

Supplementary Materials: Phenolic Profile and Antioxidant Potential of Leaves from Selected *Cotoneaster* Medik. Species

Agnieszka Kicel, Piotr Michel, Aleksandra Owczarek, Anna Marchelak, Dorota Żyżelewicz, Grażyna Budryn, Joanna Oracz and Monika Anna Olszewska

Table S1. Retention times, UV-Vis and QTOF-MS data in the *Cotoneaster* leaf extracts.

No ^a	Compound	<i>t_R</i> (min)	UV (nm)	Formula	[M – H] ⁻ <i>m/z</i>	MS Fragments (% relative abundance)
1	3- <i>O</i> -caffeoylquinic acid (NCHA) ^{b,c}	12.2	294, 325	C ₁₆ H ₁₈ O ₉	353.1	191.0 (100), 179.0 (55)
2	dicafeoylquinic acid isomer ^d	17.8	295, 325	C ₂₅ H ₂₄ O ₁₂	515.1	353.1 (6)
3	5- <i>O</i> -caffeoylquinic acid (CHA) ^{b,c}	19.7	294, 325	C ₁₆ H ₁₈ O ₉	353.1	191.0 (100), 179.0 (4)
4	4- <i>O</i> -caffeoylquinic acid (CCHA) ^{b,c}	23.6	294, 325	C ₁₆ H ₁₈ O ₉	353.1	191.0 (40), 179.0 (50), 173.0 (100)
5	procyanidin dimer B-2 ^c	26.8	280	C ₃₀ H ₂₆ O ₁₂	577.1	451.1 (5), 425.1 (20), 407.0 (22), 289.0 (8)
6	5- <i>p</i> -coumaroylquinic acid ^b	27.9	289, 310	C ₁₆ H ₁₈ O ₈	337.1	191.0 (88), 163.0 (5)
7	(–)-epicatechin ^c	30.5	280	C ₁₅ H ₁₄ O ₆	289.0	245.0 (6), 205.0 (8)
8	caffeic acid derivative ^d	33.3	290, 328		613.1 ^e	591.1 (45), 295.6 (100), 179.0 (5)
9	procyanidin trimer C-1 ^c	37.8	280	C ₄₅ H ₃₈ O ₁₈	865.2	713.1 (16), 577.1 (17), 451.1 (7), 407.0 (12), 289.0 (4)
10	procyanidin B-type tetramer ^d	41.9	280	C ₆₀ H ₅₀ O ₂₄	1153.1	1027.2 (20), 863.2 (69), 757.2 (17), 575.1 (95), 407.0 (19), 289.0 (12)
11	procyanidin B-type trimer ^d	43.9	280	C ₄₅ H ₃₈ O ₁₈	865.2	713.1 (32), 575.1 (38), 451.1 (9), 407.0 (13), 289.0 (6)
12	quercetin 3- <i>O</i> -β-glucoside-7- <i>O</i> -α-rhamnoside ^c	44.3	265, 350	C ₂₇ H ₃₀ O ₁₆	609.1	446.1 (50), 299.0 (6)
13	procyanidin B-type tetramer ^d	45.6	280	C ₆₀ H ₅₀ O ₂₄	1153.1	1027.1 (18), 863.2 (60), 575.1 (86), 449.1 (61), 407.0 (100), 289.0 (81)
14	quercetin 3- <i>O</i> -β-(2''- <i>O</i> -β-xylosyl)galactoside ^c	46.3	268, 355	C ₂₆ H ₂₈ O ₁₆	595.1	300.0 (42)
15	epicatechin derivative ^d	48.9	280		739.2	587.1 (26), 449.1 (12), 435.0 (6), 339.0 (12), 289.0 (11)
16	epicatechin derivative ^d	50.5	280		739.2	587.1 (19), 575.1 (8), 449.1 (15), 407.1 (6), 339.0 (9), 289.0 (13)
17	quercetin rhamnoside-hexoside ^d	53.7	265, 350	C ₂₇ H ₃₀ O ₁₆	609.1	300.0 (6)
18	quercetin 3- <i>O</i> -β-galactoside (hyperoside) ^c	55.0	265, 355	C ₂₁ H ₂₀ O ₁₂	463.1	300.0 (19)
19	quercetin dirhamnoside ^d	55.7	275, 345	C ₂₇ H ₃₀ O ₁₅	593.1	446.1 (74), 299.0 (10)
20	3- <i>O</i> -β-(6''- <i>O</i> -α-rhamnosyl)glucoside (rutin) ^c	56.8	260, 355	C ₂₇ H ₃₀ O ₁₆	609.1	300.0 (26)

Table S1. Cont.

No ^a	Compound	<i>t_R</i> (min)	UV (nm)	Formula	[M – H] ⁻ <i>m/z</i>	MS Fragments (% relative abundance)
21	quercetin 3- <i>O</i> -β-glucoside (isoquercitrin) ^c	58.4	275, 350	C ₂₁ H ₂₀ O ₁₂	463.1	300.0 (31)
22	procyanidin B-type dimer ^d	62.2	280	C ₃₀ H ₂₆ O ₁₂	577.1	451.2 (9), 425.1 (23), 407.0 (22), 289.0 (17)
23	procyanidin B-type trimer ^d	64.7	280	C ₄₅ H ₃₈ O ₁₈	865.2	739.1 (21), 713.1 (22), 577.1 (43), 451.1 (19), 407.0 (23), 289.0 (12)
24	quercetin hexoside derivative ^d	65.4	256, 355		505.1	463.1 (3), 300.0 (57)
25	quercetin hexoside derivative ^d	65.6	256, 355		505.1	463.1 (2), 300.0 (35)
26	kaempferol rhamnoside-hexoside ^d	66.5	273, 345	C ₂₇ H ₃₀ O ₁₅	593.1	285.0 (15)
27	quercetin rhamnoside-hexoside ^d	66.6	276, 350	C ₂₇ H ₃₀ O ₁₆	609.1	300.0 (32)
28	quercetin 3- <i>O</i> -β-rhamnoside (quercitrin) ^c	67.3	276, 350	C ₂₁ H ₂₀ O ₁₁	447.1	300.0 (21)
29	dicafeoylquinic acid isomer ^d	67.8	285, 325	C ₂₅ H ₂₄ O ₁₂	515.1	353.1 (100), 335.0 (3)
30	quercetin hexoside derivative ^d	69.2	245, 345		505.1	463.1 (4), 300.0 (58)
31	dicafeoylquinic acid isomer ^d	70.9	286, 325	C ₂₅ H ₂₄ O ₁₂	515.1	353.1 (16), 255.0 (2)
32	unknown compound	71.8	280		451.1	373.1 (4), 341.0 (24)
33	kaempferol rhamnoside-hexoside ^d	72.5	275, 345	C ₂₇ H ₃₀ O ₁₅	593.1	447.0 (20), 285.0 (11)
34	unknown compound	75.8	316		487.3	469.3 (8), 443.3 (4)

^a peak number and retention time refer to Figure 1; ^b identified based on the published literature; ^c identified with the corresponding standards; ^d tentative assignment based on MS and UV-Vis spectra; ^e [M + Na – 2H]⁻