Article

Antioxidant guided fractionation of blackberry polyphenols show synergistic role of catechins and ellagitannins

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Supplementary Materials:

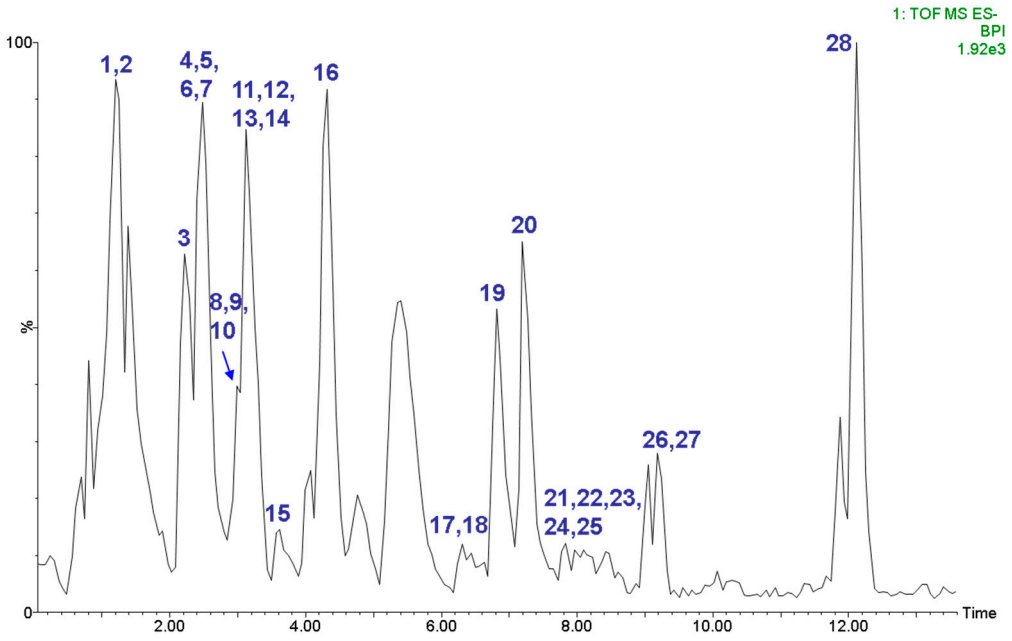

Figure S1. Representative base peak intensity (BPI) chromatogram of phenolic rich blackberry crude extract. Peak 1) Gallic acid, 2) Neochlorogenic acid, 3) Catechin, 4)Protocatechuic acid, 5) Dihydromyricetin rhamnoside, 6) Cyanidin-3-*O*-glucoside, 7) Cyanidin-3-*O*-rutinoside, 8) Procyanidin trimer C type, 9) 3-*p*-Coumaroylquinic acid, 10) Procyanthocyanidin type, 11) Cyanidin-3-*O*-sophoroside, 12) Procyanidin B2, 13) Cinnamtannin A2 14) 3-Feruloylquinic acid, 15) Procyanidin trimer C type, 16) Epicatechin, 17) Rutin, 18) Epigallocatechin, 19) Lambertianin C isomer, 20) Sanguiin H-6/Lambertianin A, 21) Ellagic acid pentoside, 22) Ellagic acid, 23) Quercetin-3-*O*-galactoside, 24) Quercetin-3-*O*-glucoside, 25) Quercetin-3-*O*-hexoside, 26) Quercetin-3-pentoside, 27) Kaempferol-3-*O*-rutinoside and 28) Quercetin.

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Table S1. Retention time (t_R), MRM transitions, collision energy and cone voltage for the standards used and the phenolic compounds that were quantified in the different fractions of the phenolic-rich blackberry extract [1,2].

Reference Compound	t_R (min.)	MRM Transition (*m*/*z*)	Cone Voltage (V)	Collision Energy (eV)
Protocatechuic acid	2.59	153.06 → 108.94	29	16
		→ 80.88		18
Cyanidin-3-*O*-glucoside	3.60	448.61 → 287.20	30	15
		→ 316.60		15
Cyanidin-3-*O*-rutinoside	3.70	594.92 → 286.80	30	20
		→ 449.20		20
Cyanidin-3,5-sophoside	3.72	611.16 → 285.10	55	24
		→ 475.20		35
Cinnamtannin A2	3.75	1155.12 → 577.32	40	40
		→ 984.45		40
Procyanidin B2	3.76	577.30 → 288.94	55	26
		→ 406.90		28
Epicatechin	4.08	289.24 → 244.95	47	14
		→ 202.74		16
Lambertianin C	4.45	1401.87 → 300.09	65	35
		→ 632.61		35
Sanguiin H-6 [2]	4.78	633.44 → 300.93	55	27
		→ 275.28		27
Ellagic acid	5.56	301.04 → 283.88	60	28
		→ 144.88		36
Rutin	5.70	609.38 → 300.20	60	34
		→ 271.00		60
Quercetin-3-*O*-galactoside	6.07	463.19 → 300.27	57	22
		→ 270.95		44
Quercetin-3-*O*-glucoside	6.42	463.19 → 300.27	57	22
		→ 270.95		44
Quercetin-3-*O*-hexoside	7.13	463.19 → 300.27	57	22
		→ 270.95		44
Kaemprferol-3-*O*-rutinoside	7.23	593.19 → 284.77	60	34
		→ 254.98		60
Quercetin	8.16	301.27 → 150.94	47	20
		→ 120.95		32

[1] The first MRM transition (*m*/*z*) constitutes the quantifier and the second the qualifier. [2] Sanguiin H-6 A was quantified using the transitions of Galloyl-HHPD glucose isomer, which is a dominant fragment of the compound.