SUPPLEMENTAL INFORMATION

SUPPLEMENTAL INFORMATION – TABLE S1. qRT-PCR primers used in this study.

Gene ID	Gene name	Primer sequences (5'–3')
MDP0000636927	*LAR*	F: GAAAATTGGCCGGACTCTCC
		R: TTCCCACTTCCACATCACGA
MDP0000575740	*CHS*	F: CTCGCTCTTCTGGATTGCAC
		R: CCACTCCAGTCCTTCTCCAG
MDP0000229348	*C4H*	F: AGTCGAAGGTGGAGGCTAAC
		R: CCCTCGGCTTCATCACAATG
MDP0000788934	*ANS*	F: GCGTGACTTGTCAATTTGGC
		R: ACTTCTTTCTCCAGCCTCCC
MDP0000306738	*β-Glu*	F: AACTTCGTATGGTGGGTGGT
		R: GGGTTGGATAGGTGTGTGGA
MDP0000190489	*F3'5'H*	F: CTGAACGTGTGCACAGTCAA
		R: GGTCAAGAAGGCATCGAACC
MDP0000774288	*MdActin*	F: TTGCAGACCGTATGAGCCG
		R: GGACCCTCCAATCCAGACAC

SUPPLEMENTAL INFORMATION – TABLE S2. Statistical table of differential metabolites.

	Compounds	Class I	VIP	Fold_Change	Log2FC	Type
1	3-Hydroxy-3-methyl butyric acid	Organic acids	1.302393073	2.100892079	1.07E+00	Up
2	2-Methylsuccinic acid*	Organic acids	1.335532711	2.163110894	1.11E+00	Up
3	Adenine*	Nucleotides and derivatives	1.318305907	2.499701233	1.32E+00	Up
4	Hypoxanthine*	Nucleotides and derivatives	1.342133308	2.122002602	1.09E+00	Up
5	Allopurinol*	Nucleotides and derivatives	1.336246669	2.052562748	1.04E+00	Up
6	Hydroxyphenethylamine	Others	1.25563481	2.12771305	1.09E+00	Up
7	Tyrosol	Phenolic acids	1.108801374	2.517590828	1.33E+00	Up
8	*O*-Phosphorylethanolamine	Others	1.063430566	6.903912927	2.79E+00	Up
9	Indole-3-carboxaldehyde	Alkaloids	1.327094176	2.168531848	1.12E+00	Up
10	p-Coumaryl alcohol	Phenolic acids	1.05809123	7.527037047	2.91E+00	Up
11	2,3-Dihydroxybenzoic Acid*	Organic acids	1.232559958	2.088511949	1.06E+00	Up
12	L-Histidine	Amino acids and derivatives	1.271872106	5.942009701	2.57E+00	Up
13	3-Hydroxy-3-methylpentane-1,5-dioic acid	Amino acids and derivatives	1.134557504	2.166174479	1.12E+00	Up
14	D-Xylonic acid	Organic acids	1.355646774	2.392459514	1.26E+00	Up
15	1-Methylhistidine*	Amino acids and derivatives	1.152024936	2.410838981	1.27E+00	Up
16	Glycyl-L-proline	Amino acids and derivatives	1.094541111	2.023982225	1.02E+00	Up
17	L-(+)-Arginine	Amino acids and derivatives	1.172714626	4.854908848	2.28E+00	Up
18	L-Citrulline	Amino acids and derivatives	1.215207864	2.314071626	1.21E+00	Up
19	Trans-4-Hydroxycinnamic Acid Methyl Ester*	Phenolic acids	1.220222568	2.21832037	1.15E+00	Up
20	4-Hydroxy-3-methoxycinnamaldehyde*	Phenolic acids	1.315797688	2.976402264	1.57E+00	Up
21	Coniferaldehyde*	Phenolic acids	1.22574538	2.321621774	1.22E+00	Up
22	Methyl p-coumarate*	Phenolic acids	1.224992938	2.235462892	1.16E+00	Up
23	Caffeic acid*	Phenolic acids	1.262571902	17.90096632	4.16E+00	Up
24	N-α-Acetyl-L-glutamine	Amino acids and derivatives	1.229615424	3.274389728	1.71E+00	Up
25	H-HomoArg-OH	Amino acids and derivatives	1.20216966	6.989366424	2.81E+00	Up
26	ferulate acid*	Others	1.374772063	6.124373923	2.61E+00	Up
27	D-Pinitol	Others	1.279046199	2.317930504	1.21E+00	Up
28	Gluconic acid	Others	1.306497767	2.611650485	1.38E+00	Up
29	L-Tryptophan	Amino acids and derivatives	1.280068734	15.10206921	3.92E+00	Up
30	Methoxyindoleacetic acid	Alkaloids	1.315674622	8.187696193	3.03E+00	Up
31	3,4-Dimethoxycinnamic acid*	Phenolic acids	1.093469052	2.070464263	1.05E+00	Up
32	Sinapinaldehyde*	Phenolic acids	1.312207691	4.633264929	2.21E+00	Up
33	N-α-Acetyl-L-arginine	Amino acids and derivatives	1.247134095	2.582601008	1.37E+00	Up
34	Glycylphenylalanine	Amino acids and derivatives	1.343015272	2.681246985	1.42E+00	Up
35	Vomifoliol	Others	1.342555998	31.11209093	4.96E+00	Up
36	11-Octadecanoic acid (Vaccenic acid)*	Lipids	1.363627597	2.084809608	1.06E+00	Up
37	Elaidic Acid*	Lipids	1.366341218	2.131044014	1.09E+00	Up
38	Guanosine	Nucleotides and derivatives	1.280964838	2.372235294	1.25E+00	Up
39	Xanthosine	Nucleotides and derivatives	1.092527327	2.496846262	1.32E+00	Up
40	Nicotinic acid-hexoside	Others	1.303489289	3.234416468	1.69E+00	Up
41	Catechin*	Flavonoids	1.358178247	2.241568089	1.16E+00	Up
42	9-Hydroxy-10,12-octadecadienoic acid*	Lipids	1.283537202	2.016113856	1.01E+00	Up
43	12,13-EODE*	Lipids	1.334540025	2.998855765	1.58E+00	Up
44	9S-Hyroxy-10E,12E-octadecadienoic acid*	Lipids	1.292796624	2.09112401	1.06E+00	Up
45	13-Hydroxy-9,11-octadecadienoic acid*	Lipids	1.298928354	2.07661559	1.05E+00	Up
46	(-)-Epigallocatechin	Flavonoids	1.050173073	7.717435836	2.95E+00	Up
47	Feruloylmalic acid	Phenolic acids	1.32309058	5.089774393	2.35E+00	Up
48	Eicosenoic acid	Lipids	1.353542199	2.253865237	1.17E+00	Up

SUPPLEMENTAL INFORMATION – TABLE S2. Statistical table of differential metabolites.

	Compounds	Class I	VIP	Fold_Change	Log2FC	Type
49	13-Oxo-9-hydroxy-10-octadecenoic acid*	Lipids	1.329224578	2.079905676	1.06E+00	Up
50	9,10-Dihydroxy-12-octadecenoic acid	Lipids	1.365699216	2.884470529	1.53E+00	Up
51	9,12,13-Trihyroxy-10,15-octadecadienoic acid	Lipids	1.19587225	2.269131453	1.18E+00	Up
52	9,10,13-Trihyroxy-11-octadecadienoic acid	Lipids	1.377129812	3.797951286	1.93E+00	Up
53	Hexadecanoic acid 2,3-dihydroxypropyl ester	Lipids	1.377295394	3.719714647	1.90E+00	Up
54	3-*O*-(E)-p-Coumaroyl quinic acid*	Phenolic acids	1.270463468	2.123912642	1.09E+00	Up
55	Chlorogenic acid*	Phenolic acids	1.359374424	11.25284069	3.49E+00	Up
56	Glyceryl linoleate*	Lipids	1.30385266	2.130057685	1.09E+00	Up
57	Pinoresinol	Lignans and Coumarins	1.11278334	2.066903216	1.05E+00	Up
58	Chlorogenic acid methyl ester*	Phenolic acids	1.281695201	3.01143296	1.59E+00	Up
59	Kaempferol-3-arabinopyranoside*	Flavonoids	1.271050464	2.811815336	1.49E+00	Up
60	Juglanin*	Flavonoids	1.247289278	2.518704387	1.33E+00	Up
61	Pinocembrin 7-*O*-β-D-glucoside (Pinocembroside)	Flavonoids	1.356884119	2.839784946	1.51E+00	Up
62	(+)-Syringaresinol	Lignans and Coumarins	1.301208034	2.418489463	1.27E+00	Up
63	Kaempferol 7-*O*-rhamnoside*	Flavonoids	1.299197159	2.236173248	1.16E+00	Up
64	Catechin-(7,8-bc)-4β-(3,4-dihydroxyphenyl)-dihydro-2-(3H)-pyranone*	Flavonoids	1.284584731	4.083814926	2.03E+00	Up
65	Cinchonain Ic*	Flavonoids	1.319640348	4.407983095	2.14E+00	Up
66	Cinchonain Id*	Flavonoids	1.181643366	3.772639183	1.92E+00	Up
67	Sanguisorbigenin	Terpenoids	1.282645693	3.309273466	1.73E+00	Up
68	24,30-Dihydroxy-12(13)-enolupi nol	Terpenoids	1.24570747	2.223739477	1.15E+00	Up
69	2-Hydroxyoleanolic acid*	Terpenoids	1.286230352	2.198229011	1.14E+00	Up
70	Maslinic acid*	Terpenoids	1.307059592	2.193477504	1.13E+00	Up
71	10-Formyl-THF	Alkaloids	1.367540268	7.197081626	2.85E+00	Up
72	1β,2α,3α,19α-Tetrahydroxyurs-12-en-28-oic acid	Terpenoids	1.022022124	2.563862063	1.36E+00	Up
73	Cynarin	Phenolic acids	1.386228237	3646.407407	1.18E+01	Up
74	Kaempferol 3-*O*-(6"-*O*-malonyl)-galactoside*	Flavonoids	1.068575887	2.192240974	1.13E+00	Up
75	Kaempferol 3-*O*-(6"-*O*-malonyl)-glucoside*	Flavonoids	1.029676977	6.155099212	2.62E+00	Up
76	Kaempferol Gallyl Glucoside	Flavonoids	1.36747713	2.495304386	1.32E+00	Up
77	p-Coumaroyleuscaphic acid	Terpenoids	1.372801773	16.78969251	4.07E+00	Up
78	Caffeoyl hawthorn acid	Terpenoids	1.08213007	2.170116488	1.12E+00	Up
79	1,1-Kestotetraose*	Others	1.32668657	2.245308819	1.17E+00	Up
80	3β-[(α-L-Arabinopyranosyl)oxy]-23-hydroxyurs-12,19(29)-dien-28-oic acid 28-β-d-glucopyranosyl ester	Terpenoids	1.093439692	2.103560454	1.07E+00	Up
81	Betaine*	Alkaloids	1.006790071	0.349096893	-1.52E+00	Down
82	Benzoic acid*	Phenolic acids	1.386505991	0.000241879	-1.20E+01	Down
83	4-Aminoindole	Alkaloids	1.385856494	3.61683E-05	-1.48E+01	Down
84	1,2-N-Methylpipecolic acid	Amino acids and derivatives	1.116748663	0.328511838	-1.61E+00	Down
85	Proline betaine (ProBet)	Amino acids and derivatives	1.152339392	0.305981212	-1.71E+00	Down
86	2-Methylglutaric acid*	Organic acids	1.357846816	0.464896403	-1.11E+00	Down
87	Orotic acid	Others	1.223798079	0.403112811	-1.31E+00	Down
88	p-Coumaric acid	Phenolic acids	1.290427328	0.1184041	-3.08E+00	Down
89	Gallacetophenone*	Others	1.37827341	0.387669753	-1.37E+00	Down
90	SubericAcid	Organic acids	1.331978621	0.382059201	-1.39E+00	Down
91	D-(+)-Galactose*	Others	1.309545393	0.411062926	-1.28E+00	Down
92	D-(+)-Mannose*	Others	1.317439679	0.462169855	-1.11E+00	Down

SUPPLEMENTAL INFORMATION – TABLE S2. Statistical table of differential metabolites.

	Compounds	Class I	VIP	Fold_Change	Log2FC	Type
93	Ayapin	Lignans and Coumarins	1.355652577	0.382198389	-1.39E+00	Down
94	Anchoic Acid	Organic acids	1.373842372	0.416779007	-1.26E+00	Down
95	2,6-Dimethyl-7-octene-2,3,6-triol	Others	1.36044115	0.371982793	-1.43E+00	Down
96	12-Hydroxydodecanoic acid	Lipids	1.340995889	0.429951384	-1.22E+00	Down
97	Dodecanedioic acid	Organic acids	1.337830441	0.372096524	-1.43E+00	Down
98	Octadecenoic amide	Others	1.334913469	0.453334609	-1.14E+00	Down
99	2-β-D-Glucopyranosyloxy-2-phenylacetic acid amide	Alkaloids	1.261053047	0.402803395	-1.31E+00	Down
100	Androsin	Others	1.35888776	0.306267219	-1.71E+00	Down
101	3-Hydroxy-4-isopropylbenzylalcohol 3-glucoside	Phenolic acids	1.367718553	0.353616201	-1.50E+00	Down
102	Cis-4,7,10,13,16,19-Docosahexaenoic Acid (C22:6n3)	Lipids	1.238565135	0.486957665	-1.04E+00	Down
103	Vanillic acid glycoside*	Phenolic acids	1.366128592	0.229337002	-2.12E+00	Down
104	1-*O*-Galloyl-β-D-glucose*	Phenolic acids	1.17038511	0.424555075	-1.24E+00	Down
105	1-*O*-p-Coumaroyl quinic acid*	Phenolic acids	1.363777659	0.300743833	-1.73E+00	Down
106	Homovanilloyl quinic acid*	Organic acids	1.35572315	0.349611723	-1.52E+00	Down
107	Byzantionoside A	Others	1.148613779	0.345531872	-1.53E+00	Down
108	Syringin	Phenolic acids	1.122427913	0.449204931	-1.15E+00	Down
109	N6-Succinyl Adenosine	Nucleotides and derivatives	1.230918244	0.479077022	-1.06E+00	Down
110	Roseoside	Others	1.340348241	0.413191043	-1.28E+00	Down
111	Penstemonoside	Terpenoids	1.341511413	0.417837638	-1.26E+00	Down
112	Di-p-Coumaroyltartaric acid	Phenolic acids	1.385946163	0.000426284	-1.12E+01	Down
113	4-hydroxycoumarin di-glucoside	Lignans and Coumarins	1.27955514	0.328481279	-1.61E+00	Down
114	5-*O*-p-Coumaroyl quinic acid *O*-hexoside*	Phenolic acids	1.341060546	0.304781751	-1.71E+00	Down
115	Sinapoyl-p-coumaroyltartaric acid	Phenolic acids	1.243903976	0.231835687	-2.11E+00	Down
116	(6S,7E,9R)-6,9-Dihydroxy-4,7-megastigmadin-3-one-9-*O*-D-xylopyranosyl(1-6)-glucopyranoside	Others	1.381644549	0.27142516	-1.88E+00	Down
117	Feruloylsinapoyltartaric acid	Phenolic acids	1.104620275	0.350073895	-1.51E+00	Down
118	β-D-Furanofructosyl-α-D-(6-mustard acyl) glucoside*	Phenolic acids	1.225146653	0.367140341	-1.45E+00	Down
119	3-Hydroxy-5-Methylphenol-1-Oxy-β-D-(6'-*O*-Digalloyl)Glucose	Phenolic acids	1.195032677	0.237312035	-2.08E+00	Down
120	Luteolin-7-*O*-rutinoside*	Flavonoids	1.248622929	0.444141575	-1.17E+00	Down
121	Quercetin glc-rha*	Flavonoids	1.224536383	0.4723189	-1.08E+00	Down
122	Bioquercetin*	Flavonoids	1.298618452	0.460358755	-1.12E+00	Down
123	Quercetin-3-*O*-(2-*O*-α-L-rhamnopyranosyl)-β-D-galactopyranoside*	Flavonoids	1.354266376	0.470029415	-1.09E+00	Down