

S4 Table. Metabolome data for the liver of irradiated mice administered 15% ethanol. Values represent the relative areas of each metabolite peak to the peak area of an internal standard.

Compound name	Relative Area												Comparative Analysis																				
	control			rad			ethanol			ethanol+rad			rad vs control		ethanol vs control		ethanol+rad vs control		ethanol+rad vs rad		ethanol+rad vs ethanol												
	1	2	3	4	5	6	7	8	9	10	11	12	Mean	S.D.	Mean	S.D.	Mean	S.D.	Mean	S.D.	Ratio [†]	p-value ^{††}	Ratio [†]	p-value ^{††}	Ratio [†]	p-value ^{††}	Ratio [†]	p-value ^{††}	Ratio [†]	p-value ^{††}			
UDP-glucose	1.2E-02	9.7E-03	1.5E-02	2.5E-02	2.3E-02	2.7E-02	1.5E-02	1.5E-02	1.6E-02	2.7E-02	2.5E-02	1.8E-02	1.2E-02	2.4E-03	2.6E-02	1.1E-03	1.6E-02	6.2E-04	2.4E-02	4.7E-03	2.1	0.004	**	1.3	0.131	2.0	0.033	*	0.9	0.517	1.5	0.092	
UDP-galactose	2.1E-04	2.4E-04	3.4E-04	5.7E-04	5.7E-04	5.2E-04	2.7E-04	3.1E-04	3.6E-04	3.3E-04	5.7E-04	3.4E-04	2.6E-04	6.9E-05	5.6E-04	3.1E-05	3.1E-04	4.6E-05	4.2E-04	1.4E-04	2.1	0.008	**	1.2	0.364	1.6	0.184	0.7	0.214	1.3	0.321		
Rhein	1.2E-04	2.4E-05	7.4E-05	7.5E-05	1.3E-04	1.9E-04	1.6E-04	7.1E-05	1.4E-04	1.5E-04	8.3E-05	N.D.	7.2E-05	4.6E-05	1.3E-04	6.0E-05	1.2E-04	4.7E-05	1.2E-04	4.7E-05	1.6	0.245	*	1.7	0.238	1.6	0.392	0.9	0.768	0.9	0.867		
Tetrahydrobiopterin	5.3E-03	6.8E-03	7.6E-03	1.0E-02	1.1E-02	1.1E-02	1.9E-02	3.8E-03	8.7E-03	7.2E-03	6.8E-03	6.4E-03	6.5E-03	1.2E-03	1.1E-02	4.9E-03	8.6E-03	6.8E-03	4.1E-03	4.1E-03	1.8	0.015	*	1.3	0.118	1.2	0.733	0.6	5.4E-04	***	0.8	0.803	
Fructose 6-phosphate	2.3E-02	3.0E-02	4.3E-02	5.2E-02	4.2E-02	3.0E-02	3.7E-02	3.6E-02	3.4E-02	3.1E-02	2.6E-02	2.9E-02	2.9E-02	5.4E-03	4.6E-02	5.2E-03	3.4E-02	3.4E-03	3.0E-02	4.1E-03	1.6	0.017	*	1.2	0.221	1.0	0.752	0.7	0.016	0.9	0.245		
Sorbitol	2.0E-04	2.4E-04	7.0E-04	8.2E-04	3.5E-04	6.3E-04	3.5E-04	3.9E-04	3.9E-04	3.7E-04	3.9E-04	3.7E-04	3.8E-04	2.8E-04	6.1E-04	2.4E-04	3.4E-04	5.1E-05	4.4E-04	1.0E-04	1.6	0.350	0.9	0.836	1.2	0.751	0.7	0.359	1.3	0.224			
XA005	2.6E-04	6.4E-04	8.0E-04	7.5E-04	9.3E-04	9.3E-04	N.D.	7.5E-04	8.7E-04	N.D.	4.6E-04	7.7E-04	5.7E-04	2.8E-04	8.7E-04	1.0E-04	8.1E-04	8.9E-05	6.3E-04	2.2E-04	1.5	0.191	1.4	0.266	1.1	0.835	0.7	0.331	0.8	0.417			
Glucose 6-phosphate	2.0E-03	3.3E-03	3.1E-03	3.8E-03	5.1E-03	3.9E-03	2.8E-03	3.8E-03	3.2E-03	3.8E-03	3.6E-03	3.0E-03	2.8E-03	7.3E-04	4.3E-03	7.0E-03	3.4E-03	4.9E-04	3.5E-03	4.3E-04	1.5	0.089	1.2	0.445	1.2	0.270	0.8	0.182	1.1	0.601			
2-Methylserine	4.7E-04	4.3E-04	4.4E-04	6.5E-04	7.9E-04	5.1E-04	7.4E-04	5.1E-04	4.8E-04	9.2E-04	7.3E-04	4.7E-04	4.5E-04	2.1E-05	6.5E-04	1.4E-04	5.8E-04	1.4E-04	7.1E-04	2.2E-04	1.4	0.130	1.3	0.244	1.4	0.183	1.1	0.716	1.2	0.460			
Uric acid	2.6E-03	3.3E-03	5.8E-03	4.8E-03	5.6E-03	6.4E-03	4.6E-03	3.6E-03	4.7E-03	5.4E-03	5.5E-03	4.4E-03	5.0E-03	3.9E-03	1.7E-03	5.6E-03	7.8E-04	4.6E-03	8.7E-04	5.0E-03	5.5E-04	1.4	0.215	1.2	0.589	1.3	0.391	0.9	0.318	1.1	0.545		
Seoanepiurone	N.D.	1.5E-04	3.5E-04	4.8E-04	3.9E-04	2.0E-04	1.2E-04	1.9E-04	1.1E-04	2.1E-04	2.6E-04	1.3E-04	2.5E-04	1.5E-04	3.6E-04	1.4E-04	4.2E-04	2.0E-04	6.5E-05	1.4	0.496	0.6	0.482	0.8	0.718	0.6	0.184	1.4	0.276				
Glyoxybisphenolone	5.7E-03	7.0E-03	8.0E-03	9.4E-03	1.2E-02	7.9E-03	6.2E-03	8.5E-03	6.0E-03	6.1E-03	7.6E-03	5.3E-03	6.9E-03	1.2E-03	9.6E-03	1.8E-03	6.9E-03	1.4E-03	6.3E-03	1.1E-03	1.4	0.104	1.0	0.984	0.9	0.572	0.7	0.065	0.9	0.620			
Ser	5.4E-02	4.7E-02	4.3E-02	7.3E-02	5.7E-02	6.8E-02	5.8E-02	4.9E-02	5.6E-02	5.8E-02	6.1E-02	5.2E-02	4.8E-02	5.9E-03	6.6E-02	8.2E-02	5.4E-02	4.3E-02	5.9E-02	7.9E-03	1.4	0.043	**	1.1	0.253	1.0	0.358	1.1	0.382				
Ribose 5-phosphate	2.5E-02	3.3E-02	4.2E-02	4.2E-02	4.9E-02	4.1E-02	3.2E-02	2.7E-02	4.5E-02	4.9E-02	3.3E-02	3.9E-02	3.3E-02	8.4E-03	4.4E-02	4.3E-03	3.5E-02	2.9E-02	4.0E-02	8.0E-03	1.3	0.133	1.0	0.848	1.2	0.341	0.9	0.507	1.2	0.459			
Glucosamine	1.7E-03	1.7E-03	2.3E-03	2.3E-03	2.5E-03	2.9E-03	2.5E-03	3.0E-03	4.0E-03	4.1E-03	3.6E-03	4.8E-03	1.9E-03	3.4E-03	2.6E-03	2.9E-03	3.1E-03	7.6E-04	4.2E-03	6.1E-03	1.3	0.089	1.6	0.092	2.2	0.010	**	1.6	0.028	*	1.3	0.140	
Homocysteine	2.1E-03	2.1E-03	2.0E-03	2.6E-03	2.9E-03	2.7E-03	3.0E-03	1.9E-03	3.1E-03	2.9E-03	2.0E-03	2.7E-03	2.1E-03	4.7E-05	2.7E-03	1.6E-04	2.7E-03	6.5E-04	2.5E-03	4.7E-04	1.3	0.013	*	1.3	0.250	1.2	0.255	0.9	0.504	0.9	0.730		
S-Methylglutathione	1.2E-03	2.2E-03	2.3E-03	2.7E-03	3.0E-03	2.7E-03	2.7E-03	2.7E-03	2.7E-03	2.7E-03	2.7E-03	2.7E-03	2.7E-03	1.3E-04	2.8E-03	1.7E-04	2.8E-03	1.0E-04	2.9E-03	1.7E-03	1.3	0.011	*	1.2	0.005	**	1.3	0.005	**	1.0	0.465	1.1	0.240
Glucosamine	9.7E-04	1.2E-03	1.1E-03	1.2E-03	1.5E-03	1.3E-03	8.2E-04	8.1E-04	8.4E-04	1.0E-03	1.0E-03	2.0E-03	1.0E-03	2.5E-04	1.3E-03	1.5E-04	8.2E-04	1.5E-05	1.4E-03	6.0E-04	1.3	0.187	0.8	0.256	1.3	0.481	1.0	0.945	1.6	0.264			
Acetyl CoA divalent	1.0E-04	1.7E-03	1.3E-03	1.2E-03	1.8E-03	1.8E-03	1.2E-03	1.1E-03	1.5E-03	9.9E-04	2.1E-03	1.3E-03	9.6E-04	1.6E-03	1.6E-03	3.5E-04	1.3E-03	2.4E-04	1.4E-03	6.5E-04	1.3	0.312	1.0	0.957	1.0	0.911	0.8	0.542	1.1	0.878			
His	7.9E-02	8.7E-02	9.5E-02	1.1E-01	1.2E-01	9.6E-02	1.0E-01	9.0E-02	1.0E-01	9.4E-02	8.0E-02	9.0E-02	8.7E-02	8.0E-03	1.1E-01	1.4E-02	1.0E-01	8.0E-03	8.8E-02	7.0E-03	1.3	0.086	1.1	0.137	1.0	0.929	0.8	0.092	0.9	0.134			
Cytosine	4.1E-05	4.2E-05	3.7E-05	6.4E-05	5.1E-05	6.6E-05	3.3E-05	3.6E-05	6.3E-05	5.3E-05	6.4E-05	4.0E-05	2.3E-06	5.0E-05	1.4E-05	4.5E-05	1.8E-05	6.0E-05	6.3E-06	1.3	0.343	1.1	0.684	1.5	0.025	1.2	0.379	1.3	0.299				
cis-4-Hydroxyproline	2.2E-04	1.7E-04	1.8E-04	2.3E-04	2.1E-04	2.8E-04	3.4E-04	3.2E-04	4.6E-04	3.9E-04	3.1E-04	4.1E-04	1.9E-04	2.3E-05	2.4E-04	3.7E-05	3.7E-04	7.5E-05	3.7E-04	5.3E-05	1.3	0.146	1.0	0.943	2.0	0.015	1.6	0.027	*	1.0	0.984		
IMP	6.2E-03	7.7E-03	7.4E-03	9.5E-03	1.0E-02	7.0E-03	8.0E-03	7.4E-03	6.4E-03	7.0E-03	5.3E-03	6.1E-03	3.1E-03	7.1E-07	8.8E-03	1.6E-05	5.0E-03	2.0E-04	6.3E-03	8.7E-04	1.2	0.193	0.8	0.058	0.9	0.281	0.7	0.089	1.1	0.243			
Asp	4.1E-02	4.9E-02	3.7E-02	4.7E-02	6.2E-02	4.7E-02	6.2E-02	5.4E-02	7.0E-02	7.1E-02	3.8E-02	4.7E-02	4.2E-02	5.8E-03	5.2E-02	8.9E-03	6.2E-02	8.2E-03	5.2E-02	1.7E-02	1.2	0.198	1.5	0.031	*	1.2	0.424	1.0	0.986	0.8	0.428		
Pyruvic acid	N.D.	4.3E-03	4.1E-03	N.D.	5.1E-03	4.2E-03	N.D.	N.D.	5.8E-03	5.3E-03	4.2E-03	1.4E-04	5.2E-03	1.3E-04	4.6E-03	5.9E-04	5.6E-03	3.1E-02	3.6E-04	1.2	0.021	*	1.1	0.547	1.3	0.069	1.1	0.372	1.2	0.211			
5-Hydroxytryptophan	8.8E-04	8.2E-04	1.3E-03	1.3E-03	1.1E-03	1.3E-03	9.9E-04	1.2E-03	1.9E-03	1.5E-03	1.2E-03	1.9E-03	1.0E-03	2.8E-04	1.2E-03	9.8E-05	1.3E-03	9.5E-04	1.5E-03	3.6E-04	1.2	0.294	1.3	0.431	1.5	0.123	1.2	0.290	1.1	0.641			
Cys	4.6E-04	3.8E-04	5.1E-04	4.7E-04	6.9E-04	4.8E-04	6.1E-04	4.5E-04	5.3E-04	6.1E-04	6.9E-04	2.7E-04	4.5E-04	8.5E-05	5.5E-04	1.2E-04	5.3E-04	9.2E-05	5.2E-04	2.2E-04	1.2	0.301	1.2	0.224	1.2	0.629	1.0	0.876	1.0	0.952			
met-enkephalin	4.1E-04	4.9E-04	4.8E-04	5.8E-04	5.4E-04	5.4E-04	4.2E-04	3.5E-04	4.1E-04	4.3E-04	4.1E-04	4.6E-04	4.3E-05	5.5E-04	2.6E-05	3.9E-04	3.0E-05	4.2E-04	1.2E-05	1.2	0.036	*	0.9	0.147	0.9	0.201	0.8	0.006	**	1.1	0.321		
Triethanolamine	1.4E-04	N.D.	1.4E-04	1.5E-04	1.8E-04	1.8E-04	2.0E-04	1.3E-04	1.4E-04	2.1E-04	1.8E-04	N.D.	1.4E-04	2.0E-06	1.7E-04	1.7E-05	1.6E-04	3.6E-05	2.0E-04	2.0E-05	1.2	0.091	1.1	0.459	1.4	0.149	1.2	0.245	1.2	0.215			
Triethanolamine	1.8E-04	2.0E-04	2.2E-04	2.2E-04	3.1E-04	1.9E-04	1.8E-04	1.9E-04	2.0E-04	2.3E-04	1.3E-04	2.9E-04	2.0E-04	2.0E-05	2.4E-04	6.5E-05	2.6E-04	1.4E-04	2.2E-04	5.9E-05	1.2	0.380	1.3	0.512	1.2	0.741	0.8	0.682					
1-Methylhistamine	7.6E-05	9.8E-05	1.2E-04	8.0E-05	1.4E-04	1.3E-04	1.2E-04	8.9E-05	1.0E-04	1.3E-04	1.0E-04	1.4E-04	9.7E-05	2.1E-05	1.2E-04	3.3E-05	1.1E-04	1.8E-05	1.2E-04	2.2E-05	1.2	0.432	1.1	0.657	1.3	0.193	1.1	0.774	1.2	0.301			
Dietaniline	2.5E-04	2.5E-04	3.6E-04	3.4E-04	3.6E-04	3.4E-04	4.1E-04	2.1E-04	3.2E-04	3.7E-04	3.5E-04	2.4E-04	2.9E-04	6.5E-05	3.5E-04	9.9E-05	3.1E-04	1.0E-04	3.2E-04	7.1E-05	1.2	0.255	1.1	0.724	1.1	0.636	0.9	0.529	1.0	0.979			
Glutathione (GSH)	4.4E-01	3.9E-01	3.8E-01	4.4E-01	5.4E-01	5.4E-01	5.6E-01	4.6E-01	4.9E-01	5.1E-01	4.6E-01	3.6E-01	4.2E-01	2.9E-02	5.0E-01	5.7E-02	5.0E-01	5.0E-02	4.4E-01	7.6E-02	1.2	0.110	1.2	0.802	1.1	0.659	0.9	0.337	0.9	0			

Thr	4.1E-02	4.3E-02	5.1E-02	4.7E-02	4.9E-02	4.6E-02	4.8E-02	4.1E-02	5.2E-02	5.2E-02	5.1E-02	4.6E-02	4.5E-02	5.4E-02	4.7E-02	1.7E-03	4.5E-02	5.6E-03	5.0E-02	2.9E-03	1.0	0.566	1.0	0.692	1.1	0.272	1.1	0.282	1.1	0.497			
Spermidine	3.3E-03	4.3E-03	5.8E-03	4.7E-03	5.0E-03	4.3E-03	5.6E-03	5.3E-03	5.7E-03	6.0E-03	5.7E-03	6.6E-03	6.9E-03	4.5E-03	1.2E-03	3.4E-04	5.6E-03	2.8E-04	6.1E-03	4.5E-04	1.0	0.813	1.3	0.250	1.4	0.142	1.3	0.014	1.1	0.211			
XC0126	3.6E-04	3.6E-04	2.5E-04	3.3E-04	3.7E-04	3.1E-04	2.7E-04	2.5E-04	2.6E-04	2.8E-04	2.7E-04	2.9E-04	3.2E-04	4.3E-04	6.3E-05	4.7E-04	2.8E-05	2.6E-04	7.2E-04	2.7E-04	2.3E-05	1.0	0.785	0.8	0.226	0.8	0.294	0.8	0.040	1.0	0.482		
GTP	4.0E-03	3.4E-03	2.2E-03	3.3E-03	3.5E-03	3.2E-03	2.9E-03	2.5E-03	3.2E-03	3.1E-03	1.6E-03	1.1E-03	8.9E-04	3.2E-03	8.9E-04	3.3E-03	1.6E-04	2.9E-03	3.8E-04	1.2E-03	3.6E-04	1.0	0.848	0.9	0.652	0.4	0.043	0.4	0.043	0.4	0.005		
XAD05	2.9E-03	2.5E-03	2.4E-03	2.6E-03	3.0E-03	3.2E-03	3.1E-03	2.8E-03	3.5E-03	2.8E-03	2.6E-03	2.6E-03	2.6E-03	3.1E-03	1.9E-03	4.4E-04	3.1E-03	4.3E-04	3.9E-03	3.2E-04	1.0	0.774	1.2	0.213	1.0	0.595	0.9	0.537	1.0	0.148			
XAD2	5.8E-03	5.4E-03	8.0E-03	5.9E-03	6.4E-03	7.4E-03	7.0E-03	8.8E-03	7.9E-03	7.5E-03	7.8E-03	6.4E-03	1.4E-03	6.8E-03	7.7E-03	8.1E-03	9.5E-04	7.7E-03	9.5E-04	7.7E-03	1.6E-04	1.0	0.857	1.2	0.168	1.2	0.245	1.2	0.120	1.0	0.563		
XAD12	1.2E-03	1.4E-03	1.1E-03	1.0E-03	1.6E-03	1.3E-03	1.5E-03	1.2E-03	1.1E-03	9.1E-04	1.0E-03	1.5E-03	1.3E-03	1.6E-04	1.3E-03	3.0E-04	1.3E-03	1.9E-04	1.2E-03	3.2E-04	1.0	0.887	1.0	0.884	0.9	0.658	0.9	0.629	0.9	0.601			
Ascorbic acid	3.2E-02	3.8E-02	3.1E-02	2.8E-02	3.8E-02	3.7E-02	3.4E-02	3.2E-02	3.4E-02	4.0E-02	5.3E-02	8.5E-03	3.4E-02	3.7E-03	3.4E-02	5.3E-03	3.3E-02	1.1E-03	3.4E-02	3.2E-02	1.0	0.848	1.0	0.933	1.0	0.985	1.0	0.974	1.0	0.974			
NMN	4.9E-04	3.3E-04	3.0E-04	3.8E-04	3.4E-04	4.2E-04	2.8E-04	3.2E-04	2.9E-04	2.6E-04	3.0E-04	3.7E-04	3.7E-04	1.0E-04	3.8E-04	4.0E-05	3.0E-04	1.7E-05	3.1E-04	5.4E-05	1.0	0.912	0.8	0.328	0.8	0.419	0.8	0.150	1.0	0.713			
Guanosine	2.1E-03	1.9E-03	2.2E-03	2.1E-03	2.1E-03	4.2E-03	2.2E-03	2.6E-03	1.9E-03	2.3E-03	2.7E-03	2.4E-03	2.1E-03	1.2E-04	2.1E-03	2.8E-06	2.3E-03	3.5E-04	2.4E-03	2.1E-04	1.0	0.609	1.1	0.389	1.2	0.062	1.2	0.099	1.1	0.503			
UTP	4.8E-03	3.8E-03	2.4E-03	3.6E-03	3.3E-03	3.7E-03	4.3E-03	2.7E-03	4.6E-03	1.8E-03	1.2E-03	9.5E-04	3.5E-03	8.9E-04	3.6E-03	2.5E-04	3.8E-03	9.9E-04	1.3E-03	4.4E-04	1.0	0.928	1.1	0.685	0.4	0.045	0.4	0.004	**	0.3	0.032		
Glycerol 3-phosphate	3.3E-02	9.0E-02	8.6E-02	8.7E-02	9.1E-02	9.1E-02	9.1E-02	8.2E-02	7.1E-02	8.2E-02	9.1E-02	8.7E-02	8.8E-02	8.8E-02	9.0E-02	2.6E-03	7.9E-02	6.8E-03	9.2E-02	5.6E-03	1.0	0.547	0.9	0.134	1.0	0.347	1.0	0.508	1.2	0.063			
Poligalonic acid	6.2E-04	5.3E-04	4.7E-04	5.6E-04	5.3E-04	N.D.	6.8E-04	4.2E-04	4.7E-04	5.9E-04	5.7E-04	4.6E-04	5.4E-04	7.6E-05	5.4E-04	2.0E-05	5.2E-04	1.4E-04	5.4E-04	6.7E-05	1.0	0.891	1.0	0.895	1.0	0.961	1.0	0.931	1.0	0.888			
Glucose	1.3E-01	1.8E-01	1.0E-01	1.2E-01	1.7E-01	1.3E-01	1.4E-01	1.5E-01	1.6E-01	1.5E-01	1.6E-01	1.6E-01	1.4E-01	3.8E-02	1.4E-01	2.8E-02	1.6E-01	2.0E-02	1.4E-01	3.2E-02	1.0	0.956	1.2	0.426	1.0	0.969	1.0	0.987	1.0	0.388			
Ala	1.2E-02	1.4E-02	1.2E-02	1.2E-02	1.4E-02	1.2E-02	1.9E-02	1.3E-02	1.7E-02	1.6E-02	1.3E-02	1.4E-02	1.3E-02	1.2E-03	1.3E-02	7.1E-04	1.6E-02	2.3E-03	1.4E-02	1.5E-03	1.0	0.879	1.3	0.108	1.1	0.108	1.1	0.243	1.1	0.246			
Hypoxanthine	6.3E-03	1.0E-02	1.6E-02	1.1E-02	1.1E-02	1.1E-02	5.7E-03	8.2E-03	6.1E-03	8.3E-03	9.9E-03	1.1E-02	1.1E-02	4.9E-03	1.1E-02	2.9E-04	6.7E-03	1.4E-03	9.7E-03	1.4E-03	1.0	0.976	0.6	0.280	0.9	0.744	0.9	0.277	1.5	0.053			
Xanthine	3.6E-03	6.1E-03	8.5E-03	5.8E-03	6.8E-03	5.6E-03	3.2E-03	4.2E-03	3.4E-03	4.0E-03	4.8E-03	4.3E-03	6.0E-03	2.4E-03	6.1E-03	6.5E-03	5.3E-04	4.4E-03	4.3E-04	1.0	0.977	0.6	0.220	0.7	0.352	0.7	0.024	*	1.2	0.127			
GDP	4.6E-03	4.2E-03	3.1E-03	3.9E-03	3.9E-03	4.1E-03	4.2E-03	3.6E-03	3.9E-03	2.2E-03	3.7E-04	1.6E-03	4.0E-03	7.8E-04	4.0E-03	1.4E-04	3.9E-03	2.9E-04	1.4E-03	9.4E-04	1.0	0.954	1.0	0.918	0.4	0.024	*	0.3	0.039	*	0.4	0.035	
Isothionic acid	3.0E-03	3.6E-03	3.1E-03	3.0E-03	3.5E-03	3.0E-03	2.3E-03	2.8E-03	2.1E-03	2.3E-03	2.6E-03	3.2E-03	3.2E-03	3.4E-03	3.3E-03	2.6E-04	2.4E-03	3.7E-04	2.7E-03	4.6E-04	1.0	0.937	0.7	0.044	*	0.8	0.160	0.8	0.143	1.1	0.491		
Histamine	1.5E-04	1.9E-04	1.8E-04	1.8E-04	1.6E-04	1.8E-04	1.4E-04	1.2E-04	1.5E-04	5.7E-05	1.5E-04	1.9E-04	1.7E-04	2.5E-05	1.8E-04	1.1E-05	1.4E-04	1.5E-05	1.3E-04	6.8E-05	1.0	0.989	0.8	0.100	0.8	0.394	0.8	0.382	1.0	0.233			
Panthenic acid	4.2E-04	3.6E-04	3.6E-04	3.2E-04	4.0E-04	4.1E-04	4.8E-04	3.6E-04	4.2E-04	3.5E-04	3.4E-04	4.2E-04	3.5E-04	3.8E-04	3.6E-05	3.8E-04	5.0E-05	4.5E-04	7.2E-05	3.7E-04	4.1E-05	1.0	0.959	1.2	0.246	1.0	0.800	1.0	0.220	0.8	0.206		
γ-Aminobutyramic acid	3.0E-04	4.6E-04	3.1E-04	3.3E-04	4.0E-04	4.4E-04	3.4E-04	3.5E-04	3.3E-04	3.1E-04	4.1E-04	3.4E-04	3.6E-04	8.9E-05	3.6E-04	4.0E-05	3.4E-04	1.0E-05	3.5E-04	5.3E-05	1.0	0.998	1.0	0.777	1.0	0.952	1.0	0.920	1.0	0.717			
Betaine	2.1E-02	2.0E-02	2.1E-02	2.2E-02	2.0E-02	2.0E-02	3.1E-02	2.4E-02	2.8E-02	2.9E-02	2.5E-02	2.8E-02	2.1E-02	4.5E-04	2.1E-02	1.4E-03	2.8E-02	4.3E-03	2.7E-02	1.9E-03	1.0	0.998	1.3	0.067	*	1.3	0.025	*	1.3	0.013	*	1.0	0.710
Imidazoleacetic acid	3.2E-04	2.8E-04	3.5E-04	2.9E-04	3.2E-04	3.3E-04	3.6E-04	4.3E-04	4.2E-04	4.6E-04	2.7E-04	3.7E-04	3.2E-04	3.5E-05	3.2E-04	2.3E-05	4.1E-04	3.7E-05	3.7E-04	9.8E-05	1.0	0.968	1.3	0.040	**	1.2	0.058	1.2	0.473	0.9	0.568		
XC0137	6.6E-03	4.7E-03	6.4E-03	5.4E-03	4.8E-03	4.8E-03	5.5E-03	5.2E-03	5.5E-03	4.9E-03	5.9E-03	5.4E-04	5.0E-03	4.9E-04	5.4E-03	1.7E-04	5.4E-03	3.9E-03	1.9E-03	1.0	0.846	1.1	0.329	0.6	0.599	0.6	0.068	0.6	0.068	0.6	0.068		
Tyr	1.2E-02	1.4E-02	1.5E-02	1.3E-02	1.4E-02	1.3E-02	1.4E-02	1.2E-02	1.7E-02	1.4E-02	1.9E-02	1.4E-02	1.5E-02	1.4E-02	1.5E-02	1.4E-02	1.5E-02	1.4E-02	1.3E-02	1.7E-02	2.2E-03	1.0	0.923	1.0	0.766	1.2	0.160	1.2	0.160	1.2	0.287		
Diphylline	5.8E-03	6.6E-03	8.6E-03	6.6E-03	6.4E-03	7.7E-03	8.0E-03	6.6E-03	6.9E-03	5.4E-03	6.1E-03	7.0E-03	1.4E-03	6.9E-03	7.0E-04	6.7E-03	1.2E-03	6.1E-03	7.3E-04	1.0	0.949	1.0	0.799	0.9	0.408	0.9	0.234	0.9	0.511				
NAD ⁺	2.1E-02	1.8E-02	1.6E-02	1.8E-02	1.7E-02	1.9E-02	1.6E-02	1.6E-02	1.7E-02	1.6E-02	1.4E-02	1.8E-02	2.9E-02	1.8E-02	1.3E-02	1.8E-02	1.3E-02	1.7E-02	1.5E-02	1.6E-03	1.0	0.933	1.0	0.772	0.8	0.216	0.8	0.080	0.9	0.150			
Gly	1.5E-01	1.5E-01	1.7E-01	1.5E-01	1.5E-01	1.7E-01	1.7E-01	1.3E-01	1.7E-01	1.6E-01	1.5E-01	1.4E-01	1.6E-01	8.9E-03	1.5E-01	1.4E-02	1.6E-01	2.4E-02	1.5E-01	1.2E-02	1.0	0.858	1.0	0.854	1.0	0.625	1.0	0.811	1.0	0.658			
γ-oxo-γ-butyro-β-methylcrotonic acid	2.3E-04	2.3E-04	2.4E-04	2.3E-04	2.5E-04	2.1E-04	2.1E-04	2.6E-04	2.7E-04	2.6E-04	2.8E-04	2.4E-04	2.3E-04	2.4E-04	1.9E-05	2.8E-04	1.5E-05	2.6E-04	2.1E-05	1.0	0.745	1.0	0.474	*	1.1	0.159	1.1	0.140	0.9	0.383			
Taurine	1.5E-01	1.6E-01	1.6E-01	1.5E-01	1.6E-01	1.5E-01	1.8E-01	1.6E-01	1.4E-01	1.1E-01	1.5E-01	1.4E-01	1.6E-01	2.8E-03	1.5E-01	8.0E-03	1.6E-01	1.8E-02	1.3E-01	1.7E-02	1.0	0.594	1.0	1.000	0.8	0.128	0.9	0.149	0.8	0.129			
Lys	7.6E-02	1.1E-01	1.0E-01	8.2E-02	1.1E-01	9.1E-02	1.3E-01	1.1E-01	1.4E-01	1.1E-01	1.0E-01	1.4E-01	1.1E-01	1.4E-01	1.1E-01	1.4E-01	1.1E-01	1.6E-02	1.2E-01	1.7E-02	1.0	0.881	1.3	0.117	1.2	0.229	1.2	0.149	0.9	0.591			
Putrescine	2.7E-04	4.2E-04	8.6E-04	5.4E-04	6.7E-04	3.0E-04	1.5E-03	1.2E-03	1.6E-03	1.8E-03	1.5E-03	1.0E-03	5.2E-04	3.1E-04	5.0E-04	1.8E-04	1.5E-03	2.3E-04	1.5E-03	4.2E-04	1.0	0.954	2.8	0.016	*	2.8	0.039	*	2.9	0.042	*	1.0	0.984
Lutamic acid	1.9E-03	2.0E-03	2.1E-03	2.1E-03	1.9E-03	1.9E-03	2.0E-03	1.9E-03	1.7E-03	2.0E-03	1.8E-03	1.4E-03	1.1E-04	2.0E-03	1.1E-04	2.0E-03	1.4E-03	2.0E-04	1.9E-03	2.0E-04	1.0	0.924	0.9	0.388	0.9	0.262	0.9	0.358	0.9	0.571			
XC0138	1.4E-03	1.3E-03	9.3E-04	1.2E-03	1.0E-03	1.3E-03	1.6E-03	1.5E-03	1.8E-03	1.4E-03	2.6E-03	1.2E-03	1.6E-03	1.2E-03	1.6E-03	1.5E-03	8.0E-05	1.9E-03	6.2E-04	1.0	0.846	1.6	0.154	1.6	0.174	1.6	0.174	1.6	0.174	1.6	0.386		
5-Hydroxylsine	7.0E-05	7.7E-05	8.8E-05	7.7E-05	8.4E-05	6.6E-05	1.4E-04	1.2E-04	1.3E-04	1.0E-04	9.1E-05	1.2E-04	7.8E-05	9.0E-06	7.8E-05	8.8E-06	1.3E-04	8.7E-06	1.1E-0														

Uracil	5.3E-04	6.4E-04	8.5E-04	5.8E-04	6.1E-04	5.8E-04	5.8E-04	8.0E-04	6.5E-04	5.5E-04	7.1E-04	7.1E-04	6.7E-04	1.6E-04	5.9E-04	1.8E-05	6.8E-04	1.1E-04	6.6E-04	9.5E-05	0.9	0.466	1.0	0.969	1.0	0.874	1.1	0.349	1.0	0.798			
Ethanolamine ribosides	8.3E-03	8.1E-03	7.9E-03	7.1E-03	7.1E-03	7.0E-03	7.8E-03	8.3E-03	6.2E-03	6.6E-03	6.6E-03	6.6E-03	8.1E-03	2.3E-04	7.1E-03	6.1E-05	7.4E-03	1.1E-03	6.4E-03	3.3E-04	0.9	0.011	0.9	0.381	0.8	0.003	**	0.9	0.072	0.9	0.259		
Argininosuccinic acid	1.6E-03	2.1E-03	2.1E-03	1.4E-03	2.1E-03	1.6E-03	1.4E-03	1.8E-03	1.6E-03	1.9E-03	1.4E-03	1.6E-03	2.0E-03	2.8E-04	1.7E-03	3.4E-04	1.8E-03	3.5E-04	1.7E-03	2.4E-04	0.9	0.380	0.9	0.525	**	0.9	0.303	1.0	0.975	1.0	0.779		
Ala-Ala	1.1E-03	1.3E-03	1.4E-03	1.3E-03	1.1E-03	9.6E-04	1.1E-03	7.9E-04	7.2E-04	7.5E-04	7.8E-04	9.4E-04	1.3E-03	1.3E-04	1.1E-03	1.3E-04	8.6E-04	1.7E-04	8.4E-04	1.0E-04	0.9	0.196	0.7	0.031	**	0.6	0.010	**	0.7	0.061	1.0	0.810	
N ¹ -Acetyllysine	4.9E-04	5.5E-04	4.5E-04	4.2E-04	4.9E-04	4.1E-04	6.9E-04	6.5E-04	5.3E-04	6.1E-04	4.8E-04	6.9E-04	5.0E-04	4.7E-05	4.3E-04	2.7E-05	5.8E-04	4.4E-05	6.9E-04	1.1E-04	0.9	0.111	1.2	0.087	1.2	0.248	**	1.4	0.136	1.0	0.855		
Biotinone	4.7E-04	5.5E-04	5.2E-04	3.7E-04	3.4E-04	5.5E-04	6.0E-04	5.2E-04	5.5E-04	5.2E-04	6.0E-04	4.8E-04	7.1E-05	4.1E-04	0.7E-05	5.6E-04	4.0E-05	5.8E-04	3.8E-05	0.9	0.398	1.2	0.167	1.2	0.182	1.4	0.105	1.0	0.901	1.0	0.904		
N ⁵ -Ethylglutamine	7.9E-04	7.4E-04	6.1E-04	6.0E-04	6.5E-04	6.0E-04	8.5E-04	9.1E-04	8.3E-04	8.0E-04	7.1E-04	8.0E-04	7.2E-04	9.2E-05	6.2E-04	2.5E-05	8.7E-04	4.2E-05	7.7E-04	5.0E-05	0.9	0.194	1.2	0.087	1.1	0.448	1.2	0.019	**	0.9	0.063		
Cystathionine	7.6E-03	1.0E-02	7.2E-03	6.4E-03	8.9E-03	6.1E-03	1.6E-02	1.1E-02	1.6E-02	8.3E-03	1.6E-02	7.2E-03	1.5E-02	1.4E-02	3.9E-03	1.4E-02	1.4E-02	2.8E-03	0.9	0.414	1.7	0.099	1.6	0.058	1.9	0.036	**	0.9	0.807	1.0	0.807		
Ergothioneine	4.8E-02	5.1E-02	4.8E-02	2.8E-02	4.6E-02	5.3E-02	4.1E-02	3.0E-02	3.8E-02	4.0E-02	3.6E-02	3.9E-02	4.9E-02	2.0E-03	4.2E-02	1.3E-02	3.6E-02	5.4E-03	3.8E-02	2.5E-03	0.9	0.448	0.7	0.043	**	0.8	0.005	**	0.9	0.688	1.1	0.588	
Citrulline	9.8E-03	1.4E-02	1.7E-02	1.1E-02	1.3E-02	1.2E-02	1.4E-02	1.0E-02	1.2E-02	1.1E-02	1.1E-02	1.5E-02	1.4E-02	3.7E-03	1.2E-02	9.8E-02	1.0E-02	2.7E-03	0.9	0.466	0.9	0.522	0.9	0.617	1.0	0.788	1.0	0.788	1.0	0.879	1.0	0.879	
Stachydine	3.6E-02	3.4E-02	3.1E-02	3.5E-02	2.5E-02	2.7E-02	4.0E-02	3.8E-02	3.5E-02	3.5E-02	3.2E-02	3.7E-02	3.4E-02	2.7E-03	2.9E-02	5.3E-03	3.8E-02	2.5E-03	3.4E-02	2.5E-03	0.9	0.233	1.1	0.160	1.0	0.854	1.2	0.205	0.9	0.189	1.0	0.189	
Gly-Gly	4.4E-04	4.8E-04	3.1E-04	3.9E-04	4.1E-04	4.2E-04	4.1E-04	3.4E-04	3.8E-04	4.4E-04	4.4E-04	5.2E-04	4.7E-04	3.6E-05	4.0E-04	1.6E-05	3.8E-04	3.1E-05	4.5E-04	6.2E-05	0.8	0.058	0.8	0.024	**	0.6	0.025	1.1	0.302	1.2	0.156		
β-hydroxyisovalinate	3.0E-03	3.4E-03	2.7E-03	2.8E-03	2.5E-03	2.4E-03	2.3E-03	2.7E-03	2.0E-03	2.1E-03	1.9E-03	4.2E-03	3.0E-03	3.3E-04	2.6E-03	2.2E-04	2.4E-03	3.6E-04	2.7E-03	1.3E-03	0.8	0.130	0.8	0.083	0.9	0.733	1.1	0.852	1.2	0.685	1.0	0.685	
Adenine	1.2E-03	1.9E-03	1.3E-03	1.6E-03	1.0E-03	1.1E-03	1.0E-03	1.7E-03	1.2E-03	1.3E-03	1.3E-03	2.1E-03	1.5E-03	3.8E-04	1.2E-03	2.9E-04	1.3E-03	3.5E-04	1.6E-03	4.7E-04	0.8	0.462	0.9	0.639	1.1	0.748	1.3	0.351	1.2	0.471	1.0	0.471	
Quantoacetic acid	2.5E-03	2.2E-03	1.8E-03	1.7E-03	2.2E-03	1.5E-03	2.3E-03	2.7E-03	1.9E-03	2.0E-03	2.1E-03	2.9E-03	2.2E-03	3.2E-04	1.9E-03	3.4E-04	2.3E-03	4.0E-04	2.3E-03	5.0E-04	0.8	0.260	1.1	0.668	1.1	0.668	1.3	0.231	1.0	0.970	1.0	0.970	
3-Methylhistidine	2.9E-03	2.8E-03	2.8E-03	2.4E-03	2.4E-03	2.3E-03	3.8E-03	3.5E-03	3.7E-03	3.1E-03	1.9E-03	3.3E-03	2.8E-03	6.1E-05	2.4E-03	5.7E-05	3.7E-03	1.5E-04	2.8E-03	7.4E-04	0.8	6.5E-04	**	1.3	0.004	**	1.0	0.923	1.2	0.428	0.7	0.158	
N-Methylalanine	2.0E-04	2.2E-04	N.D.	1.8E-04	1.6E-04	1.6E-04	2.7E-04	2.6E-04	2.5E-04	2.9E-04	2.2E-04	2.3E-04	2.1E-04	1.5E-05	1.7E-04	8.9E-06	2.6E-04	6.2E-06	2.4E-04	4.5E-05	0.8	0.139	1.3	0.094	**	1.0	0.228	1.4	0.103	0.9	0.610		
Pro	8.5E-02	9.8E-02	7.9E-02	6.7E-02	8.3E-02	9.6E-02	1.1E-01	9.0E-02	1.1E-01	1.0E-01	8.2E-02	1.2E-01	8.8E-02	9.8E-03	7.3E-02	8.4E-03	1.0E-01	1.2E-02	1.0E-01	1.6E-02	0.8	0.123	1.2	0.139	1.1	0.345	1.4	0.086	1.0	0.704	1.0	0.704	
Val	1.1E-01	1.1E-01	1.1E-01	8.6E-02	9.1E-02	9.6E-02	1.4E-01	1.2E-01	1.3E-01	1.1E-01	9.5E-02	1.2E-01	1.1E-01	1.7E-03	9.1E-02	5.3E-03	1.3E-01	1.3E-02	1.1E-01	1.3E-02	0.8	0.018	**	1.2	0.117	1.0	0.859	1.2	0.142	0.8	0.122	1.0	0.122
β-Ala-Lys	5.4E-04	7.2E-04	8.7E-04	6.7E-04	5.6E-04	5.3E-04	6.4E-04	4.3E-04	4.9E-04	5.5E-04	6.6E-04	6.5E-04	7.1E-04	1.7E-04	5.9E-04	7.1E-05	6.2E-04	1.1E-04	5.9E-04	5.5E-05	0.8	0.330	0.7	0.187	1.0	0.824	1.0	0.983	1.1	0.432	1.0	0.432	
Succinic acid	8.0E-02	8.5E-02	8.5E-02	6.5E-02	5.7E-02	6.8E-02	8.8E-02	7.5E-02	9.1E-02	7.9E-02	8.2E-02	7.7E-02	1.1E-02	6.3E-02	5.9E-03	8.1E-02	6.6E-03	8.4E-02	6.1E-03	0.8	0.141	1.1	0.577	1.1	0.383	1.3	0.013	*	1.0	0.634	1.0	0.634	
3-Aminobutyric acid	1.2E-03	7.6E-04	6.7E-04	7.5E-04	6.7E-04	7.2E-04	1.0E-03	8.4E-04	8.0E-04	8.4E-04	8.6E-04	9.8E-04	8.7E-04	2.7E-04	7.1E-04	4.2E-05	9.2E-04	9.7E-05	8.3E-04	1.5E-04	0.8	0.422	1.1	0.777	1.0	0.844	1.2	0.305	0.9	0.439	1.0	0.439	
Carboxymethylsulfonamide	9.5E-05	8.3E-05	1.3E-04	6.0E-05	5.9E-05	1.0E-04	9.1E-05	1.1E-04	1.0E-04	1.0E-04	8.2E-05	1.1E-04	1.0E-04	2.2E-05	8.1E-05	2.1E-05	1.0E-04	7.8E-06	1.0E-04	1.6E-05	0.8	0.337	1.0	0.937	1.0	0.929	1.2	0.322	1.0	0.976	1.0	0.976	
Homoserine	5.2E-04	6.3E-04	4.5E-04	4.2E-04	4.7E-04	4.1E-04	7.2E-04	6.0E-04	6.4E-04	6.5E-04	6.4E-04	6.5E-04	5.3E-04	9.2E-05	4.3E-04	3.1E-05	6.5E-04	6.0E-05	5.9E-04	8.8E-05	0.8	0.193	1.2	0.139	1.1	0.446	1.4	0.073	0.9	0.396	1.0	0.396	
Pyridoxal	1.7E-04	2.2E-04	1.7E-04	1.6E-04	1.9E-04	1.6E-04	1.9E-04	2.1E-04	1.4E-04	1.5E-04	1.6E-04	1.9E-04	1.3E-04	4.7E-05	1.3E-04	1.7E-05	1.5E-04	3.5E-05	1.9E-04	1.7E-05	0.8	0.162	0.9	0.589	1.1	0.296	1.1	0.546	0.9	0.688	1.0	0.688	
Hypoxanthine	4.6E-03	3.7E-03	3.5E-03	3.3E-03	2.8E-03	2.8E-03	4.9E-03	5.3E-03	5.9E-03	5.3E-03	5.1E-03	3.9E-03	5.8E-03	3.2E-03	3.3E-03	5.3E-03	4.5E-04	5.0E-03	1.0E-03	0.8	0.146	1.4	0.033	*	1.3	0.213	1.6	0.080	0.9	0.618	1.0	0.618	
Sarcosine	4.1E-02	3.8E-02	3.2E-02	3.2E-02	3.0E-02	2.8E-02	4.2E-02	4.0E-02	4.0E-02	4.0E-02	4.0E-02	3.9E-02	4.7E-02	3.7E-02	5.0E-03	3.0E-02	2.3E-03	4.1E-02	1.4E-03	4.2E-02	0.8	0.119	1.1	0.357	1.1	0.276	1.4	0.030	**	1.0	0.629	1.0	0.629
N-Acetyllysine	2.2E-03	2.2E-03	2.5E-03	1.8E-03	1.9E-03	1.8E-03	2.0E-03	2.2E-03	1.7E-03	1.7E-03	2.4E-03	2.3E-03	1.4E-04	1.9E-03	5.7E-03	2.1E-03	8.5E-05	1.9E-03	3.7E-04	0.8	0.021	**	1.0	0.236	1.1	0.704	0.9	0.503	1.0	0.503	1.0	0.503	
β-Ala	2.4E-02	2.5E-02	2.0E-02	1.8E-02	2.0E-02	1.8E-02	2.5E-02	2.4E-02	2.6E-02	2.6E-02	2.3E-02	2.7E-02	1.8E-02	9.8E-04	2.4E-02	2.8E-03	2.2E-02	5.0E-03	0.8	0.086	1.0	0.809	1.0	0.781	1.2	0.352	0.9	0.667	1.0	0.667	1.0	0.667	
Cystine glutathione disulfide	1.3E-04	2.1E-04	1.7E-04	1.6E-04	1.3E-04	1.2E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	1.4E-04	0.8	0.287	0.9	0.735	1.5	0.287	1.8	0.170	1.6	0.240	1.0	0.240	
N,N-Dimethylglycine	2.6E-02	2.1E-02	2.0E-02	2.0E-02	1.7E-02	1.7E-02	2.2E-02	2.3E-02	2.3E-02	2.4E-02	2.4E-02	2.2E-02	3.4E-03	1.8E-02	1.5E-03	2.2E-02	6.6E-04	2.4E-02	1.7E-04	0.8	0.137	1.0	0.961	1.1	0.469	1.4	0.018	*	1.1	0.042	1.0	0.042	
N-Acetylglycamic acid	7.8E-03	9.3E-03	6.3E-03	6.7E-03	6.7E-03	6.7E-03	9.3E-03	8.3E-03	7.2E-03	9.3E-03	8.3E-03	7.0E-03	8.4E-03	1.5E-03	6.2E-03																		

Methionine sulfoxide	1.6E-03	2.2E-03	1.7E-03	1.1E-03	1.1E-03	9.2E-04	3.3E-03	3.1E-03	2.8E-03	2.3E-03	2.2E-03	2.9E-03	1.8E-03	3.1E-04	1.0E-03	9.9E-05	3.1E-03	2.2E-04	2.4E-03	3.8E-04	0.6	0.037	*	1.7	0.007	**	1.3	0.107	2.4	0.018	*	0.8	0.085	
Butyrylcarnitine	1.1E-02	1.1E-02	7.1E-03	7.7E-03	3.1E-03	5.0E-03	4.0E-02	2.0E-02	5.4E-03	1.7E-02	1.4E-02	1.9E-02	9.6E-03	2.2E-03	5.3E-03	2.3E-03	2.2E-02	1.7E-02	1.7E-02	2.3E-03	0.6	0.079		2.3	0.353	1.7	0.020	*	3.1	0.004	**	0.8	0.661	
Glutamic acid	1.3E-03	1.1E-03	6.1E-04	N.D.	N.D.	5.3E-04	1.9E-03	1.3E-03	8.7E-04	1.2E-03	1.0E-03	1.4E-03	1.0E-03	3.7E-04	5.3E-04	N.A.	1.4E-03	5.3E-04	1.2E-03	2.1E-04	0.5	N.A.		1.3	0.423	1.2	0.446	2.3	N.A.		0.9	0.731		
¹⁵ N-acetylmethionine	1.2E-03	1.6E-03	8.4E-04	9.0E-04	4.2E-04	5.7E-04	4.0E-03	1.9E-03	4.6E-04	1.6E-03	1.7E-03	1.8E-03	1.2E-03	4.0E-04	6.3E-04	2.4E-04	2.1E-03	1.8E-03	1.7E-03	9.4E-05	0.5	0.104		1.7	0.462	1.4	0.172	2.7	0.009	**	0.8	0.723		
Glucuronic acid	4.5E-03	6.3E-03	5.1E-03	2.8E-03	1.9E-03	3.4E-03	6.7E-03	6.3E-03	6.9E-03	4.7E-03	4.9E-03	4.2E-03	5.3E-03	9.3E-04	2.8E-03	8.9E-04	6.7E-03	3.1E-04	4.6E-03	3.5E-04	0.5	0.021	*	1.3	0.116	0.9	0.329	1.8	0.043	*	0.7	0.002	**	
Isovalerylcarnitine	3.4E-03	3.1E-03	2.5E-03	1.9E-03	7.9E-04	1.5E-03	4.2E-03	4.1E-03	2.7E-03	3.7E-03	3.3E-03	4.4E-03	3.0E-03	4.5E-04	1.4E-03	5.6E-04	3.7E-03	8.3E-04	3.8E-03	5.6E-04	0.5	0.020	*	1.2	0.287	1.3	0.124	2.7	0.006	**	1.0	0.859		
Penicillamine	3.0E-04	3.4E-04	2.5E-04	N.D.	1.3E-04	N.D.	4.2E-04	3.9E-04	3.8E-04	2.9E-04	3.4E-04	4.3E-04	2.9E-04	4.2E-05	1.3E-04	N.A.	4.0E-04	2.0E-05	3.5E-04	7.1E-05	0.4	N.A.		1.3	0.036	*	1.2	0.291	2.7	N.A.		0.9	0.420	
UDP-glucuronic acid	7.2E-04	9.2E-04	7.7E-04	3.0E-04	3.1E-04	4.0E-04	2.3E-03	1.5E-03	1.7E-03	5.1E-04	4.8E-04	2.3E-04	8.0E-04	1.0E-04	3.4E-04	5.3E-05	1.8E-03	3.9E-04	4.1E-04	1.5E-04	0.4	0.006	**	2.3	0.037	*	0.5	0.025	*	1.2	0.523	0.2	0.014	*
Octanoylcarnitine	3.5E-04	4.9E-04	2.6E-04	2.0E-04	1.0E-04	1.5E-04	1.8E-03	5.9E-04	1.2E-04	6.1E-04	4.7E-04	6.9E-04	3.7E-04	1.2E-04	1.5E-04	4.8E-05	8.5E-04	8.9E-04	5.9E-04	1.1E-04	0.4	0.070		2.3	0.445	1.6	0.074	3.9	0.009	**	0.7	0.661		
Hexanoic acid	N.D.	6.1E-04	N.D.	N.D.	N.D.	N.D.	1.2E-03	6.5E-04	N.D.	4.8E-04	N.D.	7.1E-04	6.1E-04	N.A.	N.D.	N.A.	9.4E-04	4.1E-04	6.0E-04	1.7E-04	<1	N.A.		1.5	N.A.	1.0	N.A.	1<	N.A.		0.6	0.438		
Octanoic acid	N.D.	4.0E-04	N.D.	N.D.	N.D.	N.D.	6.8E-04	3.8E-04	N.D.	N.D.	3.6E-04	4.8E-04	4.0E-04	N.A.	N.D.	N.A.	5.3E-04	2.1E-04	4.2E-04	8.8E-05	<1	N.A.		1.3	N.A.	1.0	N.A.	1<	N.A.		0.8	0.604		
Methylguanidine	4.2E-04	5.2E-04	N.D.	N.D.	N.D.	N.D.	N.D.	4.0E-04	5.0E-04	4.6E-04	N.D.	5.1E-04	4.7E-04	7.5E-05	N.D.	N.A.	4.5E-04	7.3E-05	4.9E-04	3.1E-05	<1	N.A.		1.0	0.832	1.0	0.810	1<	N.A.		1.1	0.626		
¹⁵ N-methylguanidine	1.0E-04	8.1E-05	N.D.	N.D.	N.D.	N.D.	N.D.	9.1E-05	8.5E-05	8.9E-05	8.8E-05	9.4E-05	9.3E-05	1.7E-05	N.D.	N.A.	8.8E-05	4.0E-06	9.1E-05	3.3E-06	<1	N.A.		1.0	0.779	1.0	0.893	1<	N.A.		1.0	0.577		
Ethyl glucuronide	N.D.	7.3E-04	N.D.	N.D.	N.D.	N.D.	3.9E-04	N.D.	9.3E-04	N.D.	N.D.	4.7E-04	7.3E-04	N.A.	N.D.	N.A.	6.6E-04	3.8E-04	4.7E-04	N.A.	<1	N.A.		0.9	N.A.	0.7	N.A.	1<	N.A.		0.7	N.A.		
3-Amino-2-piperidone	N.D.	2.0E-04	N.D.	N.D.	N.D.	N.D.	N.D.	1.5E-04	N.D.	N.D.	2.8E-04	2.0E-04	N.A.	N.D.	N.A.	1.5E-04	N.A.	2.8E-04	N.A.	<1	N.A.		0.7	N.A.	1.4	N.A.	1<	N.A.		1.9	N.A.			
<i>N</i> -Methylproline	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	2.4E-04	2.0E-04	2.0E-04	2.1E-04	1.7E-04	2.5E-04	N.D.	N.A.	N.D.	N.A.	2.1E-04	2.1E-05	2.1E-04	3.9E-05	N.A.	N.A.		1<	N.A.	1<	N.A.	1<	N.A.		1.0	0.929		
Isobutyric acid	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	7.4E-04	5.8E-04	N.D.	4.4E-04	N.D.	N.D.	N.D.	N.A.	N.D.	N.A.	6.6E-04	1.1E-04	4.4E-04	N.A.	N.A.	N.A.	1<	N.A.	1<	N.A.	1<	N.A.		0.7	N.A.			
<i>S</i> -Methylmethionine	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	5.2E-05	4.9E-05	5.7E-05	N.D.	N.A.	N.D.	N.A.	N.D.	N.A.	5.2E-05	4.3E-06	N.A.	N.A.	N.A.	1<	N.A.	1<	N.A.	1<	N.A.		1<	N.A.			

N.D.: Not Detected.

N.A.: Not Available.

† candidate compound is predicted from HMT database based on m/z and MT of peaks.

¶ in the case of A vs B, the ratio of the average was calculated as A/B.

§ Welch's *t*-test, *p*-value (*<0.05, **<0.01, ***<0.001)

The peak signal intensities of Ala and Betaine were saturated and the relative areas of ¹³C were used.

Description of XA . . . or XC . . . in compound name indicates unknown peaks, which has been detected in some other organism samples in the HMT database for metabolic identification.