Nitrogen Starvation and Nitrate or Ammonium Availability Differently Affect Phenolic Composition in Green and Purple Basil

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SUPPLEMENTARY MATERIAL

SUPPLEMENTARY TABLE S1. Comparison of plant biomass in green ('Italiano Classico', IC) and purple ('Red Rubin', RR) basil (*Ocimum basilicum* L.). g FW plant^{-1}: grams of fresh weight per plant. L/R: ratio of the biomass of leaves and roots. Plants were exposed for 5 d to absence of N - control [con], 10 mM NO_3^- - nitrate [nit] or 10 mM NH_4^+ - ammonium [amm]. Values are the mean ± SEM (standard error of the mean, n = 6). The statistical significance within each N nutritional treatment was assessed by Student's t-test ($p < 0.05$).

Parameter	N Treatment	IC	RR	Significance (p value)
		Mean ±SEM	Mean ±SEM	Mean ±SEM
Root biomass (g FW plant^{-1})	**con**	5.65 ± 0.30 (a)	2.11 ± 0.10 (b)	< 0.001
	nit	7.44 ± 0.80 (a)	2.53 ± 0.19 (b)	< 0.001
	amm	4.99 ± 0.40 (a)	1.93 ± 0.15 (b)	< 0.001
Leaf biomass (g FW plant^{-1})	**con**	5.23 ± 0.29 (a)	4.26 ± 0.10 (b)	0.010
	nit	7.66 ± 0.44 (a)	5.23 ± 0.33 (b)	0.001
	amm	5.77 ± 0.26 (a)	4.40 ± 0.16 (b)	0.001
L/R	**con**	0.93 ± 0.02 (b)	2.03 ± 0.06 (a)	< 0.001
	nit	1.06 ± 0.08 (b)	2.08 ± 0.04 (a)	< 0.001
	amm	1.17 ± 0.04 (b)	2.32 ± 0.10 (a)	< 0.001

SUPPLEMENTARY TABLE S2. Details about compound identifications by LC-ESI-MS/MS. RT: retention time. Mod: negative (-) or positive (+) acquisition mode. $[M-H]^-$ or $[M+H]^+$ molecular ion (m/z: mass/charge). In brackets are reported the average relative abundances of each fragment ion. For further details, see ref [5] doi:10.3390/plants9010022.

Compound	RT (min)	Formula	Mod	$[M-H]^-$ or $[M+H]^+$ (m/z)	MS^2 fragmentation profile (m/z)
Salvianic acid A	2.6	$C_9H_{10}O_5$	-	197.04	197.04 (14), 179.03 (57), 135.04 (84), 123.04 (57), 72.99 (100)
Salvianolic acid K	11.7	$C_{27}H_{24}O_{13}$	-	555.11	537.10 (18), 493.11 (40), 295.06 (100)
Chicoric acid	12.0	$C_{22}H_{18}O_{12}$	-	473.07	311.04 (91), 293.03 (28), 179.03 (50), 149.01 (100)
Salvianolic acid L	14.8	$C_{36}H_{30}O_{16}$	-	717.15	717.15 (100), 673.16 (10), 537.10 (26), 519.09 (33), 321.04 (7), 295.06 (6)
Rosmarinic acid	15.2	$C_{18}H_{16}O_8$	-	359.08	359.08 (11), 197.04 (33), 179.03 (8), 161.02 (100)
Dihydroquercetin glucoside	8.0	$C_{21}H_{22}O_{12}$	+	467.12	287.06 (19), 259.06 (95), 231.07 (60), 167.03 (13), 153.02 (90), 149.02 (80), 123.04 (45)
Cyanidin glucoside	11.0	$C_{21}H_{21}O_{11}$	+	449.11	287.06 (100)
Quercetin rutinoside	11.6	$C_{27}H_{30}O_{16}$	+	611.16	303.05 (100)
Quercetin glucoside	12.0	$C_{21}H_{20}O_{12}$	+	465.10	303.05 (100)
Anthocyanin A*	12.1	$C_{51}H_{53}O_{26}$	+	1081.28	1081.28 (100), 919.23 (75), 449.11 (22), 287.06 (45)
Anthocyanin B1*	12.9	$C_{54}H_{55}O_{29}$	+	1167.28	1167.28 (100), 1005.25 (9), 919.23 (11), 535.11 (19), 287.06 (16)
Anthocyanin B2*	13.4	$C_{54}H_{55}O_{29}$	+	1167.28	1167.28 (100), 1005.23 (55), 449.11 (9), 287.06 (24)
Anthocyanin C*	13.6	$C_{51}H_{53}O_{25}$	+	1065.29	1065.29 (100), 903.23 (95), 449.11 (26), 287.06 (57)
Naringenin glucoside	13.9	$C_{21}H_{22}O_{10}$	+	435.13	273.08 (100), 153.02 (51), 147.04 (26)
Apigenin galacturonide	14.2	$C_{21}H_{18}O_{11}$	+	447.09	271.06 (100)
Anthocyanin D1*	14.4	$C_{54}H_{55}O_{28}$	+	1151.29	1151.29 (100), 903.23 (15), 535.11 (24), 287.06 (17)
Anthocyanin D2*	14.9	$C_{54}H_{55}O_{28}$	+	1151.29	1151.29 (100), 989.24 (65), 449.11 (10), 287.06 (27)

*A: cyanidin-3-(6-*p*-coumaroyl-6′-caffeoyl)sophoroside-5-glucoside; * B1: cyanidin-3-(6-*p*-coumaroyl-6′-caffeoyl)sophoroside-5-(6-malonyl)glucoside; *B2: cyanidin-3-(6-*p*-coumaroyl-malonyl-6′-caffeoyl)sophoroside-5-glucoside; * C: cyanidin-3-(6,6′-di-*p*-coumaroyl)sophoroside-5-glucoside; * D1: cyanidin-3-(6,6′-di-*p*-coumaroyl)sophoroside-5-(6-malonyl)glucoside; * D2: cyanidin-3-(6-*p*-coumaroyl-malonyl-6′-*p*-coumaroyl)sophoroside-5-glucoside.