Supplementary Material

Metabolomic analysis of the effects of cadmium and copper treatment in *Oryza sativa* L. using untargeted liquid chromatography coupled to high resolution mass spectrometry and all-ion fragmentation.

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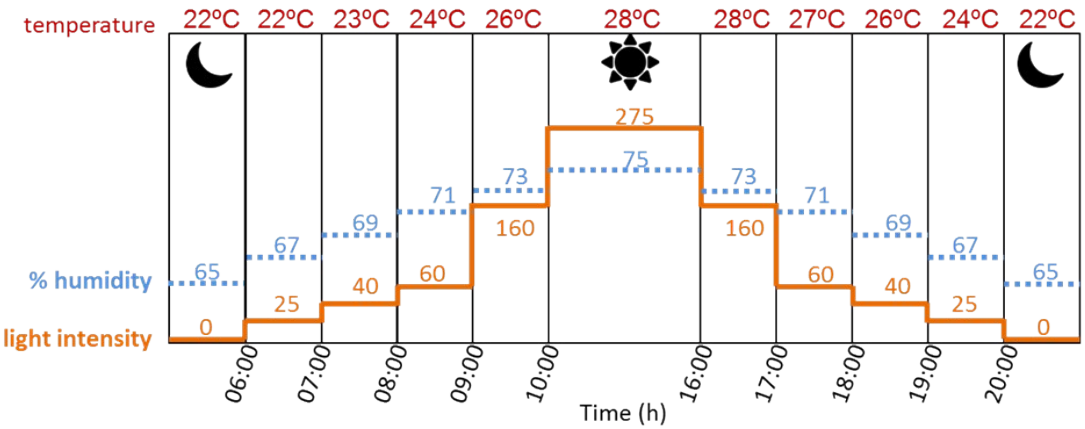

Figure S1. Experimental temperature, relative humidity and light long-day rice cultivation conditions at the growth chamber.

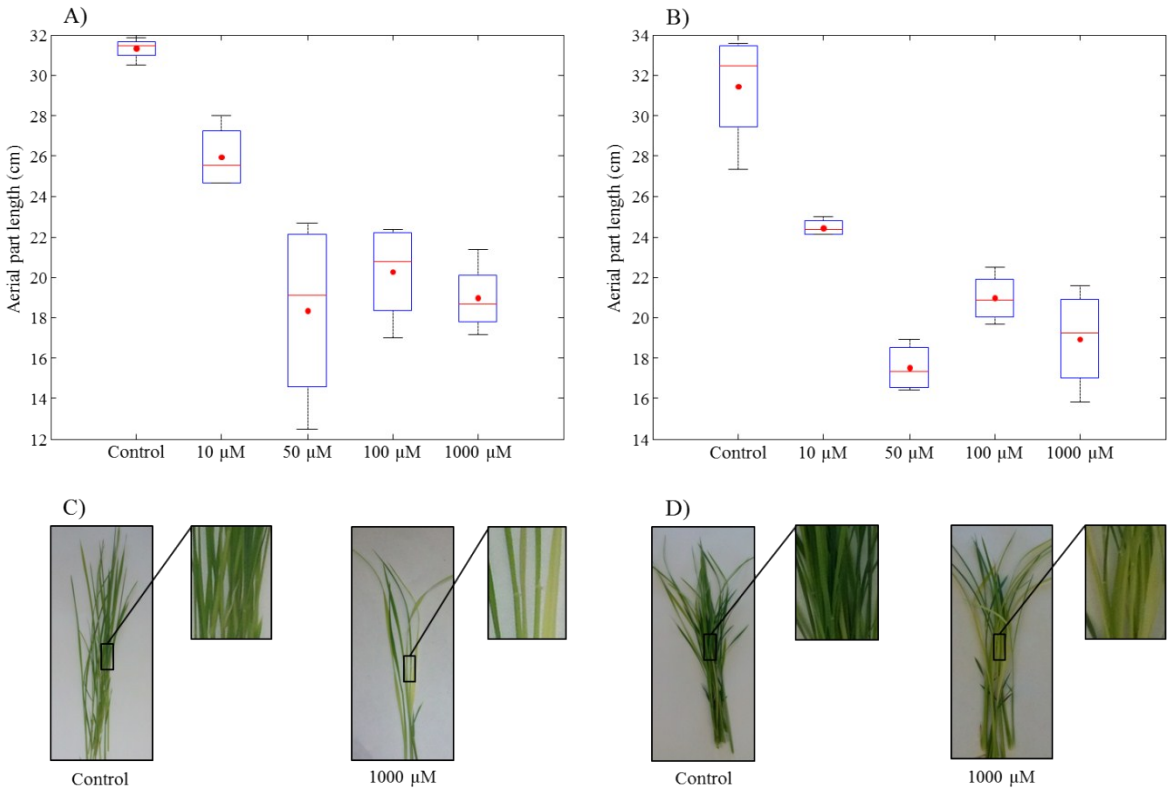

Figure S2. Phenotype information of the studied rice plants. A) Boxplot of the length of aerial parts for Control and Cd(II)-treated plants. B) Boxplot of the length of aerial parts for Control and Cu(II)-treated plants. C) Photographs of Control and 1000 µM Cd(II)-treated plants. D) Photographs of Control and 1000 µM Cu(II)-treated plants. Zooms in C and D show that treated plants were significantly yellowish compared to controls.

Analysis of metal content in root samples

In the case of root samples, 3 mL of HNO3, 1 mL of H2O2 and 0.2 mL of HF were added to 40 mg of sample, and then the mixture was digested in a Teflon reactor for three days. Finally, the samples were diluted with 30 mL of water.

Table S1. Results obtained in the determination of Cd and Cu in roots of the analysed rice samples.

Treatments	Content (µg·g^{-1} dry weight)	
	Cu	Cd
Control 1	47.0	1.18
Control 2	45.14	0.76
10 µM Cu	50.4	2.28
50 µM Cu	87.5	3.29
100 µM Cu	81.7	0.87
1000 µM Cu	176	0.6
10 µM Cd	46.2	74.1
50 µM Cd	43.4	30.2
100 µM Cd	36.9	55.4
1000 µM Cd	38.8	198.8

* Limits of detection were 0.18 µg·g^{-1} for Cd and 1.75 µg·g^{-1} for Cu.

Table S2. AIF identification results. Common metabolites obtained by both metal (Cd(II) and Cu(II)) treatments

					Cd-treatment						Cu-treatment					
Exact mass	**Compound Name**	**Ion Assignment**	**Rel. mass error (ppm)**	**AIF (*m/z*)**	**corrected *p*-value**	**Up/Dow-regulated**	**Fold Change Control vs**				**corrected *p*-value**	**Up/Dow-regulated**	**Fold Change Control vs**			
							10	**50**	**100**	**1000**			**10**	**50**	**100**	**1000**
113.0610	2-Hydroxycyclohexan-1-one *	$[M-H]^-$	1.6	99.0452	5.40E-03	Down	0.50	0.46	0.80	0.46	1.089E-01	Down	1.16	0.81	0.40	0.74
157.0508	2-Isopropylmaleate	$[M-H]^-$	0.9	127.0039/112.0531/ 123.0453	5.97E-03	Up	2.40	2.58	1.07	3.34	3.E-03	Up	1.45	1.66	3.18	1.52
223.0611	Synaptic acid	$[M-H]^-$	0.4	208.0379/93.0347/ 121.0297/149.0246/ 164.0481/1193.0146	5.115E-03	Up	1.89	1.84	2.18	1.65	8.E-03	Down	0.79	0.54	0.41	0.38
327.2186	2,3-Dinor-8-iso prostaglandin F1alpha;	$[M-H]^-$	2.7	310.2150/293.2122/ 125.0972	1.49E-04	Down	0.18	0.51	0.32	0.46	3.E-04	Down	0.20	0.13	0.18	0.09
481.2577	Stearyl citrate	$[M-2H+K]^-$	0.7	190.0149/174.0171/ 268.2727	1.430E-03	Down	0.04	0.12	0.07	0.13	9.E-05	Down	0.52	0.29	0.18	0.17
305.0184	UMP	$[M-H_2O-H]^-$	3.1	111.0201/211.0014	5.461E-03	Down	0.24	0.44	0.42	0.67	4.E-05	Down	0.26	0.23	0.19	0.16
328.0457	Cyclic-AMP	$[M-H]^-$	1.5	134.0054/107.0504/ 192.9911	3.407E-03	Down	0.24	0.44	0.35	0.61	3.E-05	Down	0.25	0.20	0.15	0.13
343.0532	Indole-3-acetyl-methionine *	$[M-2H+K]^-$	2.3	142.0512	5.443E-02	Down	0.78	0.91	0.70	0.55	6.E-01	Down	1.05	1.88	0.92	0.94
145.0619	Glutamine	$[M-H]^-$	0.2	127.0513/128.0355/ 109.0409	3.603E-03	Up	3.77	3.02	1.64	4.33	1.E-01	Up	1.40	1.53	1.72	1.44
342.1110	(6S)-Hydroxyhyoscyamine	$[M-2H+K]^-$	1.0	93.0347/139.0879	2.133E-01	Up	1.33	0.87	1.12	1.17	3.E-01	Up	1.05	1.15	2.74	1.22
401.1303	Cellobiose *	$[M-H+HAc]^-$	0.6	341.1093	2.544E-01	Up	1.31	0.86	1.12	1.17	4.E-01	Up	1.04	1.15	1.29	1.23
102.0563	GABA *	$[M-H]^-$	2.4	-	9.492E-02	Down	0.63	0.60	0.61	0.96	2.E-03	Down	0.49	0.50	0.49	0.56

127.0517	5,6-Dihydrothymine *	$[M-H]^-$	2.7	-	4.08E-03	Up	3.36	2.66	1.58	3.69	4.E-01	Up	1.39	1.51	1.71	3.45
439.0865	3,5-Dihydroxyphenyl 1-O-(6-O-galloyl-beta-D-glucopyranoside)	$[M-H]^-$	3.9	125.0245/93.0347/ 179.0565/147.0662/ 149.0457/133.0509	3.367E-01	Down	1.12	0.85	0.89	0.93	3.E-01	Up	1.17	1.20	1.28	1.07
487.1789	Ptelatoside B	$[M-H+HAc]^-$	4.6	179.0563/147.0661/ 149.0456/133.0505/ 93.0347	5.747E-02	Up	2.50	1.97	0.98	2.65	3.E-01	Up	1.43	1.65	2.18	1.87

* Metabolites identified with less than four IPs.

Table S3. AIF identification results. Metabolites identified only for Cd(II).

Exact mass	Compound Name	Ion Assignment	Rel. mass error (ppm)	AIF (*m/z*)	corrected *p*-value	Up/Dow-regulated	Fold Change Control vs			
							10	50	100	1000
111.0453	Acrolein *	$[2M-H]^-$	1.4	-	1.06.E-01	Down	0.76	0.90	1.41	0.88
134.0374	(Medicarpin	$[M-2H]^{2-}$	0.5	269.1031/254.0956	1.18.E-02	Down	0.49	0.45	0.66	0.48
137.0243	4-Hydroxybenzoate *	$[M-H]^-$	0.8	93.0347	2.10.E-01	Up	1.05	1.26	1.59	1.35
145.0659	Eugenol	$[M-H_2O-H]^-$	4.0	163.0402/148.0533/ 130.0875/102.0279	4.67.E-01	Up	0.84	1.01	1.22	1.04
193.0509	Ferulic acid	$[M-H]^-$	1.1	134.0374/149.0609/ 178.0274	9.92.E-04	Down	0.35	0.45	0.54	0.49
205.0356	(R)-Lipoate	$[M-H]^-$	3.3	100.0487/160.0406	1.12.E-01	Up	1.35	1.28	1.50	1.05
213.1498	(-)-Menthone	$[M-H+HAc]^-$	0.9	111.0453/152.9959/ 138.0199	1.72.E-02	Down	0.95	0.51	1.17	0.64
227.1290	6(E)-8-Oxogeraniol	$[M-H+HAc]^-$	0.4	167.1079/152.0845/ 137.0609/151.1009	3.28.E-03	Down	0.44	0.50	0.66	0.42
241.0120	Galactose 1-phosphate	$[M-H+HAc]^-$	2.7	259.0225/96.9697/ 138.9874	1.55.E-01	Up	1.18	1.20	1.58	1.28
319.0466	Dihydromyricetin	$[M-H]^-$	2.1	194.0284/124.0168/ 177.0196/160.0169/ 143.0139/107.0140	1.49.E-03	Down	0.59	0.58	1.10	0.65
337.0932	Columbamine	$[M-H]^-$	0.8	275.0952/289.1108	1.97.E-02	Down	1.09	0.77	1.60	0.87

367.1041	O-Feruloylquinic acid	$[M-H]^-$	1.9	202.1086/122.0375/ 199.0615/174.0561/ 129.0559/192.0432	1.29.E-02	Up	1.82	1.83	1.63	2.67
515.1231	b-D-Glucuronopyranosyl-(1->3)-a-D-galacturonopyranosyl-(1->2)-L-rhamnose	$[M-H]^-$	4.4	131.0352/192.0262/ 500.0988	2.92.E-01	Down	0.60	0.74	1.11	0.72
671.4685	PA(16:0/18:2(9Z,12Z))	$[M-H]^-$	4.2	391.2256/255.2329/ 433.2364/409.2363/ 415.2257/279.2329	1.20.E-02	Down	0.32	0.43	0.67	0.29
719.4904	PG(16:0/16:1(9Z))	$[M-H]^-$	4.9	687.4284/254.2207	2.48.E-01	Down	0.65	0.85	0.81	0.56
721.5055	PG(16:0/16:0)	$[M-H]^-$	4.2	254.2207/706.4765/ 689.4425	9.19.E-02	Down	0.62	1.06	0.91	0.51
741.4741	1-18:3-2-trans-16:1-phosphatidylglycerol	$[M-H]^-$	3.9	488.2498/464.2501/ 276.2049	3.25.E-01	Down	0.69	0.81	0.79	0.54
793.5193	1-18:1-2-16:0-monogalactosyldiacylglycerol	$[M-2H+K]^-$	4.9	255.2329/295.2643	4.63.E-04	Down	0.46	0.67	0.54	0.36
99.0089	4 -Fumaryl-acetoacetate	$[M-2H]^{2-}$	1.7	100.0123/154.0273/ 112.0123/98.0011	1.76.E-02	Down	1.06	1.06	1.59	0.98
105.0195	Glycerate *	$[M-H]^-$	1.5	-	3.31.E-02	Down	0.98	0.62	1.21	0.81
133.0143	Malic acid *	$[M-H]^-$	0.6	115.0038	3.04.E-03	Down	0.77	0.88	0.93	0.47
145.0143	2-Oxoglutarate *	$[M-H]^-$	0.5	101.0246	8.11.E-03	Up	1.17	1.32	1.15	1.05
153.0323	n-Butyl acetate *	$[M-2H+K]^-$	0.2	-	3.59.E-01	Up	1.47	1.22	1.19	1.26
157.0369	Allantoin	$[M-H]^-$	1.1	129.0196/114.0311	1.63.E-03	Up	4.65	4.17	2.56	5.78
171.0302	3-Dehydroshikimate	$[M-H]^-$	1.6	109.0297/127.0403/ 108.0219/91.0191/ 99.0406	8.31.E-02	Down	0.78	0.71	1.03	0.62
179.0565	Glucose *	$[M-H]^-$	1.9	119.03515	3.94.E-01	Down	0.81	0.78	0.69	0.95
243.0620	Uridine	$[M-H]^-$	1.0	110.0249/140.0356/ 152.0356/200.0569	4.90.E-01	Down	0.43	1.11	0.84	0.81
311.1353	4-Hydroxybutanoate *	$[3M-H]^-$	1.7	-	2.86.E-03	Up	2.01	3.41	2.81	3.18
315.0727	2,5-Dihydroxybenzoate 5-O-β-D-glucoside	$[M-H]^-$	1.6	131.0352/152.0116/ 107.0141/161.0459/ 145.0508/239.0561/ 247.0611	9.70.E-02	Up	1.22	1.26	1.71	1.21

321.1559	Butyl (S)-3-hydroxybutyrate glucoside	$[M-H]^-$	1.3	249.0615/247.0822/ 287.1502/253.1446	2.80.E-01	Up	1.18	1.24	1.44	1.05
337.0570	5-Amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxamide	$[M-H]^-$	4.5	96.96978/125.04167	9.75.E-03	Down	0.73	0.74	1.19	0.68
343.1042	Benzoate β-D-glucose ester	$[M-H+HAc]^-$	2.1	179.056/163.0616/ 149.0456/165.0405/ 121.0297	4.50.E-01	Up	2.28	1.16	1.61	1.15
344.0407	cyclic-GMP	$[M-H]^-$	1.7	133.0151/150.0422	5.01.E-04	Down	0.23	0.42	0.34	0.53
371.0990	Syringin	$[M-H]^-$	1.8	209.0820/433.1508	3.81.E-02	Up	2.13	2.14	1.95	1.93
563.1421	Apigenin 7-O-[beta-D-apiosyl-(1->2)-beta-D-glucoside]	$[M-H]^-$	2.6	269.0666/431.0988	1.04.E-03	Down	0.52	0.49	1.12	0.67
799.2141	6'''-O-Sinapoylsaponarin	$[M-H]^-$	4.8	92.0256/131.0352/ 142.0053/756.1915	4.51.E-03	Down	0.28	0.30	1.68	0.66
130.0876	Leucine*	$[M-H]^-$	1.6	-	3.29.E-01	Up	1.00	0.98	0.66	1.29
164.0720	Phenylalanine	$[M-H]^-$	1.5	147.04529/103.0554	6.09.E-01	Down	0.69	0.81	0.43	0.86
173.0458	Shikimate	$[M-H]^-$	1.2	93.0347/99.0453/ 111.0453/137.0245/ 155.0352	1.82.E-02	Down	0.87	0.61	1.14	0.60
191.0560	L-Quinic acid*	$[M-H]^-$	0.6	96.96971	3.96.E-03	Down	0.76	0.50	0.99	0.51
237.0615	3-Deoxy-D-(manno)-octulosonate	$[M-H]^-$	0.5	221.0665/165.0752	4.67.E-01	Down	0.95	0.94	1.16	0.94
251.1037	2,6-Dihydroxy-N-methylmyosmine	$[M-H+HAc]^-$	0.1	109.01709/157.0316 7/176.67197	3.29.E-03	Down	0.38	0.53	0.49	0.63
301.0537	Cysteine *	$[2M-H+HAc]^-$	1.0	-	1.58.E-01	Down	0.78	1.07	1.11	0.86

311.1353	4-Hydroxybutyric acid *	$[3M-H]^-$	1.7	-	3.84.E-01	Up	0.90	1.55	1.19	1.64
347.0599	Maclurin 3-C-(2"-galloyl-6"-p-hydroxybenzoyl-glucoside)	$[M-2H]^{2-}$	2.5	695.1251/93.0347/109.0296/124.0166/125.0245/136.0166	2.50.E-08	Up	1000.00	1000.00	1000.00	1000.00
363.0337	Xanthylic acid	$[M-H]^-$	3.0	96.9697/108.0219/120.9698/151.0264/211.0013	1.49.E-01	Down	1.24	0.97	1.51	0.70
365.1092	cis-3,4-Leucopelargonidin	$[M-H+HAc]^-$	4.9	109.02960/137.0245/289.07368	1.46.E-04	Down	0.67	0.42	1.00	0.40
385.0547	Shoyuflavone A *	$[M-H]^-$	4.7	133.0144	4.91.E-02	Down	0.72	0.43	0.82	0.39
623.1642	Apigenin 7-O-beta-D-glucoside	$[M-H+HAc]^-$	3.9	432.1024/431.0988/270.0420/269.0454/239.0345/151.0040	9.80.E-04	Down	0.47	0.57	1.28	0.72
785.2200	Kaempferol 3-(2G-apiosylrobinobioside)	$[M-H+HAc]^-$	4.9	93.0347/177.0198/131.0351/147.0303/117.0194/101.0245	3.24.E-05	Down	0.35	0.28	0.85	0.28
815.2290	Cyanidin-3-O-rutinoside-5-O-ß-D-glucoside	$[M-H+HAc]^-$	4.8	93.0347/177.0197/163.0616/179.0565/149.0457/133.0508	1.80.E-06	Down	0.22	0.25	0.86	0.24
96.9698	Phosphate *	$[M-H]^-$	1.5	-	3.61.E-01	Up	1.00	1.01	1.35	1.73
132.0305	Aspartic acid	$[M-H]^-$	2.0	115.0039/114.0562	3.27.E-01	Up	1.79	2.28	3.70	1.68
171.0068	Glycerol 3-phosphate	$[M-H]^-$	2.1	96.9697/152.9597	9.85.E-06	Down	0.39	0.39	0.48	0.51
176.9363	Diphosphate	$[M-H]^-$	2.1	133.0146/114.9489	2.21.E-04	Down	0.49	0.45	0.78	0.35
195.0515	Gluconic acid	$[M-H]^-$	2.2	98.9561/111.0089/128.9598/130.9439/140.9886/149.0536/151.0153	3.25.E-01	Down	1.00	1.12	1.09	0.77
244.0227	3-Phosphoserine	$[M-H+HAc]^-$	0.4	184.0021/96.9697	1.89.E-02	Up	1.95	1.86	1.65	1.51
253.0567	D-Glucuronic acid	$[M-H+HAc]^-$	0.7	193.0358/113.0246/103.0037/101.0246	1.74.E-01	Down	0.71	0.87	1.06	0.82
259.0225	Glucose 1-phosphate	$[M-H]^-$	0.1	96.9155/138.9805/181.0511/240.9522	1.36.E-02	Down	0.65	0.59	0.66	0.59

277.0333	Caffeoylmalic acid	$[M-H_2O-H]^-$	4.9	134.0351/278.0457/ 227.0337/186.0163/ 141.0182/116.0107/ 178.0240	2.68.E-05	Down	0.36	0.43	0.51	0.34
299.0990	D-Ribulose	$[2M-H]^-$	2.1	149.0459/133.0509	6.11.E-03	Down	0.29	0.64	0.46	0.44
313.1145	(2R)-1-O-beta-D-Galactopyranosylglycerol	$[M-H+HAc]^-$	1.7	259.0945/236.0954/ 191.0509/162.0499	1.43.E-05	Down	0.25	0.56	0.37	0.36
331.0554	S-7-Methylthioheptylhydroximoyl-L-cysteine	$[M-2H+K]^-$	1.1	293.0990/130.0876/ 277.0839/278.0763/ 219.0772	3.88.E-03	Up	9.23	7.69	3.23	9.55
423.1797	Sophoraflavanone G	$[M-H]^-$	3.9	93.0347/109.0297/ 179.0387/163.0431/ 147.0456	3.87.E-01	Up	1.57	1.79	1.70	1.73
104.0355	Serine*	$[M-H]^-$	1.9	-	1.90.E-02	Up	2.20	1.96	1.45	2.46
118.0511	Threonine*	$[M-H]^-$	1.0	-	6.53.E-03	Up	2.78	2.46	1.38	3.47
239.0773	Galactose	$[M-H+HAc]^-$	0.1	179.0565/161.0458	1.32.E-02	Down	1.01	0.92	0.99	0.95
274.0120	6-Pyruvoyltetrahydropterin	$[M-2H+K]^-$	1.2	192.0903/162.0489	2.36.E-02	Down	0.66	0.66	0.34	0.60
315.0717	3'-Hydroxy-N-methyl-(S)-coclaurine	$[M-H]^-$	1.4	108.02183/122.0375 /191.0955	5.19.E-03	Up	1.32	0.87	1.12	1.18
341.1092	Trehalose	$[M-H]^-$	2.3	101.0245/113.0246/ 119.0305/143.0349/ 161.0456	3.68.E-03	Down	0.87	0.77	0.81	0.69
377.0857	1-O-Feruloylglucose	$[M-2H+Na]^-$	0.7	179.0565/149.0457/ 133.0509	5.37.E-01	Down	0.87	0.80	0.80	0.68
402.1047	2,4-Dihydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one 2-glucoside	$[M-H]^-$	1.3	179.0565/170.0438	5.50.E-01	Down	0.59	0.45	0.13	1.89
404.1370	Dimethylsulfoniopropanoate*	$[3M-H]^-$	0.8	133.0338	3.23.E-01	Down	1.19	0.74	1.00	0.97
683.2288	Resveratrol	$[3M-H]^-$	0.3	185.0935/227.0647/ 183.0180/159.9910/ 143.0349/157.0987	1.32.E-01	Up	3.32	2.67	1.59	3.63
128.0356	5-Oxoproline*	$[M-H]^-$	2.1	-	3.89.E-03	Up	3.61	2.97	1.13	4.56
329.0874	1-O-vanilloyl-beta-D-glucose	$[M-H]^-$	1.1	179.0565/149.0457/ 165.0406/93.0347	2.92.E-02	Up	9.52	7.42	0.93	61.69
743.2493	Cellobiose	$[2M-H+HAc]^-$	4.1	341.1093/179.0565/ 149.0457/133.0509	1.75.E-01	Down	1.20	0.74	1.01	0.98

* Metabolites identified with less than four IPs.

Table S4. AIF identification results. Metabolites identified only for Cu(II).

Exact mass	Compound Name	Ion Assignment	Rel. mass error (ppm)	AIF (*m/z*)	corrected *p*-value	Up/Dow-regulated	Fold Change Control vs			
							10	50	100	1000
409.2365	1-Palmitoylglycerol 3-phosphate	$[M-H]^-$	1.0	152.9959/255.2329/171.0065	1.35E-04	Down	0.27	0.25	0.19	0.17
431.2209	6-Aminopenicillanate	$[2M-H]^-$	4.4	215.1078/171.0066	4.893E-05	Down	0.45	0.31	0.14	0.14
433.2365	LPA(0:0/18:2(9Z,12Z))	$[M-H]^-$	1.1	278.2207/153.9993/169.9923/416.2294	2.20E-05	Down	0.43	0.33	0.14	0.14
459.2337	Fusicoplagin A*	$[M-2H+Na]^-$	4.8	347.2593	4.90E-05	Down	0.11	0.03	0.07	0.03
503.2417	PG(18:4(6Z,9Z,12Z,15Z)/0:0)	$[M-H]^-$	1.4	152.9959/90.0350	1.990E-05	Down	0.70	0.41	0.24	0.24
134.0474	Adenine	$[M-H]^-$	1.5	106.0664/107.0365	3.97E-03	Down	0.52	0.52	0.43	0.42
179.0387	Methyl-5-thio-D-ribose	$[M-H]^-$	2.2	161.0403/144.0305/130.0229/116.0072/102.0279	7.104E-03	Up	2.03	1.85	2.21	1.15
226.9966	3-Dehydroquinate	$[M-2H+K]^-$	1.0	127.0403/171.0302/109.0295/153.0194/125.0245/189.0199/117.0348	1.260E-04	Up	1.80	1.65	1.62	2.51
266.0895	Adenosine	$[M-H]^-$	0.0	134.0474/107.0365	1.37E-03	Down	0.52	0.45	0.41	0.40
267.1084	2'-Deoxyribose	$[2M-H]^-$	0.5	133.0509/103.0403	5.405E-04	Up	24.43	22.25	30.03	14.04

299.0776	1R,6R)-6-Hydroxy-2-succinylcyclohexa-2,4-diene-1-carboxylate	$[M-H+HAc]^-$	1.1	239.0561/137.0246/101.0246/222.0532/194.0588	3.914E-07	Up	0.80	1.36	5.65	5.64
312.0954	5-(3'-Carboxy-3'-oxopropenyl)-4,6-dihydroxypicolinate	$[M-H+HAc]^-$	1.3	99.0088/151.0262/219.0161	1.936E-03	Down	0.48	0.42	0.34	0.34
430.1568	Oxynarcotine	$[M-H]^-$	4.6	137.0246/196.0986/193.0511	9.E-01	Up	1.01	1.20	1.14	1.29
110.0251	3,4-Dihydroxypyridine *	$[M-H]^-$	3.5	-	5.E-01	Down	0.68	2.09	0.64	0.69
113.0245	Prop-2-ynal *	$[M-H+HAc]^-$	1.0	-	1.E-01	Down	0.63	0.86	0.72	0.74
242.0800	Pantothenol	$[M-2H+K]^-$	0.2	102.0562/126.0938	1.60E-03	Up	1.44	1.45	1.34	1.62
316.1173	Glycerophosphocholine *	$[M-H+HAc]^-$	2.0	199.0341	4.36E-03	Up	1.46	1.47	1.37	1.62
489.1643	Phloroacetophenone 6'-[xylosyl-(1->6)-glucoside]	$[M-H]^-$	4.9	195.0615/179.0561/149.0457/165.0406	6.E-01	Up	1.30	1.28	0.90	1.05
175.0251	Ascorbic acid	$[M-H]^-$	1.8	113.02462/157.03676/115.07661/139.08801/130.28988	2.686E-05	Up	5.62	7.40	36.71	22.14
336.0875	S-(Hydroxymethyl)glutathione	$[M-H]^-$	1.3	320.0678/319.0844/305.0689/277.0738/185.0571	3.201E-07	Up	3.65	5.67	13.53	9.87

* Metabolites identified with less than four IPs.