Supplementary Materials of the article:

Crop Productivity, Phytochemicals, and Bioactivities of Wild and Cultivated Slender Amaranth (*Amaranthus viridis* L.)

Supplementary Table S3. Phenolic compounds identified by LC-MS in the hydroalcoholic extracts (MeOH:H_2O, 60:40 v/v) of *Amaranthus viridis* leaves and identification basis.

Phenolic compound	Retention time (min)	Formula	Adduct	Mass *m/z*	*m/z* (Delta) (ppm)	Fragment	Identification basis
Gallocatechin (−)	1.44	$C_{15}H_{14}O_7$	$[M+H]^+$	307.08123	4.89497	139.03884	Molecular ion $[M+H]^-$ *m/z* 307, and fragment *m/z* 139, that is probably produced due to the cleavage of C-ring via Retro Diels-Alder (RDA) mechanism fission [68]
Protocatechuic acid	4.27	$C_7H_6O_4$	$[M+H]^+$	153.01933	−4.86733	109.02970	Molecular ion $[M-H]^-$ *m/z* 153, and at *m/z* 109, produced after the neutral loss of CO_2 (44 Da)
DL-*p*-hydroxyphenyllactic acid	6.63	$C_9H_{10}O_4$	$[M-H]^-$	181.05063	−3.71567	137.04410	Molecular ion $[M-H]^-$ *m/z* 181 and its characteristic product ion *m/z* 137, due to the loss of the CO_2 group
Isorhamnetin-3-*O*-glucoside	7.47	$C_{22}H_{22}O_{12}$	$[M+H]^+$	479.11584	−5.33328	314.04263	Molecular ion $[M+H]^+$ *m/z* 479, and fragment *m/z* 314, due to the loss of a hexose (162 Da)
Vanillic acid	7.57	$C_8H_8O_4$	$[M-H]^-$	167.03498	5.26530	152.00996	Molecular ion $[M-H]^-$ *m/z* 167 and its characteristic product ion 152 due to the loss of CH_4
Sinapic acid	7.60	$C_{11}H_{12}O_5$	$[M-H]^-$	223.06120	−1.28626	121.02821	Molecular ion $[M-H]^-$ m/z 223, and the loss of $2CH_3$–CO_2–CO (*m/z* 121) [69]
Trans-*p*-coumaric acid	7.72	$C_9H_8O_3$	$[M-H]^-$	163.03917	−5.52434	119.04881	Molecular ion $[M-H]^-$ m/z 163 and its characteristic product ion 119, due to the loss of the CO_2 group
Ferulic acid	7.94	$C_{10}H_{10}O_4$	$[M-H]^-$	193.05063	−2.45718	134.03690	Molecular ion $[M-H]^-$ *m/z* 193, and *m/z* 134 corresponding to the loss of CO_2 and CH_3
Chlorogenic acid	8.05	$C_{16}H_{18}O_9$	$[M-H]^-$	353.08792	1.00622	191.02567	Molecular ion $[M-H]^-$ *m/z* 353 and a fragment of *m/z* 191 ($C_7H_{11}O_6$) corresponding to [Quinic acid-H]
Rutin (quercetin-3-*O*-rutinoside)	8.27	$C_{27}H_{30}O_{16}$	$[M-H]^-$	609.14563	−0.78818	301.03474	Molecular ion $[M-H]^-$ *m/z* 609, and fragment *m/z* 301 due to the loss of 308 Da (rutinose)
Caffeic acid	8.30	$C_9H_8O_4$	$[M-H]^-$	179.03416	−3.95878	135.04810	Molecular ion $[M-H]^-$ *m/z* 179 and its characteristic product ion 135, due to the loss of the CO_2 group
Isoquercetin (quercetin-7-*O*-glucoside)	8.31	$C_{21}H_{20}O_{12}$	$[M-H]^-$	463.08807	−0.27267	302.03696	Molecular ion $[M-H]^-$ *m/z* 463, and *m/z* 302, corresponding to the aglycone of quercetin following the loss of a hexose ($[M-H-162]^-$
4-hydroxybenzoic acid	8.41	$C_7H_6O_3$	$[M-H]^-$	137.02339	−7.50433	93.03325	Molecular ion $[M-H]^-$ *m/z* 137 and its characteristic product ion 93,

							generated by the loss of the CO_2 group
Kaempferol-3-*O*-rutinoside	8.64	$C_{27}H_{30}O_{15}$	$[M-H]^-$	593.15131	0.19582	285.03973	Molecular ion $[M-H]^-$ *m/z* 593, and *m/z* 285 corresponding to a deprotonated kaempferol aglycone, and further loss of the rutinoside moiety
Naringenin	9.19	$C_{15}H_{12}O_5$	$[M-H]^-$	271.06104	−0.60814	119.04879	Molecular ion $[M-H]^-$ *m/z* 271, and *m/z* 119 that correspond to fragmentation of the B ring ($^{1,3}B^-$), as described by Fabre et al. [70]
Isoquercetin (quercetin-3-*O*-glucoside)	9.26	$C_{21}H_{20}O_{12}$	$[M-H]^-$	463.08820	2.52640	302.03699	Retention time after the "−7−*O*− isomer", molecular ion $[M-H]^-$ *m/z* 463, and *m/z* 302, corresponding to the aglycone of quercetin following the loss of a hexose ($[M-H-162]^-$
Lithospermic acid	10.02	$C_{27}H_{22}O_{12}$	$[M-H]^-$	537.10385	−4.48623	493.02461	Molecular ion $[M-H]^-$ *m/z* 537 and its characteristic product *m/z* 493 ($[M-H-CO_2]^-$)
Apigenin-7-*O*-glucuronide	10.46	$C_{21}H_{18}O_{11}$	$[M+H]^+$	447.09219	1.02599	253.04783	Molecular ion $[M+H]^+$ *m/z* 447, and fragment at *m/z* 253 [M+H−glucuronic (176 Da) − H_2O]$^+$
Apigenin-7-*O*-glucoside	10.53	$C_{21}H_{20}O_{10}$	$[M+H]^+$	433.11292	−2.54805	271.05908	Molecular ion $[M+H]^-$ *m/z* 433, and *m/z* 271 corresponding to the aglycon apigenin, by the loss of glucose (162 Da)