

Supplementary Materials

Table S1. Changes in concentration, presented as fold values, for all metabolites detected in the BBD community after 24 h exposure to 50 µg/L MC-LR as calculated from MetaboAnalyst 2.5 processed data. Metabolites in the microcystin treated community with the most robust differences ($p \leq 0.05$ and fold change ≥ 1.5) from the control (t = 24, no exposure to microcystin) are bolded. Other potentially interesting metabolites with less robust changes ($p \leq 0.1$ and/or fold change ≥ 1.25) are bolded and italicized.

Metabolite	Fold Change	p Value
Pyruvate	0.644	0.454
Sarcosine	1.185	0.189
L-Alanine	1.041	0.922
Lactate	0.755	0.369
<i>N,N-Dimethylglycine</i>	1.299	0.012
4-Aminobutanoate	1.397	0.017
L-Serine	1.015	0.965
L-Proline	1.141	0.170
Fumarate	0.491	0.406
L-Valine	1.344	0.132
<i>Betaine</i>	1.281	0.051
Succinate	1.120	0.862
Methylmalonate	0.947	0.855
L-Threonine	1.575	0.149
Purine	1.108	0.636
Nicotinate	1.435	0.238
Taurine	1.296	0.429
<i>Thymine</i>	1.703	0.082
5-Oxoproline	0.990	0.972
2-Methylmaleate	1.307	0.323
<i>N</i> -Acetyl-beta-Alanine	1.177	0.193
trans-4-Hydroxy- L-Proline	1.146	0.191
L-Leucine	1.249	0.369
L-Isoleucine	1.202	0.510
L-Asparagine	2.486	0.020
Hydroxyisocaproic Acid	0.751	0.363
L-Ornithine	1.086	0.725
L-Aspartate	1.133	0.448
Malate	1.031	0.944
Adenine	1.280	0.442
Hypoxanthine	0.768	0.365
<i>p</i> -Hydroxybenzoate	1.072	0.938
<i>p</i> -Hydroxybenzoate	1.021	0.988
Carbamoyl phosphate	0.829	0.642
2-Oxoglutarate	2.132	0.112

Table S1. Cont.

Metabolite	Fold Change	p Value
L-Glutamine	2.392	0.044
<i>L-Glutamate</i>	1.378	0.005
2-Hydroxy-2-Methylbutanedioic Acid	0.746	0.622
L-Methionine	1.318	0.244
Guanine	0.806	0.300
<i>Xanthine</i>	1.388	0.103
2-Hydroxyphenylacetate	0.837	0.680
Orotate	1.056	0.818
Allantoin	0.976	0.644
L-2-Aminoadipate	1.559	0.144
Methionine sulfoxide	1.146	0.435
Pyridine-2-3-Dicarboxylate	1.072	0.811
Phosphoenolpyruvate	0.630	0.285
Urate	2.218	0.082
Glycerone Phosphate	0.163	0.441
<i>sn</i> -Glycerol 3-phosphate	0.434	0.390
2-Isopropyl-3-Oxosuccinate	1.573	0.597
L-Arginine	1.588	0.039
L-Citrulline	1.349	0.308
<i>N-Carbamoyl- L-Aspartate</i>	1.349	0.086
Allantoate	1.085	0.866
2-Isopropylmalate	1.490	0.332
D-Glucono-1,5-Lactone	1.363	0.129
L-Homocysteic acid	1.672	0.168
3-Phosphoglycerate	0.448	0.424
<i>N</i> -acetyl-Glutamine	1.127	0.439
2-Dehydro-D-Gluconate	1.240	0.556
D-Erythrose-4-phosphate	0.448	0.359
Acetylcarnitine	1.583	0.172
Xanthurenic Acid	0.908	0.711
Lipoate	1.031	0.792
Kynurenine	1.719	0.508
D-Glucarate	1.116	0.556
Deoxyribose-phosphate	0.362	0.462
Cystathionine	1.086	0.708
Flavone	1.101	0.662
Prephenate	1.022	0.767
<i>Deoxyuridine</i>	2.015	0.056
Ribose-phosphate	1.125	0.682
5-Methoxytryptophan	1.084	0.430
Cystine	0.915	0.711

Table S1. Cont.

Metabolite	Fold Change	p Value
Cytidine	1.099	0.576
Uridine	0.964	0.881
Deoxyadenosine	0.924	0.655
Deoxyinosine	1.346	0.478
Shikimate-3-phosphate	1.124	0.582
D-gluconolactone-6-phosphate	0.339	0.151
Glucose-6-phosphate	1.219	0.470
Glucose-1-phosphate	1.254	0.394
Thiamine	1.630	0.018
Adenosine	1.481	0.385
Inosine	2.956	0.142
1-Methyladenosine	1.836	0.253
Guanosine	0.967	0.764
D-Sedoheptulose-1 or 7-phosphate ¹	0.910	0.836
D-Sedoheptulose-1 or 7-phosphate ¹	0.983	0.969
L-Argininosuccinate	1.125	0.539
S-Methyl-5'-Thioadenosine	1.666	0.048
7-Methylguanosine	1.477	0.381
N-Acetyl-Glucosamine-1/6-Phosphate	1.423	0.019
dCMP	0.923	0.672
Glutathione	1.063	0.960
dUMP	2.840	0.037
dTMP	1.676	0.386
CMP	1.112	0.198
UMP	1.151	0.294
Cyclic-AMP	1.453	0.357
Nicotinamide ribotide	0.933	0.641
Aminoimidazole Carboxamide Ribonucleotide	1.471	0.001
Fructose-1-6-bisphosphate	1.754	0.345
Trehalose/Sucrose	1.431	0.365
Thiamine-Phosphate	1.512	0.081
dGMP	1.684	0.371
AMP	0.917	0.332
IMP	0.979	0.849
GMP	1.027	0.895
Riboflavin	1.562	0.373
S-adenosyl-L-Homocysteine	1.243	0.282
dCDP	1.965	0.445
5-Phosphoribosyl-1-Pyrophosphate	0.899	0.510
dTDP	3.747	0.192

Table S1. Cont.

Metabolite	Fold Change	p Value
<i>UDP</i>	1.452	0.051
Thiamine Pyrophosphate	0.883	0.519
Adenosine 5--Phosphosulfate	0.833	0.770
ADP	1.014	0.944
UTP	0.846	0.863
<i>CDP-Choline</i>	1.426	0.078
ATP	0.958	0.927
UDP-D-Glucose	1.394	0.094
UDP- D-Glucuronate	1.243	0.184
ADP- D-Glucose	1.342	0.175
<i>UDP-N-Acetyl-glucosamine</i>	1.373	0.034
Glutathione disulfide	1.899	0.310
<i>NAD⁺</i>	1.435	0.008
NADH	1.522	0.611
<i>Cyclic bis-3,5-dimeric GMP</i>	1.802	0.065
NADP ⁺	1.175	0.422
NADPH	3.008	0.133
<i>FAD</i>	1.367	0.042
Acetyl-CoA	1.147	0.736

Note: the method used cannot differentiate between D-Sedoheptulose-1-phosphate and D-Sedoheptulose-7-phosphate. Therefore, the two observed peaks are both ambiguously labeled as D-Sedoheptulose-1 or 7-phosphate.