

Table S1. Chromatographic and spectrometric parameters including retention time, adduct ion, theoretical and measured mass (m/z), accuracy and sensibility for anthocyanins (n=20) in the investigated red cabbage extract. RT = Retention Time

Tentative assignment	RT (min)	Chemical Formula	[M] ⁺ or [M+H] ⁺ theoretical mass (m/z)	[M] ⁺ or [M+H] ⁺ found Mass (m/z)	MS/MS fragment ions (m/z)	Accuracy (Δ ppm)	LOD (mg/kg)	LOQ (mg/kg)
Cyanidin 3-diglucoside 5-glucoside	3.07	C ₃₃ H ₄₁ O ₂₁	773.21348	773.21057	611.06012- 449.16882-287.05219	-3.763	-	-
Cyanidin 3-soph 5-xyloside	3.17	C ₃₂ H ₃₉ O ₂₀	743.20292	743.20294	611.06012- 287.97883	0.026	-	-
Cyanidin 3,5-diglucoside	3.18	C ₂₇ H ₃₁ O ₁₆	611.16066	611.16022	449.19708-287.06469	-0.719	0.013	0.039
Cyanidin 3-galactoside	3.23	C ₂₁ H ₂₁ O ₁₁	449.10784	449.10654	287.05576	-2.894	0.026	0.078
Cyanidin 3-(sin)soph-5-glucoside	3.25	C ₄₄ H ₅₁ O ₂₅	979.27139	979.27136	817.19598-447.61975-287.05479	-0.030	-	-
Cyanidin 3-(sin) triglucoside-5-glucoside	3.32	C ₅₀ H ₆₁ O ₂₄	1141.32422	1141.32544	979.27155-817.21722-449.10831-287.05466	1.068	-	-
Cyanidin 3-(glucofer)-diglucoside-5-glucoside	3.34	C ₄₉ H ₅₉ O ₂₉	1111.29252	1111.29602	949.26074-703.49890-449.10782-287.05457-177.00717	3.419	-	-
Cyanidin 3-(<i>p</i> -coum)glucoside-5-glucoside	3.39	C ₄₂ H ₅₇ O ₂₇	757.19744	757.19641	449.10791-287.14624	-1.360	-	-
Cyanidin 3-(caf)diglu-5-glucoside	3.47	C ₄₂ H ₄₇ O ₂₄	935.24518	935.24414	773.21832-449.10736-287.05432	-1.112	-	-
Cyanidin 3-(fer)glucoside-5-glucoside	3.52	C ₃₇ H ₃₉ O ₁₉	787.20800	787.20679	449.10709-287.14661	-1.537	-	-
Cyanidin 3-(sin)glucoside-5-glucoside	3.54	C ₃₈ H ₄₁ O ₂₀	817.21857	817.21796	449.10709-287.10703	-0.746	-	-
Cyanidin 3-(<i>p</i> -coum)diglucoside-5-glucoside	3.54	C ₄₂ H ₄₇ O ₂₃	919.25026	919.24945	757.19755-287.05457-147.06674	-0.881	-	-
Cyanidin 3-(fer)soph-5-glucoside	3.56	C ₄₃ H ₄₉ O ₂₄	949.26083	949.26025	747.42340-449.20041-287.05457-177.00108	-0.881	-	-
Cyanidin	3.57	C ₁₅ H ₁₁ O ₆	287.05501	287.05472	207.05879-147.07649	-0.611	0.013	0.039
Cyanidin 3-(sin)-diglucoside-5-glucoside	3.58	C ₄₄ H ₅₁ O ₂₅	979.27139	979.27106	817.21771-447.22711-207.06528	-0.336	-	-
Cyanidin 3-(caf)(<i>p</i> -coum)diglucoside-5-glucoside	3.60	C ₅₁ H ₅₃ O ₂₆	1081.28196	1081.28271	919.24951-756.43555-287.14618-147.06679	0.693	-	-
Cyanidin 3-(caf)(sin)soph-5-glucoside	3.61	C ₅₃ H ₅₇ O ₂₈	1141.30309	1141.30261	979.27087-817.21808-287.05457-207.06522-163.03885	-0.420	-	-
Cyanidin 3-(sin)(<i>p</i> -coum)soph-5-glucoside	3.63	C ₅₃ H ₅₇ O ₂₇	1125.30817	1125.30872	979.27112-287.28288-207.00906-147.06674	0.488	-	-
Cyanidin 3-(sin)(fer)soph-5-glucoside	3.65	C ₅₄ H ₅₉ O ₂₈	1155.31874	1155.31836	993.28876-949.26105-287.05457-207.06522-177.00697	-0.330	-	-
Cyanidin 3-(sin)(sin)soph-5-glucoside	3.69	C ₅₅ H ₆₁ O ₂₉	1185.32930	1185.32959	1023.27771-449.10782-287.05499-207.06532	0.240	-	-

*sin= sinapoyl; soph= sophoroside; fer= feruloyl; *p*-coum=*p*-cumaroyl; caf=caffeoyl; glucofer=glucoferoyl.

Table S2. Chromatographic and spectrometric parameters including retention time, adduct ion, theoretical and measured mass (m/z), accuracy and sensibility for phenolic acids and flavonoids (n=20) in the investigated red cabbage extract. RT = Retention Time

Tentative assignment	RT (min)	Chemical Formula	[M-H] ⁻ theoretical mass (m/z)	[M-H] ⁻ found mass (m/z)	MS/MS fragment ions (m/z)	Accuracy (Δ ppm)	LOD (mg/kg)	LOQ (mg/kg)
Protocatechuic acid	2.42	C ₇ H ₆ O ₄	153.01930	153.01857	109.02840	-4.77064	0.026	0.078
Epigallocatechin	2.93	C ₁₅ H ₁₄ O ₇	305.06675	305.06650	219.06580-159.10190- 121.02846-109.02807	-0.81949	0.013	0.039
Chlorogenic acid	3.00	C ₁₆ H ₁₈ O ₉	353.08780	353.08798	191.05594-84.98998	0.50979	0.013	0.039
Epicatechin	3.17	C ₁₅ H ₁₄ O ₇	289.07176	289.07202	221.94647-203.09201- 161.04478	0.89943	0.013	0.039
Gallocatechin	3.19	C ₁₅ H ₁₄ O ₈	305.06676	305.06681	219.06254-159.10185- 109.02836-121.02847	0.16390	0.013	0.039
Caffeic acid	3.25	C ₉ H ₈ O ₄	179.03498	179.03455	134.99960	-2.40177	0.013	0.039
Vanillic acid	3.30	C ₈ H ₈ O ₄	167.03490	167.03428	151.03905-123.04387	-3.71180	0.026	0.078
Catechin	3.34	C ₁₅ H ₁₄ O ₆	289.07175	289.07205	247.02241-205.10712- 151.03923-125.02335	1.03780	0.026	0.078
Syringic acid	3.39	C ₉ H ₁₀ O ₅	197.04555	197.04503	182.02153-166.99791	-2.63898	0.026	0.078
Daidzein	3.40	C ₁₅ H ₉ O ₄	253.05063	253.04977	209.96429-225.00984	-3.39853	0.103	0.310
<i>p</i> -coumaric acid	3.47	C ₉ H ₈ O ₃	163.04001	163.03937	119.04917	-3.92542	0.026	0.078
Isoquercetin	3.65	C ₂₁ H ₂₀ O ₁₂	463.08820	463.08853	431.09848-187.09698- 174.95542	0.71261	0.013	0.039
Rutin	3.65	C ₂₇ H ₃₀ O ₁₆	609.14611	609.14673	300.99911-271.05026- 255.12390	1.01782	0.013	0.039
Ellagic acid	3.74	C ₁₄ H ₆ O ₈	300.99899	300.99911	245.91669-229.93712- 185.01208-117.00336	0.39867	0.013	0.039
Quercetin	3.97	C ₁₅ H ₁₀ O ₇	301.03538	301.03508	174.95551	-0.99656	0.013	0.039
Naringenin	4.10	C ₁₅ H ₁₂ O ₅	271.06120	271.06110	235.92595-151.03917	-0.36892	0.013	0.039
Kaempferol	4.13	C ₁₅ H ₁₀ O ₆	285.04046	285.04086	93.00679	1.40331	0.013	0.039
Genistein	4.18	C ₁₅ H ₁₀ O ₅	269.04554	269.04562	241.14435-213.14908- 151.03935	0.29735	0.013	0.039
Ferulic acid	4.84	C ₁₀ H ₁₀ O ₄	193.05063	193.05016	178.02666-149.06009- 134.99963	-2.43459	0.013	0.039
Sinapic acid	5.07	C ₁₁ H ₁₂ O ₅	223.06120	223.06100	208.93591-179.03423	-0.89661	0.026	0.078