dehydrocarnitine*	LC/MS pos	0.97	1.01	0.12	0.10	0.13	0.10	1.01	1.05	0.81
		acetylcarnitine	LC/MS pos	1.34	1.07	0.25	0.22	0.19	0.21	0.77	0.62	0.69
		hexanoylcarnitine	LC/MS pos	0.78	0.99	0.54	0.82	0.69	0.83	0.66	0.84	1.00
		octanoylcarnitine	LC/MS pos	0.84	1.04	0.62	0.71	0.74	0.68	0.88	1.09	1.00
		palmitoylcarnitine	LC/MS pos	2.11	1.06	0.60	0.15	0.29	0.15	1.62	0.91	0.47
		stearoylcarnitine	LC/MS pos	1.75	1.05	0.70	0.25	0.40	0.24	1.48	0.89	0.54
		oleoylcarnitine	LC/MS pos	1.99	0.93	0.37	0.09	0.18	0.10	1.67	0.87	0.47
	Glycerolipid metabolism	choline phosphate	LC/MS pos	0.69	1.25	0.13	0.23	0.19	0.18	0.54	0.97	0.96
		choline	LC/MS pos	1.14	1.19	1.04	1.25	0.92	1.05	1.01	1.06	1.21
		glycerol 3-phosphate (G3P)	GC/MS	0.91	0.94	0.11	0.07	0.13	0.07	0.92	0.95	0.55
		glycerophosphorylcholine (GPC)	LC/MS pos	0.79	1.16	0.36	0.28	0.46	0.24	0.63	0.93	0.49
		cytidine 5'-diphosphocholine	LC/MS pos	0.85	1.00	0.29	0.29	0.34	0.29	0.71	0.84	0.72
	Inositol metabolism	myo-inositol	GC/MS	0.90	0.88	0.04	0.03	0.04	0.03	1.09	1.06	0.79
		inositol 1-phosphate (1IP)	GC/MS	0.89	1.11	0.95	1.36	1.06	1.23	0.75	0.93	1.09
		scyllo-inositol	GC/MS	0.90	0.65	0.45	0.35	0.50	0.54	1.29	0.92	1.00
		1-palmitoylglycerophosphoethanolamine	LC/MS pos	2.21	1.14	3.94	0.97	1.78	0.85	1.74	0.90	0.43
		2-palmitoylglycerophosphoethanolamine*	LC/MS pos	1.74	1.15	2.51	0.68	1.44	0.59	1.41	0.94	0.38
		2-palmitoleoylglycerophosphoethanolamine*	LC/MS pos	1.53	1.35	2.17	0.84	1.41	0.62	1.14	1.00	0.44

0.0508	0.0533	0.8433	0.4434	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.5718	0.5759	0.2116	0.9444	0.5771	0.8939	< 0.001	0.0000	0.9340	0.6657	0.3353	0.3397
0.4671	0.2576	0.0847	0.1766	0.0110	0.0018	< 0.001	0.0001	0.0549	0.0183	0.0233	0.0029	0.8880	0.6963	0.2412	0.9574	0.1212	0.3561	< 0.001	0.0000	0.1013	0.1825	0.5719	0.4621
0.0567	0.0578	0.0260	0.1698	0.0013	0.0003	0.0031	0.0007	0.1155	0.0351	0.3706	0.0347	0.4044	0.4932	0.2342	0.9574	0.6219	0.9346	< 0.001	0.0000	0.1511	0.2477	0.8788	0.5822
0.4039	0.2314	0.3157	0.2697	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.5922	0.5868	0.7162	0.9875	1.0000	1.0000	< 0.001	0.0000	0.6038	0.5983	0.9263	0.6005
0.3024	0.1919	0.0684	0.1730	0.0027	0.0005	0.0817	0.0142	< 0.001	0.0001	0.0011	0.0002	0.1381	0.2616	0.5034	0.9875	1.0000	1.0000	< 0.001	0.0000	0.2135	0.3149	0.5618	0.4619
0.0067	0.0117	0.4268	0.3201	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.0084	0.0393	0.4828	0.9875	0.2004	0.4884	< 0.001	0.0000	0.0093	0.0345	0.3072	0.3217
0.7780	0.3440	0.0624	0.1730	0.0061	0.0011	0.4834	0.0697	0.0119	0.0051	0.2260	0.0224	0.3235	0.4235	0.0132	0.2203	0.2102	0.5025	0.0461	0.0018	0.1789	0.2782	0.0326	0.0608
0.0043	0.0088	0.6197	0.3791	0.0276	0.0043	0.2022	0.0317	0.4300	0.1057	0.0822	0.0091	0.0036	0.0218	0.5642	0.9875	0.6735	0.9445	0.0449	0.0018	0.0621	0.1301	0.0440	0.0785
0.5949	0.3009	0.8151	0.4409	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.9054	0.7062	0.8567	0.9875	< 0.001	0.0009	< 0.001	0.0000	0.0133	0.0419	0.0043	0.0120
0.3511	0.2097	0.9879	0.4842	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.0088	0.0393	0.0673	0.5278	< 0.001	0.0014	< 0.001	0.0000	0.8102	0.6243	< 0.001	0.0003
< 0.001	0.0037	0.5063	0.3403	< 0.001	0.0000	< 0.001	0.0000	0.0204	0.0080	< 0.001	0.0001	0.0198	0.0716	0.5631	0.9875	0.3016	0.6526	< 0.001	0.0000	0.0998	0.1816	0.1141	0.1566
0.4914	0.2652	0.1928	0.2318	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.6963	0.6350	0.8076	0.9875	0.8100	1.0000	< 0.001	0.0000	0.8229	0.6256	0.8943	0.5899
0.6955	0.3234	0.3095	0.2697	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0002	< 0.001	0.0000	0.5007	0.5529	0.9672	0.9875	0.6630	0.9402	< 0.001	0.0000	0.8711	0.6460	0.7303	0.5500
0.8345	0.3568	0.4522	0.3228	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.9370	0.7120	0.3018	0.9875	0.1132	0.3561	< 0.001	0.0000	0.7713	0.6224	0.1761	0.2150
0.6659	0.3170	0.7697	0.4266	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.8574	0.6963	0.9680	0.9875	0.1110	0.3561	< 0.001	0.0000	0.2894	0.3867	0.4614	0.4064
0.2188	0.1535	0.9005	0.4614	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0003	< 0.001	0.0000	0.4219	0.4932	0.7524	0.9875	0.0326	0.1260	< 0.001	0.0000	0.1234	0.2132	0.2073	0.2416
0.0242	0.0301	0.1027	0.1829	< 0.001	0.0000	< 0.001	0.0000	0.0072	0.0032	< 0.001	0.0002	0.6278	0.6025	0.8287	0.9875	0.5388	0.8795	< 0.001	0.0000	0.6098	0.5983	0.8159	0.5622
0.0080	0.0128	0.1329	0.1969	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0001	< 0.001	0.0000	0.3326	0.4323	0.7295	0.9875	0.3782	0.7534	< 0.001	0.0000	0.3837	0.4554	0.5788	0.4621
0.0473	0.0503	0.9804	0.4833	< 0.001	0.0001	0.0024	0.0006	0.0817	0.0264	0.0023	0.0003	0.0563	0.1393	0.9135	0.9875	0.1492	0.3976	< 0.001	0.0000	0.0623	0.1301	0.3139	0.3265
0.0596	0.0596	0.4835	0.3320	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0004	< 0.001	0.0000	0.5249	0.5693	0.5409	0.9875	0.9935	1.0000	< 0.001	0.0000	0.9924	0.6769	0.6743	0.5175
0.0340	0.0390	0.0537	0.1730	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.9346	0.7120	0.7649	0.9875	0.6570	0.9402	< 0.001	0.0000	0.6341	0.5983	0.9666	0.6079
0.0261	0.0313	0.0440	0.1730	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.4012	0.4932	0.5483	0.9875	0.6068	0.9230	< 0.001	0.0000	0.2631	0.3572	0.9707	0.6079
0.2620	0.1706	0.1542	0.2062	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.9639	0.7153	0.7842	0.9875	0.4337	0.8054	< 0.001	0.0000	0.5586	0.5845	0.8360	0.5709
0.0256	0.0311	0.3562	0.2926	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.3975	0.4932	0.5685	0.9875	0.6366	0.9399	< 0.001	0.0000	0.6639	0.5983	0.5807	0.4621
0.1216	0.0975	0.0105	0.0919	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.2058	0.3339	0.8997	0.9875	0.4089	0.7834	< 0.001	0.0000	0.7376	0.6140	0.3336	0.3397
0.1218	0.0975	0.2405	0.2462	0.0092	0.0015	0.0023	0.0006	0.2312	0.0630	0.0374	0.0045	0.5396	0.5759	0.3165	0.9875	0.9624	1.0000	< 0.001	0.0000	0.3381	0.4189	0.7882	0.5529
0.2221	0.1535	0.0185	0.1419	0.0854	0.0122	< 0.001	0.0003	0.5936	0.1343	0.2319	0.0229	0.1976	0.3262	0.9602	0.9875	0.5313	0.8795	0.0021	0.0001	0.6728	0.5994	0.3863	0.3696
0.0835	0.0753	0.8364	0.4416	< 0.001	0.0000	< 0.001	0.0000	0.0044	0.0021	< 0.001	0.0000	0.9358	0.7120	0.1063	0.6350	0.8106	1.0000	< 0.001	0.0000	0.3897	0.4554	0.3630	0.3584
0.9014	0.3743	0.1449	0.2023	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.1942	0.3262	0.9638	0.9875	0.4561	0.8139	< 0.001	0.0000	0.7613	0.6172	0.3388	0.3403
0.3997	0.2305	0.0800	0.1730	0.0487	0.0072	< 0.001	0.0001	0.2346	0.0634	0.0262	0.0032	0.0997	0.2076	0.4655	0.9875	0.6861	0.9568	< 0.001	0.0000	0.2493	0.3494	0.3403	0.3403
0.8876	0.3717	0.0314	0.1698	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.0715	0.1636	0.7993	0.9875	0.1249	0.3589	< 0.001	0.0000	0.9826	0.6769	0.0647	0.1024
0.5155	0.2710	0.1501	0.2029	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.2875	0.4058	0.3001	0.9875	0.5585	0.8795	< 0.001	0.0000	0.7472	0.6172	0.2976	0.3160
0.6143	0.3019	0.2881	0.2690	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.8851	0.6963	0.4773	0.9875	0.0166	0.0706	< 0.001	0.0000	0.0583	0.1263	0.2204	0.2512
0.0748	0.0712	0.1074	0.1861	0.0257	0.0040	< 0.001	0.0000	0.6103	0.1362	0.0095	0.0013	0.7574	0.6692	0.6198	0.9875	0.0844	0.2863	< 0.001	0.0000	0.5748	0.5853	0.2162	0.2501
0.1817	0.1348	0.1032	0.1829	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.6380	0.6059	0.8759	0.9875	0.1951	0.4828	< 0.001	0.0000	0.6903	0.6025	0.4073	0.3849
0.2582	0.1692	0.4835	0.3320	0.0069	0.0012	0.0093	0.0020	0.0847	0.0269	0.0017	0.0003	0.9241	0.7120	0.0888	0.5745	0.9758	1.0000	< 0.001	0.0000	0.3339	0.4189	0.3517	0.3495
0.7327	0.3331	0.6993	0.4020	0.9911	0.1091	0.3976	0.0595	0.7411	0.1598	0.6423	0.0551	0.4183	0.4932	0.9312	0.9875	0.9613	1.0000	0.7973	0.0256	0.6233	0.5983	0.8038	0.5563
0.2515	0.1659	0.1290	0.1968	0.6867	0.0801	0.0680	0.0121	0.4507	0.1097	0.7376	0.0612	0.7343	0.6626	0.9575	0.9875	0.2576	0.5987	0.1343	0.0049	0.6200	0.5983	0.5534	0.4587
0.4589	0.2545	0.0628	0.1730	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0001	0.2936	0.4058	0.0323	0.3528	0.7143	0.9721	< 0.001	0.0000	0.0987	0.1816	0.1951	0.2326
0.3021	0.1919	0.9467	0.4748	0.0022	0.0004	0.0034	0.0008	0.0256	0.0098	0.0040	0.0006	0.6064	0.5944	0.6461	0.9875	0.7373	0.9844	< 0.001	0.0000	0.8210	0.6256	0.7614	0.5500
< 0.001	0.0030	0.0706	0.1730	< 0.001	0.0000	< 0.001	0.0000	0.1794	0.0507	0.0024	0.0004	0.0699	0.1636	0.9160	0.9875	0.0694	0.2453	< 0.001	0.0000	0.0435	0.1019	0.2805	0.3062
0.1556	0.1181	0.0556	0.1730	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0001	< 0.001	0.0000	0.4417	0.5080	0.8150	0.9875	0.7918	0.9996	< 0.001	0.0000	0.6681	0.5983	0.7617	0.5500
0.7545	0.3399	0.7196	0.4064	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.0172	0.0670	0.0035	0.1251	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0002	< 0.001	0.0000
0.4831	0.2625	0.8636	0.4483	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.6635	0.6257	0.9226	0.9875	0.1821	0.4658	< 0.001	0.0000	0.3316	0.4189	0.5813	0.4621
0.0026	0.0064	0.3084	0.2697	0.3182	0.0402	0.0059	0.0013	< 0.001	0.0001	< 0.001	0.0001	0.0570	0.1393	0.7557	0								

0.3421	0.2055	0.4693	0.3299	0.0016	0.0003	0.0049	0.0011	0.0157	0.0064	0.0267	0.0033	0.8370	0.6963	0.9794	0.9912	0.7925	0.9996	< 0.001	0.0000	0.9616	0.6718	0.9455	0.6079
0.4463	0.2502	0.4131	0.3145	0.0047	0.0009	0.4181	0.0620	0.0279	0.0104	0.1106	0.0118	0.5677	0.5759	0.3143	0.9875	0.1000	0.3303	0.0129	0.0005	0.2246	0.3256	0.2702	0.2971
0.7693	0.3431	0.3066	0.2697	0.0026	0.0005	0.0683	0.0121	0.0053	0.0024	0.0069	0.0010	0.4146	0.4932	0.6140	0.9875	0.5408	0.8795	< 0.001	0.0000	0.8634	0.6450	0.5297	0.4487
0.0190	0.0240	0.5908	0.3752	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0001	< 0.001	0.0001	0.0945	0.2014	0.8204	0.9875	0.4552	0.8139	< 0.001	0.0000	0.6678	0.5983	0.1977	0.2339
0.3061	0.1928	0.2189	0.2401	< 0.001	0.0001	< 0.001	0.0001	0.0050	0.0023	0.0109	0.0015	0.8839	0.6963	0.7188	0.9875	0.9720	1.0000	< 0.001	0.0000	0.7547	0.6172	0.9725	0.8079
0.0138	0.0194	0.0636	0.1730	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0002	0.0018	0.0003	0.4160	0.4932	0.9081	0.9875	0.5951	0.9108	< 0.001	0.0000	0.8168	0.6256	0.6325	0.4977
0.0131	0.0189	0.2879	0.2690	< 0.001	0.0001	0.0191	0.0038	0.1686	0.0482	0.0014	0.0002	0.2886	0.4058	0.6170	0.9875	< 0.001	0.0001	0.0001	0.0017	0.0087	0.0331	< 0.001	0.0012
0.0324	0.0380	0.4078	0.3135	0.0011	0.0002	0.0125	0.0025	0.1667	0.0481	0.0017	0.0003	0.2240	0.3540	0.8586	0.9875	< 0.001	0.0002	0.1009	0.0038	0.0270	0.0680	< 0.001	0.0016
0.0057	0.0103	0.2563	0.2585	< 0.001	0.0000	0.0106	0.0022	0.1591	0.0473	< 0.001	0.0001	0.1666	0.2900	0.6597	0.9875	< 0.001	0.0000	0.0226	0.0009	0.0099	0.0359	< 0.001	0.0005
0.1594	0.1200	0.1416	0.2023	< 0.001	0.0001	0.2172	0.0339	0.0114	0.0049	0.0102	0.0014	0.2711	0.3976	0.2441	0.9574	< 0.001	0.0014	0.0746	0.0028	0.2570	0.3530	< 0.001	0.0027
< 0.001	0.0032	0.0786	0.1730	< 0.001	0.0000	0.0101	0.0021	0.2522	0.0678	< 0.001	0.0000	0.2055	0.3339	0.4831	0.9875	< 0.001	0.0000	0.0019	0.0001	0.0022	0.0109	< 0.001	0.0002
0.0014	0.0048	0.5235	0.3468	< 0.001	0.0000	0.0016	0.0004	0.3223	0.0841	< 0.001	0.0001	0.0500	0.1300	0.3729	0.9875	< 0.001	0.0000	0.0160	0.0007	0.0084	0.0326	< 0.001	0.0002
0.0038	0.0079	0.2014	0.2326	< 0.001	0.0000	0.0016	0.0004	0.1028	0.0320	< 0.001	0.0000	0.0909	0.1961	0.9008	0.9875	< 0.001	0.0000	0.0118	0.0005	0.0076	0.0316	< 0.001	0.0001
0.0028	0.0064	0.7267	0.4064	< 0.001	0.0000	0.0031	0.0007	0.0483	0.0166	0.0013	0.0002	0.0901	0.1961	0.2403	0.9574	< 0.001	0.0000	0.0499	0.0019	0.0012	0.0073	< 0.001	0.0001
0.0175	0.0232	0.1003	0.1829	0.0020	0.0004	0.0437	0.0081	0.3673	0.0939	< 0.001	0.0001	0.5113	0.5578	0.8619	0.9875	< 0.001	0.0004	0.0183	0.0008	0.0170	0.0485	0.0011	0.0039
< 0.001	0.0030	0.9805	0.4833	< 0.001	0.0000	0.0935	0.0159	0.6399	0.1422	0.0979	0.0105	0.0076	0.0376	0.3199	0.9875	0.0037	0.0184	0.0335	0.0013	0.4559	0.5165	< 0.001	0.0032
< 0.001	0.0021	0.4185	0.3158	< 0.001	0.0000	0.1176	0.0196	0.0740	0.0242	0.0221	0.0028	0.4175	0.4932	0.0200	0.2868	< 0.001	0.0000	0.0032	0.0001	< 0.001	0.0007	< 0.001	0.0004
0.0035	0.0076	0.2830	0.2690	< 0.001	0.0000	0.0015	0.0004	0.0926	0.0292	< 0.001	0.0000	0.0710	0.1636	0.8070	0.9875	< 0.001	0.0000	0.0166	0.0007	0.0078	0.0317	< 0.001	0.0001
0.0026	0.0064	0.3910	0.3096	< 0.001	0.0001	0.0035	0.0008	0.4357	0.1065	< 0.001	0.0001	0.0754	0.1685	0.5347	0.9875	< 0.001	0.0001	0.0157	0.0007	0.0204	0.0562	< 0.001	0.0005
0.0017	0.0054	0.5945	0.3752	< 0.001	0.0001	0.0801	0.0140	0.4889	0.1162	0.0263	0.0032	0.0344	0.1035	0.4613	0.9875	< 0.001	0.0049	0.0275	0.0011	0.1922	0.2952	0.0011	0.0039
0.0050	0.0098	0.1480	0.2023	< 0.001	0.0000	< 0.001	0.0002	0.1792	0.0507	< 0.001	0.0000	0.2458	0.3663	0.6900	0.9875	< 0.001	0.0000	0.0063	0.0003	0.0011	0.0067	< 0.001	0.0001
0.0019	0.0058	0.2301	0.2408	< 0.001	0.0000	0.5699	0.0801	0.1631	0.0476	0.0832	0.0092	0.1194	0.2406	0.5339	0.9875	< 0.001	0.0044	0.0044	0.0002	0.1077	0.1919	0.0027	0.0081
0.8096	0.3507	0.0353	0.1698	0.5163	0.0615	0.0877	0.0151	0.6817	0.1484	0.6569	0.0560	0.0451	0.1234	0.8997	0.9875	0.3309	0.7089	0.1557	0.0056	0.0742	0.1425	0.3855	0.3696
0.0512	0.0533	0.0178	0.1419	0.6764	0.0795	0.6759	0.0923	0.1163	0.0352	0.0067	0.0009	0.9779	0.7170	0.6068	0.9875	0.4215	0.8005	0.0039	0.0002	0.8782	0.6475	0.6375	0.4991
0.0930	0.0816	0.0013	0.0329	0.0047	0.0009	< 0.001	0.0001	0.1857	0.0516	0.5910	0.0515	0.5513	0.5759	0.2144	0.9444	0.6514	0.9402	< 0.001	0.0000	0.5209	0.5605	0.4245	0.3879
0.5998	0.3009	0.6981	0.4020	0.2094	0.0273	0.0136	0.0027	0.4558	0.1104	0.0324	0.0039	0.2672	0.3949	0.2145	0.9444	0.8141	1.0000	0.0258	0.0010	0.2216	0.3240	0.5068	0.4338
0.0755	0.0712	0.2329	0.2408	0.0032	0.0006	0.0026	0.0006	0.1679	0.0482	0.0430	0.0050	0.9879	0.7215	0.5221	0.9875	0.9480	1.0000	< 0.001	0.0000	0.7325	0.6140	0.8585	0.5806
0.4838	0.2625	0.5203	0.3468	0.0121	0.0020	< 0.001	0.0000	0.0564	0.0187	< 0.001	0.0000	0.2934	0.4058	0.2684	0.9875	0.1613	0.4218	< 0.001	0.0000	0.6639	0.5983	0.1364	0.1777
0.9525	0.3907	0.2886	0.2690	0.2872	0.0366	0.6537	0.0903	0.2620	0.0698	0.1368	0.0144	0.3124	0.4149	0.9945	0.9945	0.6944	0.9629	0.1838	0.0065	0.4151	0.4733	0.7675	0.5500
0.8134	0.3508	0.1121	0.1864	0.8455	0.0946	0.0063	0.0014	0.6670	0.1470	0.1917	0.0193	0.0243	0.0796	0.3306	0.9875	0.4396	0.8054	0.1528	0.0056	0.1448	0.2404	0.0987	0.1443
0.2282	0.1548	0.4766	0.3313	0.5123	0.0613	0.2528	0.0387	0.5729	0.1307	0.6577	0.0560	0.7803	0.6746	0.8188	0.9875	0.4380	0.8054	0.3172	0.0108	0.6325	0.5983	0.7730	0.5500
0.7805	0.3440	0.3181	0.2699	0.3724	0.0455	0.0927	0.0159	0.5365	0.1251	0.0106	0.0014	0.9401	0.7120	0.2323	0.9574	0.3677	0.7442	0.0589	0.0022	0.8949	0.6542	0.3286	0.3373
0.0026	0.0064	0.2813	0.2690	0.0004	0.0032	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.0520	0.1305	0.8326	0.9875	< 0.001	0.0001	< 0.001	0.0000	0.0414	0.0983	< 0.001	0.0003
0.0017	0.0054	0.2996	0.2690	0.2380	0.0307	< 0.001	0.0000	0.0288	0.0107	< 0.001	0.0000	0.0511	0.1300	0.6766	0.9875	< 0.001	0.0000	< 0.001	0.0000	0.0081	0.0321	< 0.001	0.0001
0.0808	0.0741	0.0613	0.1730	< 0.001	0.0001	< 0.001	0.0001	0.0419	0.0145	0.0380	0.0045	0.7611	0.6692	0.5682	0.9875	0.7105	0.9721	< 0.001	0.0000	0.5200	0.5605	0.9951	0.6146
0.1305	0.1037	0.2041	0.2326	0.0061	0.0011	0.0018	0.0005	0.1617	0.0475	0.0786	0.0045	0.6778	0.5991	0.9875	0.8281	1.0000	< 0.001	0.0000	0.7382	0.6140	0.8650	0.5806	
0.0465	0.0500	0.0430	0.1730	< 0.001	0.0000	< 0.001	0.0000	0.0267	0.0102	0.0178	0.0023	0.8663	0.6963	0.8368	0.9875	0.6992	0.9643	< 0.001	0.0000	0.6608	0.5983	0.9862	0.6139
0.2685	0.1737	0.2865	0.2690	0.0875	0.0125	0.4246	0.0626	0.5227	0.1226	0.7835	0.0645	0.4074	0.4932	0.4312	0.9875	0.9010	1.0000	0.1617	0.0058	0.3895	0.4554	0.7437	0.5500
0.6561	0.3153	0.4320	0.3202	0.3347	0.0418	0.4984	0.0716	0.5985	0.1343	0.9119	0.0739	0.7375	0.6626	0.4985	0.9875	0.9669	1.0000	0.4804	0.0159	0.5432	0.5771	0.9013	0.5920
0.3152	0.1951	0.4986	0.3371	< 0.001	0.0000	< 0.001	0.0002	< 0.001	0.0000	< 0.001	0.0000	0.0181	0.0677	0.0083	0.1898	1.0000	1.0000	< 0.001	0.0000	0.0046	0.0202	0.1058	0.1499
0.0027	0.0064	0.0011	0.0919	0.0058	0.0010	0.9165	0.1205	0.7489	0.1608	0.0129	0.0017	0.0287	0.0923	0.0893	0.5745	0.5590	0.8795	< 0.001	0.0000	0.0542	0.1205	0.1118	0.1548
0.0585	0.0590	0.0010	0.0322	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0002	0.5545	0.5759	0.0279	0.3184	0.5557	0.8795	< 0.001	0.0000	0.0523	0.1192	0.3787	0.3673
0.6896	0.3234	0.7643	0.4254	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.5451	0.5759	0.9261	0.9875	0.0157	0.0681	< 0.001	0.0000	0.2417	0.3417	0.0775	0.1178
0.9906	0.3999	0.2995	0.2690	0.0118	0.0019	< 0.001	0.0000	0.0114	0.0049	< 0.001	0.0000	0.0960	0.2023	0.5155	0.9875	0.1319	0.3678	< 0.001	0.0000	0.6349	0.5983	0.0795	0.1185
0.0053	0.0100	0.0280	0.1698	0.0027	0.0005	< 0.001	0.0001	0.7780	0.1657	0.0481	0.0055	0.8889	0.6963	0.3950	0.9875	0.3610	0.7366	< 0.001	0.0000	0.9653	0.6718	0.4533	0.4016
0.0986	0.0850																						

Cofactors and vitamins	Nicotinate and nicotinamide metabolism	nicotinamide adenine dinucleotide (NAD+)	LC/MS pos	1.00	0.99	0.52	0.29	0.52	0.29	1.01	1.00	0.56
		nicotinamide adenine dinucleotide reduced (NADH)	LC/MS neg	0.91	1.64	0.65	0.66	0.71	0.40	0.87	1.55	0.88
		nicotinate adenine dinucleotide (NAAD+)	LC/MS neg	0.73	0.90	0.41	0.34	0.57	0.38	1.01	1.24	0.83
	Pantothenate and CoA metabolism	pantothenate	LC/MS pos	1.37	1.13	0.43	0.24	0.32	0.22	1.65	1.36	0.92
		phosphopantetheine	LC/MS neg	0.82	0.97	0.33	0.81	0.40	0.83	0.61	0.72	1.49
		coenzyme A	LC/MS neg	1.03	1.12	0.40	0.50	0.39	0.44	0.96	1.04	1.18
		3'-dephosphocoenzyme A	LC/MS neg	1.03	0.94	0.44	0.55	0.43	0.59	0.80	0.74	1.00
	Riboflavin metabolism	flavin adenine dinucleotide (FAD)	LC/MS neg	1.07	1.13	0.78	0.67	0.73	0.59	0.96	1.01	0.82
	Tocopherol metabolism	alpha-tocopherol	GC/MS	1.30	1.11	1.61	1.19	1.24	1.08	1.21	1.03	0.89
	Xenobiotics	Chemical	glycerol 2-phosphate	GC/MS	1.14	0.87	0.19	0.08	0.16	0.09	1.18	0.90

0.9004	0.3743	0.9077	0.4614	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.8251	0.6963	0.9840	0.9919	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000
0.5004	0.2672	0.0040	0.0615	0.0032	0.0006	0.0064	0.0014	0.0163	0.0066	< 0.001	0.0000	0.3053	0.4084	0.0095	0.1956	0.4526	0.8139	< 0.001	0.0000	0.5657	0.5845	0.0197	0.0412
0.0074	0.0125	0.2941	0.2690	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.8764	0.6963	0.0659	0.4837	0.1164	0.3561	< 0.001	0.0000	0.7590	0.6172	0.0538	0.0897
0.0081	0.0128	0.2967	0.2690	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0017	0.0101	0.1956	0.4572	0.8139	< 0.001	0.0000	< 0.001	0.0054	0.0030	0.0088
0.3077	0.1928	0.8209	0.4410	< 0.001	0.0000	0.3829	0.0575	< 0.001	0.0000	0.5155	0.0462	0.0086	0.0393	0.0518	0.4647	0.0348	0.1324	< 0.001	0.0000	0.1365	0.2335	0.0030	0.0086
0.5914	0.3009	0.0696	0.1730	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.5533	0.5759	0.4584	0.9875	0.0050	0.0235	< 0.001	0.0000	0.0732	0.1423	0.0466	0.0803
0.9610	0.3926	0.6025	0.3752	< 0.001	0.0000	0.0011	0.0003	< 0.001	0.0000	0.0040	0.0006	0.1806	0.3065	0.0622	0.5035	1.0000	1.0000	< 0.001	0.0000	0.0661	0.1330	0.3791	0.3673
0.1889	0.1381	0.0301	0.1698	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.4389	0.5060	0.8702	0.9875	< 0.001	0.0045	< 0.001	0.0000	0.0162	0.0478	0.0232	0.0474
0.0445	0.0488	0.4497	0.3228	< 0.001	0.0002	0.1935	0.0308	0.1063	0.0329	0.5746	0.0506	0.1213	0.2417	0.8017	0.9875	0.4011	0.7834	0.0051	0.0002	0.5670	0.5845	0.2392	0.2662
0.2218	0.1535	0.2222	0.2401	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	< 0.001	0.0000	0.1325	0.2564	0.3514	0.9875	< 0.001	0.0000	< 0.001	0.0000	0.0023	0.0109	< 0.001	0.0002