

Article

Antioxidant and Anti-Inflammatory Effects of Nettle Polyphe-nolic Extract: Impact on Human Colon Cells and Cytotoxicity Against Colorectal Adenocarcinoma.

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Table S1. Mass data of the compounds found in the extracts from *Urtica dioica*.

R _T (min.)	Mass Data (m/z-H)	Fragment (m/z-H)	Formula	Δ ppm	Component
4.79	315.07261	(152)	C ₁₃ H ₁₆ O ₉	1.44	Dihydroxybenzoic acid hexoside
4.04	371.06231	(209, 135, 179)	C ₁₅ H ₁₆ O ₁₁	0.87	Caffeoylglucaric acid
5.98	371.06167	(209, 135, 179)	C ₁₅ H ₁₆ O ₁₁	-0.85	Caffeoylglucaric acid
6.84	371.06218	(209, 135, 179)	C ₁₅ H ₁₆ O ₁₁	0.62	Caffeoylglucaric acid
8.58	353.08872	(191, 135, 179)	C ₁₆ H ₁₈ O ₉	2.58	Neochlorogenic acid *
8.88	371.06192	(209, 135, 179)	C ₁₅ H ₁₆ O ₁₁	-0.17	Caffeoylglucaric acid
13.78	353.08891	(191, 135, 179)	C ₁₆ H ₁₈ O ₉	3.12	Chlorogenic acid *
15.68	353.08863	(191, 135, 179)	C ₁₆ H ₁₈ O ₉	2.33	Cryptochlorogenic acid *
13.43	179.03551	(135)	C ₉ H ₈ O ₄	2.93	Caffeic acid *
16.80	295.04581	(135, 179)	C ₁₃ H ₁₂ O ₈	-0.44	Caffeoylmalic acid
18.45	497.12909	(135, 179)	C ₂₂ H ₂₆ O ₁₃	-1.96	Caffeic acid derivative
17.38	337.09136	(191, 163, 173)	C ₁₆ H ₁₈ O ₈	-4.53	p-Coumaroylquinic acid (I)
18.73	335.07777	(191, 135, 179)	C ₁₆ H ₁₆ O ₈	1.57	Caffeoylshikimic acid
18.91	337.09253	(191, 163)	C ₁₆ H ₁₈ O ₈	-1.07	p-Coumaroylquinic acid (II)
19.55	367.10304	(191)	C ₁₇ H ₂₀ O ₉	-1.13	Feruloylquinic acid
20.43	279.05133	(133, 163)	C ₁₃ H ₁₂ O ₇	1.08	p-Coumaroylmalic acid
23.11	193.05111		C ₁₀ H ₁₀ O ₄	2.46	Ferulic acid *
23.65	531.24299		C ₂₅ H ₃₉ O ₁₂	-3.21	unknown
28.22	609.14785	(300)	C ₂₇ H ₃₀ O ₁₆	2.85	Quercetin derivative
28.87	609.14681	(300, 463)	C ₂₇ H ₃₀ O ₁₆	1.15	Rutin *
29.09	463.08785	(300)	C ₂₁ H ₂₀ O ₁₂	-0.75	Isoquercetin *
32.02	505.09783	(300, 463)	C ₂₃ H ₂₂ O ₁₃	-1.85	Quercetin acetylglucoside
33.95	593.14999	(285)	C ₂₇ H ₃₀ O ₁₅	-2.03	Kaempferol rutinoside *
36.25	515.24943		C ₂₅ H ₄₀ O ₁₁	-0.69	unknown
36.30	623.16183		C ₂₈ H ₃₂ O ₁₆	0.11	Unknown flavonoid

* identification was confirmed using standard

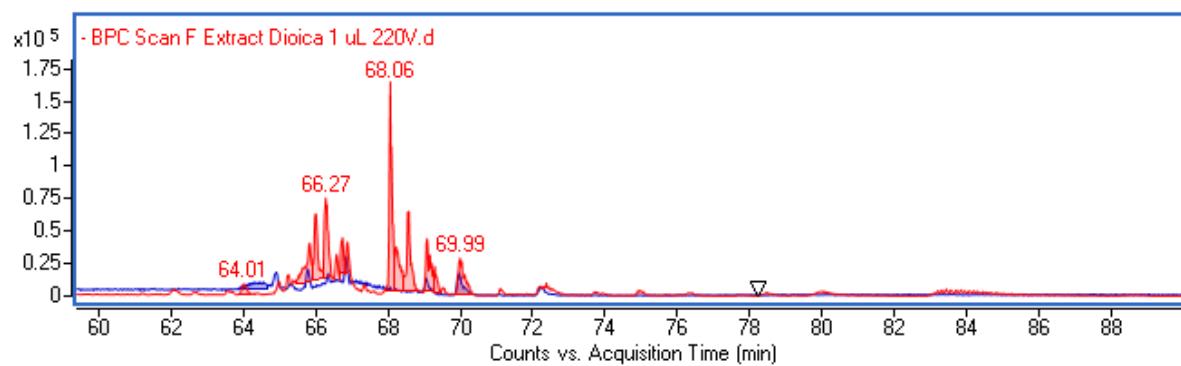


Figure S1. Overlapped base peak chromatograms (BPC) of ethanol-water extract of *U. dioica* (red line) and the polyphenolic fraction isolated from ethanol-water extract (blue line).