Supplemental table 1. Other putative metabolites in negative ionization mode (ESI-)

Baseline	Control 4 weeks	Cocoa 4 weeks	RT (min)	Detected mass (m/z)	Metabolite putative identification	Assignation	Mass difference (mDa)
nd	10.15	7.75	4.086	246.0463	Phenylephrine 3-O-sulfate	$[M-H]^-$	-2.1
0.87	5.00	10.68	6.131	197.0678	5-Acetylamino-6-amino-3-methyluracil	$[M-H]^-$	0.2
13.25	5.71	8.89	6.367	232.0278	Dopamine 4-O-sulfate	$[M-H]^-$	0.7
			6.367	232.0278	Dopamine 3-O-sulfate	$[M-H]^-$	0.7
3.96	6.90	13.06	6.944	165.0424	7-Methylxanthine	$[M-H]^-$	-0.6
			6.944	165.0424	3-Methylxanthine	$[M-H]^-$	-0.6
1.21	11.55	8.55	7.971	261.0113	2,4-dichlorophenoxybutyric acid. methyl ester	$[M-H]^-$	-2.2
			7.971	261.0113	phenylglycol 3-O-sulfate	$[M+HCOO]^-[-H_2O]$	-2.3
			7.971	261.0113	4-Sulfobenzoate	$[M+CH_3COO]^-$	-3.9
2.20	10.66	6.96	8.267	375.1325	Asp Trp Gly	$[M-H]^-$	-1.5
			8.267	375.1325	Riboflavin	$[M-H]^-$	-1.5
			8.267	375.1325	Asp Ile Trp	$[M-H]^-$	-1.5
			8.267	375.1325	Trp Asp Gly	$[M-H]^-$	-1.5

			8.312	137.0244	(2S,3S)-2,3-Dihydro-2,3-dihydroxybenzoate	$[M-H]^-[-H_2O]$	0.0
			8.312	137.0244	3-Methyl-cis.cis-hexadienedioate	$[M-H]^-[-H_2O]$	0.0
			8.312	137.0244	3-Methylmuconolactone	$[M-H]^-[-H_2O]$	-0.5
			8.312	137.0244	4-Methylmuconolactone	$[M-H]^-[-H_2O]$	-0.5
0.93	1.64	14.92	8.312	137.0244	1,6-Dihydroxycyclohexa-2,4-diene-1-carboxylate	$[M-H]^-[-H_2O]$	-0.5
			8.312	137.0244	2-Hydroxy-6-keto-2,4-heptadienoate	$[M-H]^-[-H_2O]$	-0.5
			8.312	137.0244	(1R,6S)-1.6-Di,hydroxycyclohexa-2,4-diene-1-carboxylate	$[M-H]^-[-H_2O]$	-0.5
			8.312	137.0244	2-Hydroxy-5-methyl-cis,cis-muconic semialdehyde	$[M-H]^-[-H_2O]$	-0.5
			8.312	137.0244	4-Methyl-3-oxoadipate-enol-lactone	$[M-H]^-[-H_2O]$	-0.5
nd	2.50	16.16	8.317	216.9812	5-Sulfosalicylate	$[M-H]^-$	0.0
			8.318	389.1019	Ser-Tyr-OH	$[M-H]^-$	-2.8
			8.318	389.1019	Tyr-Ser-OH	$[M-H]^-$	-2.8
			8.318	389.1019	Dopaxanthin	$[M-H]^-$	-2.8
2.09	6.59	11.50	8.318	389.1019	3,5-Pyridinedicarboxylic acid. 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-carboxymethyl methyl est	$[M-H]^-$	-2.8
			8.318	389.1019	Glabrescin	$[M-H]^-[-H_2O]$	0.6

			8.318	389.1019	Dehydroamorphigenin	$[M-H]^-[-H_2O]$	0.6
			8.318	389.1019	Ferrugone	$[M-H]^-[-H_2O]$	0.6
			8.318	389.1019	5-Methoxydurmillone	$[M-H]^-[-H_2O]$	0.6
6.02	15.16	8.45	8.352	330.0318	C13H9N5O4S	$[M-H]^-$	-1.5
			8.600	125.0240	(E)-2-Methylglutaconic acid	$[M-H]^-[-H_2O]$	-0.1
			8.600	125.0240	3-hexenedioic acid	$[M-H]^-[-H_2O]$	-0.1
			8.600	125.0240	2,3-Dimethylmaleate	$[M-H]^-[-H_2O]$	-0.1
			8.600	125.0240	(E)-3-methylglutaconic acid	$[M-H]^-[-H_2O]$	-0.1
4.58	11.76	5.08	8.600	125.0240	(E)-hex-2-enedioic acid	$[M-H]^-[-H_2O]$	-0.1
			8.600	125.0240	1,5-Anhydro-4-deoxy-D-glycero-hex-1-en-3-ulose	$[M-H]^-[-H_2O]$	-0.1
			8.600	125.0240	1,5-Anhydro-4-deoxy-D-glycero-hex-3-en-2-ulose	$[M-H]^-[-H_2O]$	-0.1
			8.600	125.0240	Allylmalonic acid	$[M-H]^-[-H_2O]$	-0.1
			8.600	125.0240	Methylitaconate	$[M-H]^-[-H_2O]$	-0.1
0.40	9.94	3.36	8.681	273.0116	C6H10O12	$[M-H]^-$	-1.7
			8.685	193.0506	Scytalone	$[M-H]^-$	-1.6

			8.685	193.0506	Isoferulic acid	$[M-H]^-$	-1.6
			8.685	193.0506	Monoethyl phthalate	$[M-H]^-$	-1.6
			8.685	193.0506	5-Hydroxyconiferaldehyde	$[M-H]^-$	-1.6
13.74	6.69	6.07	8.723	476.1172	Isorhamnetin 7-alpha-D-Glucosamine	$[M-H]^-$	2.7
nd	0.84	11.43	8.107	415.1278	Asp Asp Trp	$[M-H]^-[-H_2O]$	-2.4
			8.107	415.1278	Trp Asp Asp	$[M-H]^-[-H_2O]$	-2.4
			8.107	415.1278	Asp Trp Asp	$[M-H]^-[-H_2O]$	-2.4
			8.107	415.1278	N5-Dinitrophenyl-L-ornithine methyl ester	$[M+HCOO]^-[-H_2O]$	-1.9
			8.107	415.1278	HoPhe-Phe-OH	$[M-H]^-[-H_2O]$	1.6
			8.107	415.1278	Phe-HoPhe-OH	$[M-H]^-[-H_2O]$	1.6

Abbreviations: nd, no detected; RT, retention time.
The following comparisons were $p<0.01$: baseline vs. control, baseline vs. cocoa and control vs. cocoa.
The data in baseline, control and cocoa columns refers to mean intensity of metabolites and are presented as log 2.