

Supplementary material

Antioxidant activity and discrimination of organic apples (*Malus domestica* Borkh.) cultivated in the western region of Romania: a DPPH· kinetics – PCA approach

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Abstract: Apple (*Malus domestica* Borkh.) is one of the most used fruit for beverages in Romania. The goal of the study was to evaluate the antioxidant activity and discrimination of various parts of organic and non-organic apple varieties cultivated in the western region of Romania using the DPPH· kinetics – PCA (principal component analysis) approach. Organic and non-organic apples have been subjected to solid-liquid ethanol extraction. Core and shell extracts were mixed with DPPH· and spectrophotometrically monitored at 517 nm. Antioxidant activity and mean DPPH· reaction rate at various time ranges reveals significant differences between organic and non-organic samples, as well as apple parts. Organic core and shell extracts had higher antioxidant activities than the corresponding non-organic samples (74.5-96.9% and 61.9-97.2%, respectively 23.5-94.3% and 59.5-95.5%). Significant differences were observed for the DPPH· reaction rate for the first ½ min, especially in the presence of organic core extracts (3.7-4.8 μM/s). The organic samples were well discriminated by DPPH· kinetics – PCA, the most important variables being the DPPH· reaction rate for the first time range. This is the first DPPH· kinetics – PCA approach applied for discriminating between organic and non-organic fruits and can be useful for evaluating the quality of such type of fruits.

Keywords: apple; *Malus domestica* Borkh.; antioxidant activity; organic and non-organic orchards; DPPH· kinetics; mean DPPH· reaction rate; principal component analysis discrimination

1. Radical scavenging activity of apple extracts

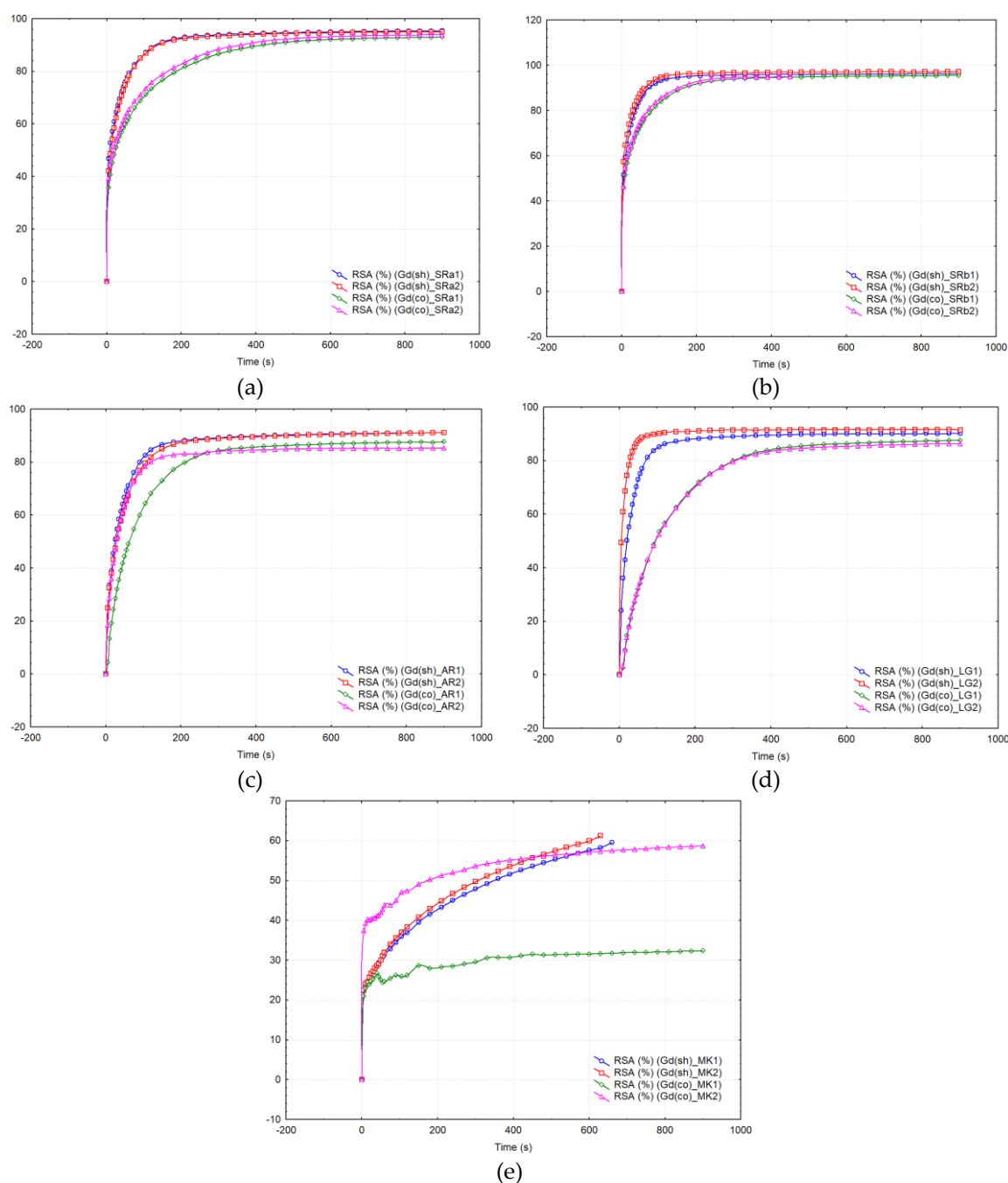


Figure S1. Variation of the radical scavenging activity (RSA, %) during the spectrophotometric monitoring for the extracts obtained from the “Golden Delicious” apple varieties in the presence of the DPPH \cdot solution: (a) organic shell and core apple extracts, *Gd(sh)_SRa* and *Gd(co)_SRa*; (b) organic shell and core apple extracts, *Gd(sh)_SRb* and *Gd(co)_SRb*; (c) non-organic shell and core apple extracts, *Gd(sh)_AR* and *Gd(co)_AR*; (d) non-organic shell and core apple extracts, *Gd(sh)_LG* and *Gd(co)_LG*; (e) non-organic shell and core apple extracts, *Gd(sh)_MK* and *Gd(co)_MK* (all determinations are presented as duplicates “1” and “2”).

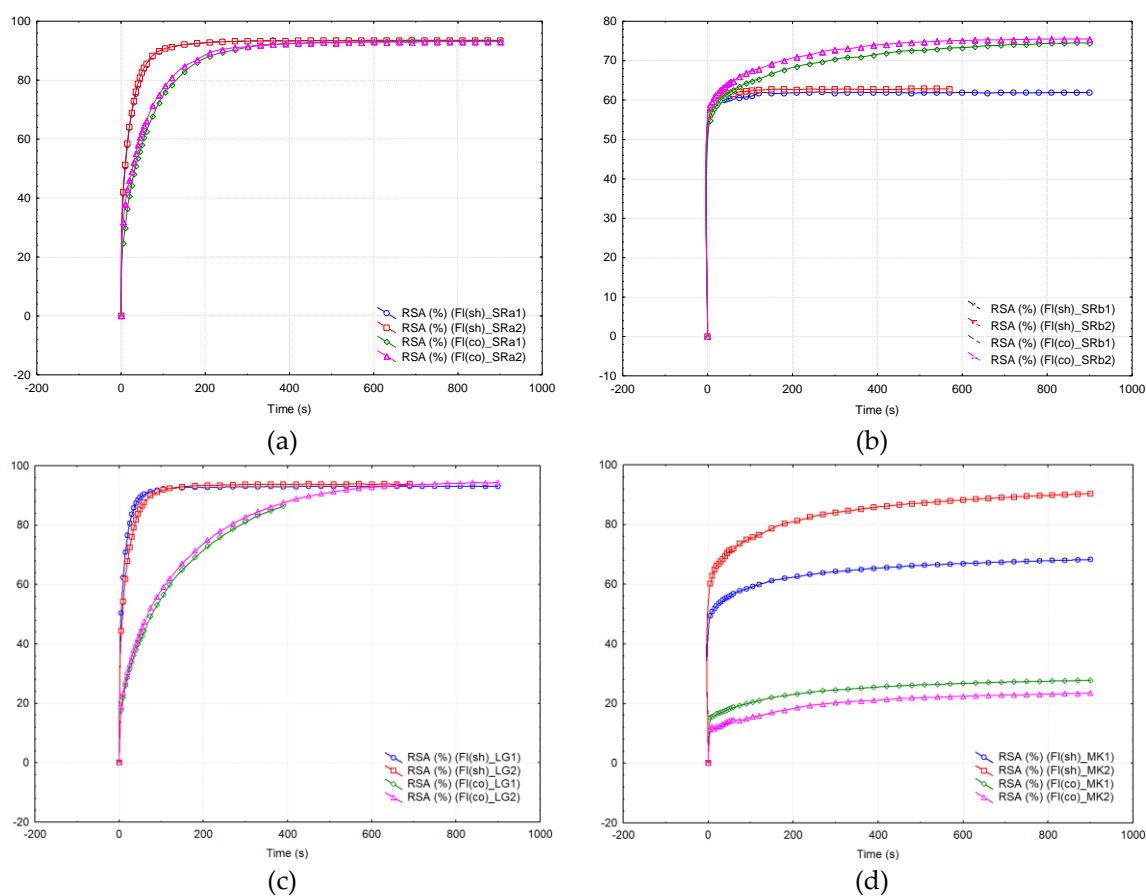


Figure S2. Variation of the radical scavenging activity (RSA, %) during the spectrophotometric monitoring for the extracts obtained from the “Florina” apple varieties in the presence of the DPPH \cdot solution: (a) organic shell and core apple extracts, *Fl(sh)_SRa* and *Fl(co)_SRa*; (b) organic shell and core apple extracts, *Fl(sh)_SRb* and *Fl(co)_SRb*; (c) non-organic shell and core apple extracts, *Fl(sh)_LG* and *Fl(co)_LG*; (d) non-organic shell and core apple extracts, *Fl(sh)_MK* and *Fl(co)_MK* (all determinations are presented as duplicates “1” and “2”).

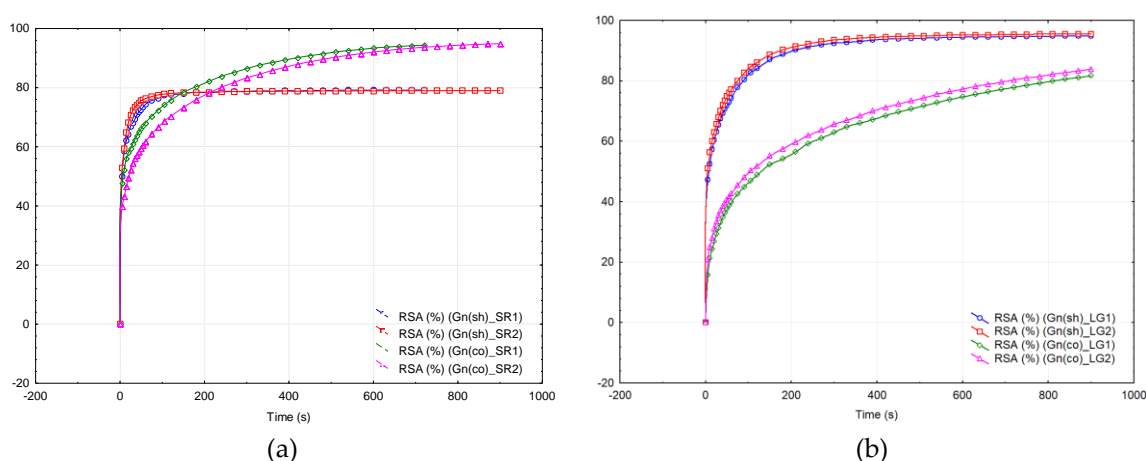


Figure S3. Variation of the radical scavenging activity (RSA, %) during the spectrophotometric monitoring for the extracts obtained from the “Generos” apple varieties in the presence of the DPPH \cdot solution: (a) organic shell and core apple extracts, *Gn(sh)_SR* and *Gn(co)_SR*; (b) non-organic shell and core apple extracts, *Gn(sh)_LG* and *Gn(co)_LG* (all determinations are presented as duplicates “1” and “2”).

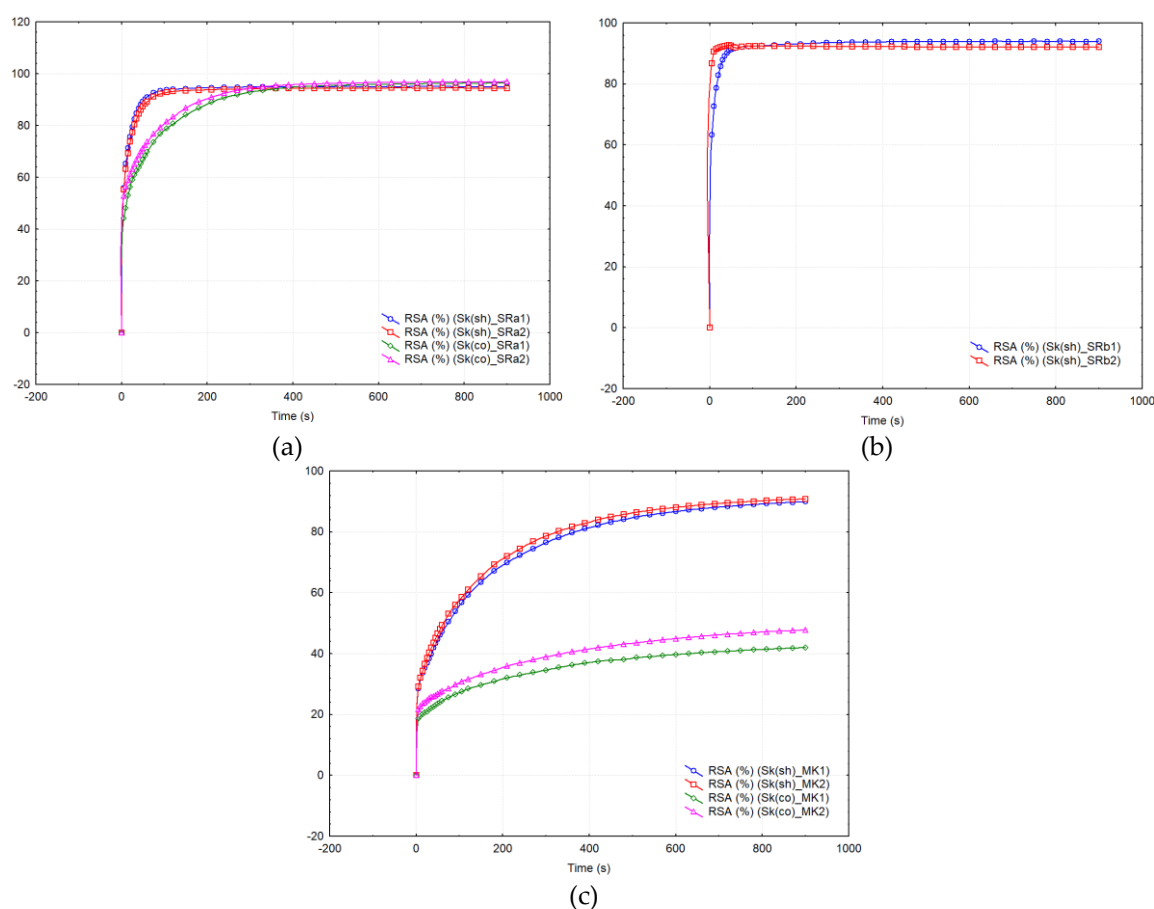


Figure S4. Variation of the radical scavenging activity (RSA, %) during the spectrophotometric monitoring for the extracts obtained from the “Starkrimson” apple varieties in the presence of the DPPH \cdot solution: (a) organic shell and core apple extracts, *Sk(sh)_SRa* and *Sk(co)_SRa*; (b) organic shell apple extracts, *Sk(sh)_SRb*; (c) non-organic shell and core apple extracts, *Sk(sh)_MK* and *Sk(co)_MK* (all determinations are presented as duplicates “1” and “2”).

Table S1. Radical scavenging activity (RSA, %) at various times of monitoring for the standard antioxidant compound solutions (*Rv_1mM/0.2mM/0.1mM* – resveratrol solutions at concentrations of 1 mM/0.2 mM/0.1 mM; *PG_0.2mM* – propyl gallate solution at a concentration of 0.2 mM). Values are expressed as mean (\pm standard deviation, SD).

Code	Antioxidant type	RSA (1 min) (%)	RSA (3 min) (%)	RSA (5 min) (%)	RSA (15 min) (%)
<i>Rv_1mM</i>	Natural	57.97 (± 0.13)	68.11 (± 0.24)	72.99 (± 0.41)	84.17 (± 0.62)
<i>Rv_0.2mM</i>	Natural	48.89 (± 0.25)	52.86 (± 0.22)	54.86 (± 0.17)	59.55 (± 0.03)
<i>Rv_0.1mM</i> *	Natural	45.22	47.53	48.71	51.41
<i>PG_0.2mM</i> *	Synthetic	67.96	73.74	76.76	82.46

*Single determination.

Table S2. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Golden Delicious” apple extracts (*RSA* – radical scavenging activity, %, at 1 min; organic shell apple extracts: *Gd(sh)_SRa* and *Gd(sh)_SRb*; organic core apple extracts: *Gd(co)_SRa* and *Gd(co)_SRb*; non-organic shell apple extracts: *Gd(sh)_AR*, *Gd(sh)_LG* and *Gd(sh)_MK*; non-organic core apple extracts: *Gd(co)_AR*, *Gd(co)_LG* and *Gd(co)_MK*). *p*-level values lower than 0.05 are bolded.

[illegible]

Table S3. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Golden Delicious” apple extracts (*RSA* – radical scavenging activity, %, at 3 min; organic shell apple extracts: *Gd(sh)_SRa* and *Gd(sh)_SRb*; organic core apple extracts: *Gd(co)_SRa* and *Gd(co)_SRb*; non-organic shell apple extracts: *Gd(sh)_AR*, *Gd(sh)_LG* and *Gd(sh)_MK*; non-organic core apple extracts: *Gd(co)_AR*, *Gd(co)_LG* and *Gd(co)_MK*). *p*-level values lower than 0.05 are bolded.

[illegible]

Table S4. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Golden Delicious” apple extracts (*RSA* – radical scavenging activity, %, at 5 min; organic shell apple extracts: *Gd(sh)_SRa* and *Gd(sh)_SRb*; organic core apple extracts: *Gd(co)_SRa* and *Gd(co)_SRb*; non-organic shell apple extracts: *Gd(sh)_AR*, *Gd(sh)_LG* and *Gd(sh)_MK*; non-organic core apple extracts: *Gd(co)_AR*, *Gd(co)_LG* and *Gd(co)_MK*). *p*-level values lower than 0.05 are bolded.

[illegible]

Table S5. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Golden Delicious” apple extracts (RSA – radical scavenging activity, %, at 15 min; organic shell apple extracts: *Gd(sh)_SRa* and *Gd(sh)_SRb*; organic core apple extracts: *Gd(co)_SRa* and *Gd(co)_SRb*; non-organic shell apple extracts: *Gd(sh)_AR*, *Gd(sh)_LG* and *Gd(sh)_MK*; non-organic core apple extracts: *Gd(co)_AR*, *Gd(co)_LG* and *Gd(co)_MK*). *p*-level values lower than 0.05 are bolded.

[illegible]

Table S6. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Florina” apple extracts (RSA – radical scavenging activity, %, at 1 min; organic shell apple extracts: *Fl(sh)_SRa* and *Fl(sh)_SRb*; organic core apple extracts: *Fl(co)_SRa* and *Fl(co)_SRb*; non-organic shell apple extracts: *Fl(sh)_LG* and *Fl(sh)_MK*; non-organic core apple extracts: *Fl(co)_LG* and *Fl(co)_MK*). *p*-level values lower than 0.05 are bolded.

	<i>Fl(sh)_SRa</i>	<i>Fl(co)_SRa</i>	<i>Fl(sh)_SRb</i>	<i>Fl(co)_SRb</i>	<i>Fl(sh)_LG</i>	<i>Fl(co)_LG</i>	<i>Fl(sh)_MK</i>	<i>Fl(co)_MK</i>
<i>Fl(sh)_SRa</i>		0.027098	0.039373	0.022688	0.983522	0.000823	0.026934	0.000240
<i>Fl(co)_SRa</i>			0.999054	1.000000	0.011265	0.048304	1.000000	0.000381
<i>Fl(sh)_SRb</i>				0.999863	0.018646	0.214254	0.999105	0.001194
<i>Fl(co)_SRb</i>					0.009581	0.058291	1.000000	0.000398
<i>Fl(sh)_LG</i>						0.000544	0.011203	0.000239
<i>Fl(co)_LG</i>							0.048612	0.004340
<i>Fl(sh)_MK</i>								0.000381
<i>Fl(co)_MK</i>								

Table S7. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Florina” apple extracts (RSA – radical scavenging activity, %, at 3 min; organic shell apple extracts: *Fl(sh)_SRa* and *Fl(sh)_SRb*; organic core apple extracts: *Fl(co)_SRa* and *Fl(co)_SRb*; non-organic shell apple extracts: *Fl(sh)_LG* and *Fl(sh)_MK*; non-organic core apple extracts: *Fl(co)_LG* and *Fl(co)_MK*). *p*-level values lower than 0.05 are bolded.

	<i>Fl(sh)_SRa</i>	<i>Fl(co)_SRa</i>	<i>Fl(sh)_SRb</i>	<i>Fl(co)_SRb</i>	<i>Fl(sh)_LG</i>	<i>Fl(co)_LG</i>	<i>Fl(sh)_MK</i>	<i>Fl(co)_MK</i>
<i>Fl(sh)_SRa</i>		0.922382	0.026205	0.030315	1.000000	0.040164	0.049479	0.000245
<i>Fl(co)_SRa</i>			0.076107	0.114097	0.890435	0.153669	0.190584	0.000276
<i>Fl(sh)_SRb</i>				0.965683	0.024010	0.916234	0.863625	0.003643
<i>Fl(co)_SRb</i>					0.027200	0.999992	0.999678	0.000600
<i>Fl(sh)_LG</i>						0.035951	0.044213	0.000244
<i>Fl(co)_LG</i>							0.999999	0.000538
<i>Fl(sh)_MK</i>								0.000493
<i>Fl(co)_MK</i>								

Table S8. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Florina” apple extracts (RSA – radical scavenging activity, %, at 5 min; organic shell apple extracts: *Fl(sh)_SRa* and *Fl(sh)_SRb*; organic core apple extracts: *Fl(co)_SRa* and *Fl(co)_SRb*; non-organic shell apple extracts: *Fl(sh)_LG* and *Fl(sh)_MK*; non-organic core apple extracts: *Fl(co)_LG* and *Fl(co)_MK*). *p*-level values lower than 0.05 are bolded.

	<i>Fl(sh)_SRa</i>	<i>Fl(co)_SRa</i>	<i>Fl(sh)_SRb</i>	<i>Fl(co)_SRb</i>	<i>Fl(sh)_LG</i>	<i>Fl(co)_LG</i>	<i>Fl(sh)_MK</i>	<i>Fl(co)_MK</i>
<i>Fl(sh)_SRa</i>		0.999901	0.030882	0.059906	1.000000	0.500284	0.103185	0.000275
<i>Fl(co)_SRa</i>			0.043073	0.091623	0.999887	0.683938	0.158556	0.000281
<i>Fl(sh)_SRb</i>				0.868982	0.030671	0.218954	0.693211	0.006921
<i>Fl(co)_SRb</i>					0.059381	0.598877	0.999512	0.000756
<i>Fl(sh)_LG</i>						0.496658	0.102264	0.000275
<i>Fl(co)_LG</i>							0.828447	0.000364
<i>Fl(sh)_MK</i>								0.000597
<i>Fl(co)_MK</i>								

Table S9. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Florina” apple extracts (RSA – radical scavenging activity, %, at 15 min; organic shell apple extracts: *Fl(sh)_SRa* and *Fl(sh)_SRb*; organic core apple extracts: *Fl(co)_SRa* and *Fl(co)_SRb*; non-organic shell apple extracts: *Fl(sh)_LG* and *Fl(sh)_MK*; non-organic core apple extracts: *Fl(co)_LG* and *Fl(co)_MK*). *p*-level values lower than 0.05 are bolded.

	<i>Fl(sh)_SRa</i>	<i>Fl(co)_SRa</i>	<i>Fl(sh)_SRb</i>	<i>Fl(co)_SRb</i>	<i>Fl(sh)_LG</i>	<i>Fl(co)_LG</i>	<i>Fl(sh)_MK</i>	<i>Fl(co)_MK</i>
<i>Fl(sh)_SRa</i>		1.000000	0.059998	0.199107	1.000000	0.999781	0.424263	0.000372
<i>Fl(co)_SRa</i>			0.062027	0.207429	1.000000	0.999878	0.439695	0.000375
<i>Fl(sh)_SRb</i>				0.758658	0.059828	0.088732	0.479451	0.022706
<i>Fl(co)_SRb</i>					0.198413	0.317788	0.994823	0.001532
<i>Fl(sh)_LG</i>						0.999770	0.422965	0.000372
<i>Fl(co)_LG</i>							0.622299	0.000417
<i>Fl(sh)_MK</i>								0.000977
<i>Fl(co)_MK</i>								

Table S10. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Generos” apple extracts (RSA – radical scavenging activity, %, at 1 min; organic shell apple extract: *Gn(sh)_SR*; organic core apple extract: *Gn(co)_SR*; non-organic shell apple extract: *Gn(sh)_LG*; non-organic core apple extract: *Gn(co)_LG*). *p*-level values lower than 0.05 are bolded.

	<i>Gn(sh)_SR</i>	<i>Gn(co)_SR</i>	<i>Gn(sh)_LG</i>	<i>Gn(co)_LG</i>
<i>Gn(sh)_SR</i>		0.064085	0.997978	0.001100
<i>Gn(co)_SR</i>			0.055782	0.003931
<i>Gn(sh)_LG</i>				0.001055
<i>Gn(co)_LG</i>				

Table S11. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Generos” apple extracts (RSA – radical scavenging activity, %, at 3 min; organic shell apple extract: *Gn(sh)_SR*; organic core apple extract: *Gn(co)_SR*; non-organic shell apple extract: *Gn(sh)_LG*; non-organic core apple extract: *Gn(co)_LG*). *p*-level values lower than 0.05 are bolded.

	<i>Gn(sh)_SR</i>	<i>Gn(co)_SR</i>	<i>Gn(sh)_LG</i>	<i>Gn(co)_LG</i>
<i>Gn(sh)_SR</i>		0.998480	0.017927	0.001438
<i>Gn(co)_SR</i>			0.016259	0.001505
<i>Gn(sh)_LG</i>				0.000472
<i>Gn(co)_LG</i>				

Table S12. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Generos” apple extracts (RSA – radical scavenging activity, %, at 5 min; organic shell apple extract: *Gn(sh)_SR*; organic core apple extract: *Gn(co)_SR*; non-organic shell apple extract: *Gn(sh)_LG*; non-organic core apple extract: *Gn(co)_LG*). *p*-level values lower than 0.05 are bolded.

	<i>Gn(sh)_SR</i>	<i>Gn(co)_SR</i>	<i>Gn(sh)_LG</i>	<i>Gn(co)_LG</i>
<i>Gn(sh)_SR</i>		0.047922	0.002524	0.002490
<i>Gn(co)_SR</i>			0.019332	0.000786
<i>Gn(sh)_LG</i>				0.000386
<i>Gn(co)_LG</i>				

Table S13. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Generos” apple extracts (RSA – radical scavenging activity, %, at 15 min; organic shell apple extract: *Gn(sh)_SR*; organic core apple extract: *Gn(co)_SR*; non-organic shell apple extract: *Gn(sh)_LG*; non-organic core apple extract: *Gn(co)_LG*). *p*-level values lower than 0.05 are bolded.

	<i>Gn(sh)_SR</i>	<i>Gn(co)_SR</i>	<i>Gn(sh)_LG</i>	<i>Gn(co)_LG</i>
<i>Gn(sh)_SR</i>		0.000387	0.000374	0.036497
<i>Gn(co)_SR</i>			0.922697	0.000654
<i>Gn(sh)_LG</i>				0.000593
<i>Gn(co)_LG</i>				

Table S14. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Starkrimson” apple extracts (RSA – radical scavenging activity, %, at 1 min; organic shell apple extracts: *Sk(sh)_SRa* and *Sk(sh)_SRb*; organic core apple extract: *Sk(co)_SRa*; non-organic shell apple extract: *Sk(sh)_MK*; non-organic core apple extract: *Sk(co)_MK*). *p*-level values lower than 0.05 are bolded.

	<i>Sk(sh)_SRa</i>	<i>Sk(co)_SRa</i>	<i>Sk(sh)_SRb</i>	<i>Sk(sh)_MK</i>	<i>Sk(co)_MK</i>
<i>Sk(sh)_SRa</i>		0.001069	0.890317	0.000272	0.000271
<i>Sk(co)_SRa</i>			0.000784	0.000475	0.000271
<i>Sk(sh)_SRb</i>				0.000271	0.000271
<i>Sk(sh)_MK</i>					0.000548
<i>Sk(co)_MK</i>					

Table S15. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Starkrimson” apple extracts (RSA – radical scavenging activity, %, at 3 min; organic shell apple extracts: *Sk(sh)_SRa* and *Sk(sh)_SRb*; organic core apple extract: *Sk(co)_SRa*; non-organic shell apple extract: *Sk(sh)_MK*; non-organic core apple extract: *Sk(co)_MK*). *p*-level values lower than 0.05 are bolded.

	<i>Sk(sh)_SRa</i>	<i>Sk(co)_SRa</i>	<i>Sk(sh)_SRb</i>	<i>Sk(sh)_MK</i>	<i>Sk(co)_MK</i>
<i>Sk(sh)_SRa</i>		0.056558	0.902596	0.000300	0.000271
<i>Sk(co)_SRa</i>			0.131536	0.000499	0.000271
<i>Sk(sh)_SRb</i>				0.000316	0.000271
<i>Sk(sh)_MK</i>					0.000272
<i>Sk(co)_MK</i>					

Table S16. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Starkrimson” apple extracts (RSA – radical scavenging activity, %, at 5 min; organic shell apple extracts: *Sk(sh)_SRa* and *Sk(sh)_SRb*; organic core apple extract: *Sk(co)_SRa*; non-organic shell apple extract: *Sk(sh)_MK*; non-organic core apple extract: *Sk(co)_MK*). *p*-level values lower than 0.05 are bolded.

	<i>Sk(sh)_SRa</i>	<i>Sk(co)_SRa</i>	<i>Sk(sh)_SRb</i>	<i>Sk(sh)_MK</i>	<i>Sk(co)_MK</i>
<i>Sk(sh)_SRa</i>		0.982634	0.856420	0.001030	0.000271
<i>Sk(co)_SRa</i>			0.987631	0.001261	0.000271
<i>Sk(sh)_SRb</i>				0.001553	0.000271
<i>Sk(sh)_MK</i>					0.000271
<i>Sk(co)_MK</i>					

Table S17. Significance *p*-levels from the Tukey HSD test (honestly significant difference) for the antioxidant activity of “Starkrimson” apple extracts (RSA – radical scavenging activity, %, at 15 min; organic shell apple extracts: *Sk(sh)_SRa* and *Sk(sh)_SRb*; organic core apple extract: *Sk(co)_SRa*; non-organic shell apple extract: *Sk(sh)_MK*; non-organic core apple extract: *Sk(co)_LG*). *p*-level values lower than 0.05 are bolded.

	<i>Sk(sh)_SRa</i>	<i>Sk(co)_SRa</i>	<i>Sk(sh)_SRb</i>	<i>Sk(sh)_MK</i>	<i>Sk(co)_MK</i>
<i>Sk(sh)_SRa</i>		0.862829	0.901720	0.321557	0.000271
<i>Sk(co)_SRa</i>			0.455069	0.119220	0.000271
<i>Sk(sh)_SRb</i>				0.698331	0.000271
<i>Sk(sh)_MK</i>					0.000272
<i>Sk(co)_MK</i>					

2. DPPH· kinetics approach for the apple extracts

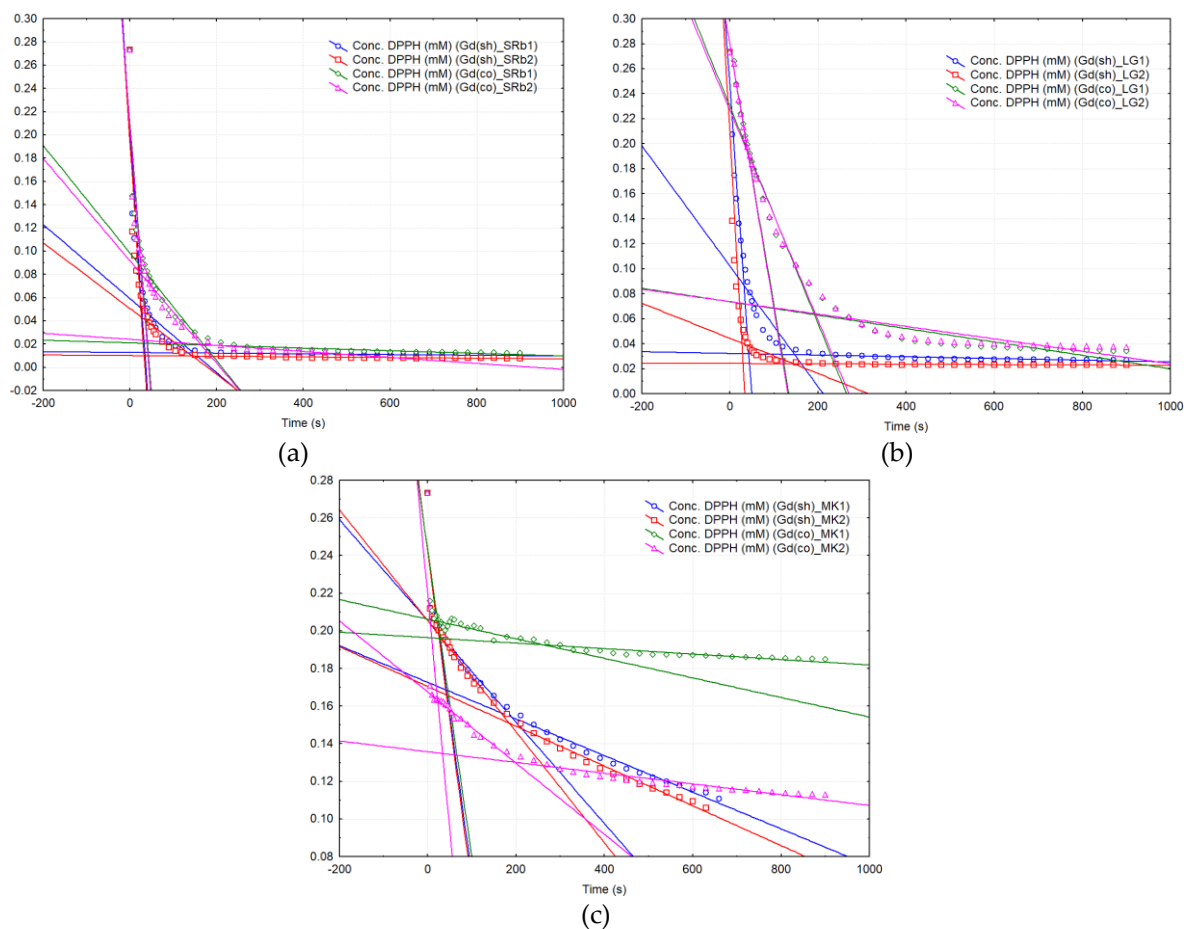


Figure S5. Variation of the DPPH· concentration during the reaction with antioxidant compounds from the extracts obtained from: (a) organic shell and core “Golden Delicious” apple variety (*Gd(sh)_SRa* and *Gd(co)_SRa*); (b) non-organic shell and core “Golden Delicious” apple variety (*Gd(sh)_LG* and *LG(co)_AR*); (c) non-organic shell and core “Golden Delicious” apple variety (*Gd(sh)_MK* and *Gd(co)_MK*) (all determinations are presented as duplicates “1” and “2”).

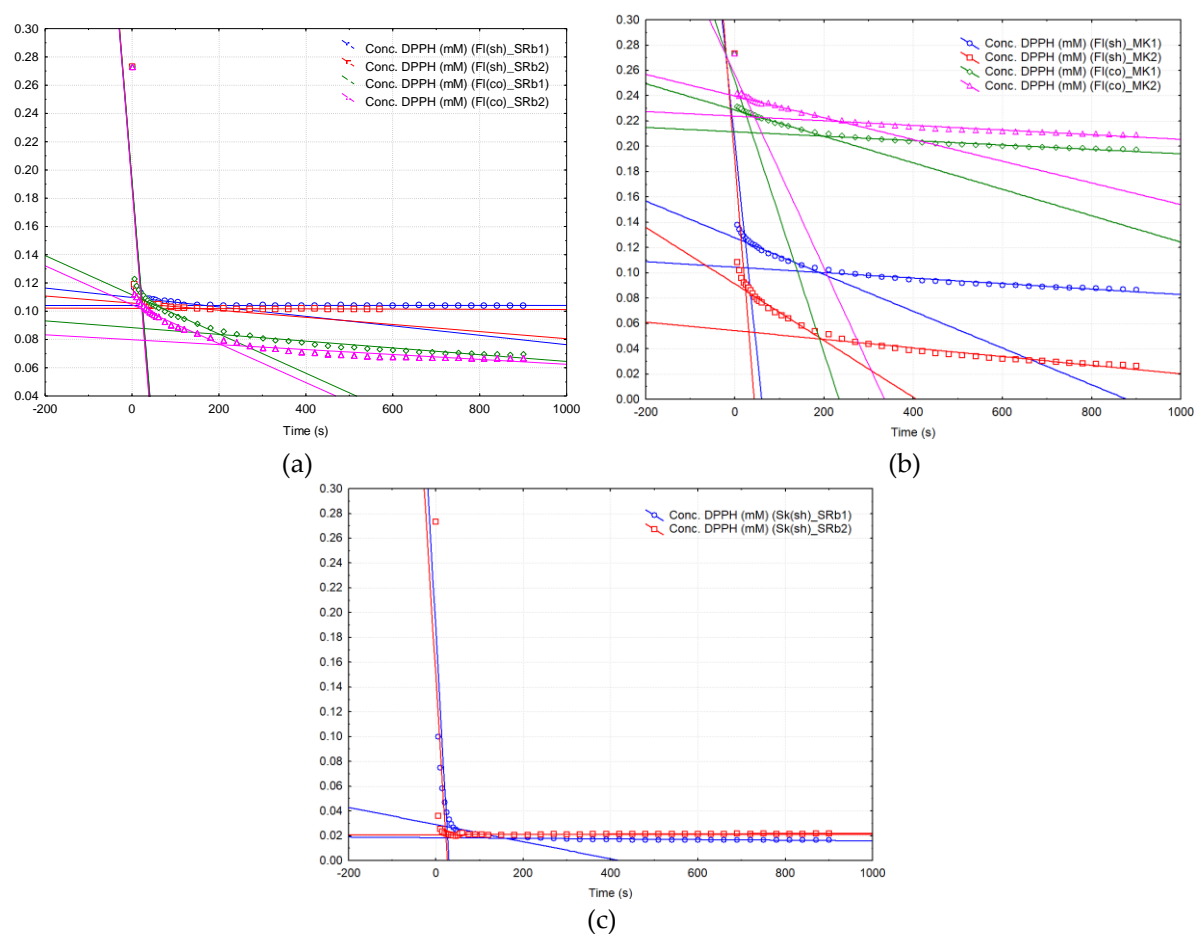


Figure S6. Variation of the DPPH· concentration during the reaction with antioxidant compounds from the extracts obtained from: (a) organic shell and core “Florina” apple variety (*Fl(sh)_SRb* and *Fl(co)_SRb*); (b) non-organic shell and core “Florina” apple variety (*Fl(sh)_MK* and *Fl(co)_MK*); (c) organic shell “Starkrimson” apple variety (*Sk(sh)_SRb*) (all determinations are presented as duplicates “1” and “2”).

Table S18. Values of the mean DPPH· reaction rates (\bar{v}_1 , \bar{v}_2 and \bar{v}_3) for the standard antioxidant compound solutions (*Rv_1mM/0.2mM/0.1mM* – resveratrol solutions at concentrations of 1 mM/0.2 mM/0.1 mM; *PG_0.2mM* – propyl gallate solution at a concentration of 0.2 mM). Values are expressed as mean (\pm standard deviation, SD).

Code	Antioxidant type	DPPH· reaction rate	DPPH· reaction rate	DPPH· reaction rate
		on t_1 time range, \bar{v}_1 ($\mu\text{M/s}$)	on t_2 time range, \bar{v}_2 ($\mu\text{M/s}$)	on t_3 time range, \bar{v}_3 ($\mu\text{M/s}$)
<i>Rv_1mM</i>	<i>Natural</i>	3.40 (± 0.00)	0.30 (± 0.00)	0.057 (± 0.001)
<i>Rv_0.2mM</i>	<i>Natural</i>	2.85 (± 0.07)	0.10 (± 0.00)	0.024 (± 0.001)
<i>Rv_0.1mM*</i>	<i>Natural</i>	2.60	0.06	0.014
<i>PG_0.2mM*</i>	<i>Synthetic</i>	4.20	0.20	0.030

*Single determination.

Table S19. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_1 = 0\text{--}30$ s in the presence of “Golden Delicious” apple extracts (\bar{v}_1 , $\mu\text{M/s}$; organic shell apple extracts: $Gd(sh)_{SRa}$ and $Gd(sh)_{SRb}$; organic core apple extracts: $Gd(co)_{SRa}$ and $Gd(co)_{SRb}$; non-organic shell apple extracts: $Gd(sh)_{AR}$, $Gd(sh)_{LG}$ and $Gd(sh)_{MK}$; non-organic core apple extracts: $Gd(co)_{AR}$, $Gd(co)_{LG}$ and $Gd(co)_{MK}$). p -level values lower than 0.05 are bolded.

[illegible]

Table S20. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_2 = 30\text{--}180$ s in the presence of “Golden Delicious” apple extracts (\bar{v}_2 , $\mu\text{M/s}$; organic shell apple extracts: $Gd(sh)_{SRA}$ and $Gd(sh)_{SRB}$; organic core apple extracts: $Gd(co)_{SRA}$ and $Gd(co)_{SRB}$; non-organic shell apple extracts: $Gd(sh)_{AR}$, $Gd(sh)_{LG}$ and $Gd(sh)_{MK}$; non-organic core apple extracts: $Gd(co)_{AR}$, $Gd(co)_{LG}$ and $Gd(co)_{MK}$). p -level values lower than 0.05 are bolded.

[illegible]

Table S21. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_3 = 180\text{--}900$ s in the presence of “Golden Delicious” apple extracts (\bar{v}_3 , $\mu\text{M/s}$; organic shell apple extracts: $Gd(sh)_{SRa}$ and $Gd(sh)_{SRb}$; organic core apple extracts: $Gd(co)_{SRa}$ and $Gd(co)_{SRb}$; non-organic shell apple extracts: $Gd(sh)_{AR}$, $Gd(sh)_{LG}$ and $Gd(sh)_{MK}$; non-organic core apple extracts: $Gd(co)_{AR}$, $Gd(co)_{LG}$ and $Gd(co)_{MK}$). p -level values lower than 0.05 are bolded.

	$Gd(sh)_{SRa}$	$Gd(co)_{SRa}$	$Gd(sh)_{SRb}$	$Gd(co)_{SRb}$	$Gd(sh)_{AR}$	$Gd(co)_{AR}$	$Gd(sh)_{LG}$	$Gd(co)_{LG}$	$Gd(sh)_{MK}$	$Gd(co)_{MK}$
$Gd(sh)_{SRa}$		0.017361	0.984368	0.879938	0.999653	0.946999	0.995897	0.001429	0.000225	0.655124
$Gd(co)_{SRa}$			0.004507	0.138460	0.040365	0.101565	0.005686	0.623085	0.000268	0.259677
$Gd(sh)_{SRb}$				0.377600	0.819871	0.482708	1.000000	0.000565	0.000225	0.209722
$Gd(co)_{SRb}$					0.994389	1.000000	0.463340	0.008468	0.000225	0.999953
$Gd(sh)_{AR}$						0.999357	0.893729	0.002814	0.000225	0.923374
$Gd(co)_{AR}$							0.578600	0.006327	0.000225	0.998962
$Gd(sh)_{LG}$								0.000654	0.000225	0.266166
$Gd(co)_{LG}$									0.000690	0.015990
$Gd(sh)_{MK}$										0.000226
$Gd(co)_{MK}$										

Table S22. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_1 = 0\text{--}30$ s in the presence of “Florina” apple extracts (\bar{v}_1 , $\mu\text{M/s}$; organic shell apple extracts: $Fl(sh)_{SRa}$ and $Fl(sh)_{SRb}$; organic core apple extracts: $Fl(co)_{SRa}$ and $Fl(co)_{SRb}$; non-organic shell apple extracts: $Fl(sh)_{LG}$ and $Fl(sh)_{MK}$; non-organic core apple extracts: $Fl(co)_{LG}$ and $Fl(co)_{MK}$). p -level values lower than 0.05 are bolded.

	$Fl(sh)_{SRa}$	$Fl(co)_{SRa}$	$Fl(sh)_{SRb}$	$Fl(co)_{SRb}$	$Fl(sh)_{LG}$	$Fl(co)_{LG}$	$Fl(sh)_{MK}$	$Fl(co)_{MK}$
$Fl(sh)_{SRa}$		0.008713	0.022322	0.006380	0.716882	0.000608	0.008713	0.000240
$Fl(co)_{SRa}$			1.000000	0.999950	0.002081	0.088110	1.000000	0.000566
$Fl(sh)_{SRb}$				1.000000	0.005858	0.224680	1.000000	0.001717
$Fl(co)_{SRb}$					0.001625	0.129777	0.999950	0.000657
$Fl(sh)_{LG}$						0.000349	0.002081	0.000238
$Fl(co)_{LG}$							0.088110	0.007442
$Fl(sh)_{MK}$								0.000566
$Fl(co)_{MK}$								

Table S23. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_3 = 30\text{--}180$ s in the presence of “Florina” apple extracts (\bar{v}_2 , $\mu\text{M/s}$; organic shell apple extracts: $Fl(sh)_{SRa}$ and $Fl(sh)_{SRb}$; organic core apple extracts: $Fl(co)_{SRa}$ and $Fl(co)_{SRb}$; non-organic shell apple extracts: $Fl(sh)_{LG}$ and $Fl(sh)_{MK}$; non-organic core apple extracts: $Fl(co)_{LG}$ and $Fl(co)_{MK}$). p -level values lower than 0.05 are bolded.

	$Fl(sh)_{SRa}$	$Fl(co)_{SRa}$	$Fl(sh)_{SRb}$	$Fl(co)_{SRb}$	$Fl(sh)_{LG}$	$Fl(co)_{LG}$	$Fl(sh)_{MK}$	$Fl(co)_{MK}$
$Fl(sh)_{SRa}$		0.013312	0.111716	0.172921	0.776893	0.006349	0.405884	0.152349
$Fl(co)_{SRa}$			0.001582	0.001052	0.003231	0.990386	0.001773	0.000984
$Fl(sh)_{SRb}$				0.971984	0.454293	0.001042	0.762975	0.983318
$Fl(co)_{SRb}$					0.776893	0.000682	0.990386	1.000000
$Fl(sh)_{LG}$						0.001773	0.990386	0.723953
$Fl(co)_{LG}$							0.001052	0.000647
$Fl(sh)_{MK}$								0.980223
$Fl(co)_{MK}$								

Table S24. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_3 = 180\text{--}900$ s in the presence of “Florina” apple extracts (\bar{v}_3 , $\mu\text{M/s}$; organic shell apple extracts: $Fl(sh)_{SRa}$ and $Fl(sh)_{SRb}$; organic core apple extracts: $Fl(co)_{SRa}$ and $Fl(co)_{SRb}$; non-organic shell apple extracts: $Fl(sh)_{LG}$ and $Fl(sh)_{MK}$; non-organic core apple extracts: $Fl(co)_{LG}$ and $Fl(co)_{MK}$). p -level values lower than 0.05 are bolded.

	$Fl(sh)_{SRa}$	$Fl(co)_{SRa}$	$Fl(sh)_{SRb}$	$Fl(co)_{SRb}$	$Fl(sh)_{LG}$	$Fl(co)_{LG}$	$Fl(sh)_{MK}$	$Fl(co)_{MK}$
$Fl(sh)_{SRa}$		0.999826	1.000000	0.998759	1.000000	0.062393	0.991061	0.999570
$Fl(co)_{SRa}$			0.999915	1.000000	0.999791	0.099255	0.999919	1.000000
$Fl(sh)_{SRb}$				0.999463	1.000000	0.139493	0.996299	0.999803
$Fl(co)_{SRb}$					0.998593	0.117372	0.999998	1.000000
$Fl(sh)_{LG}$						0.061604	0.990302	0.999498
$Fl(co)_{LG}$							0.150630	0.106424
$Fl(sh)_{MK}$								0.999976
$Fl(co)_{MK}$								

Table S25. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_1 = 0\text{--}30$ s in the presence of “Generos” apple extracts (\bar{v}_1 , $\mu\text{M/s}$; organic shell apple extract: $Gn(sh)_{SR}$; organic core apple extract: $Gn(co)_{SR}$; non-organic shell apple extract: $Gn(sh)_{LG}$; non-organic core apple extract: $Gn(co)_{LG}$). p -level values lower than 0.05 are bolded.

	$Gn(sh)_{SR}$	$Gn(co)_{SR}$	$Gn(sh)_{LG}$	$Gn(co)_{LG}$
$Gn(sh)_{SR}$		0.014238	0.401220	0.000763
$Gn(co)_{SR}$			0.047895	0.004838
$Gn(sh)_{LG}$				0.001129
$Gn(co)_{LG}$				

Table S26. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_2 = 30$ –180 s in the presence of “Generos” apple extracts (\bar{v}_2 , $\mu\text{M/s}$; organic shell apple extract: $Gn(sh)_{SR}$; organic core apple extract: $Gn(co)_{SR}$; non-organic shell apple extract: $Gn(sh)_{LG}$; non-organic core apple extract: $Gn(co)_{LG}$). p -level values lower than 0.05 are bolded.

	$Gn(sh)_{SR}$	$Gn(co)_{SR}$	$Gn(sh)_{LG}$	$Gn(co)_{LG}$
$Gn(sh)_{SR}$		0.007443	0.007443	0.007443
$Gn(co)_{SR}$			1.000000	1.000000
$Gn(sh)_{LG}$				1.000000
$Gn(co)_{LG}$				

Table S27. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_3 = 180$ –900 s in the presence of “Generos” apple extracts (\bar{v}_3 , $\mu\text{M/s}$; organic shell apple extract: $Gn(sh)_{SR}$; organic core apple extract: $Gn(co)_{SR}$; non-organic shell apple extract: $Gn(sh)_{LG}$; non-organic core apple extract: $Gn(co)_{LG}$). p -level values lower than 0.05 are bolded.

	$Gn(sh)_{SR}$	$Gn(co)_{SR}$	$Gn(sh)_{LG}$	$Gn(co)_{LG}$
$Gn(sh)_{SR}$		0.307240	0.974877	0.458049
$Gn(co)_{SR}$			0.450686	0.971691
$Gn(sh)_{LG}$				0.647153
$Gn(co)_{LG}$				

Table S28. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_1 = 0$ –30 s in the presence of “Starkrimson” apple extracts (\bar{v}_1 , $\mu\text{M/s}$; organic shell apple extracts: $Sk(sh)_{SRa}$ and $Sk(sh)_{SRb}$; organic core apple extract: $Sk(co)_{SRa}$; non-organic shell apple extract: $Sk(sh)_{MK}$; non-organic core apple extract: $Sk(co)_{MK}$). p -level values lower than 0.05 are bolded.

	$Sk(sh)_{SRa}$	$Sk(co)_{SRa}$	$Sk(sh)_{SRb}$	$Sk(sh)_{MK}$	$Sk(co)_{MK}$
$Sk(sh)_{SRa}$		0.004159	1.000000	0.000356	0.000275
$Sk(co)_{SRa}$			0.004159	0.004159	0.000476
$Sk(sh)_{SRb}$				0.000356	0.000275
$Sk(sh)_{MK}$					0.014434
$Sk(co)_{MK}$					

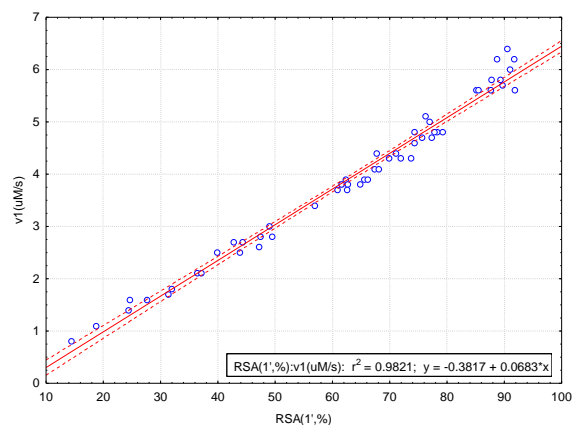
Table S29. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_2 = 30$ –180 s in the presence of “Starkrimson” apple extracts (\bar{v}_2 , $\mu\text{M/s}$; organic shell apple extracts: $Sk(sh)_{SRa}$ and $Sk(sh)_{SRb}$; organic core apple extract: $Sk(co)_{SRa}$; non-organic shell apple extract: $Sk(sh)_{MK}$; non-organic core apple extract: $Sk(co)_{MK}$). p -level values lower than 0.05 are bolded.

	$Sk(sh)_{SRa}$	$Sk(co)_{SRa}$	$Sk(sh)_{SRb}$	$Sk(sh)_{MK}$	$Sk(co)_{MK}$
$Sk(sh)_{SRa}$		0.006906	0.038351	0.003110	1.000000
$Sk(co)_{SRa}$			0.000816	0.703256	0.006906
$Sk(sh)_{SRb}$				0.000558	0.038351
$Sk(sh)_{MK}$					0.003110
$Sk(co)_{MK}$					

Table S30. Significance p -levels from the Tukey HSD test (honestly significant difference) for the DPPH· reaction rate on the $\Delta t_3 = 180\text{--}900$ s in the presence of “Starkrimson” apple extracts (\bar{v}_3 , $\mu\text{M/s}$; organic shell apple extracts: $Sk(sh)_{SRa}$ and $Sk(sh)_{SRb}$; organic core apple extract: $Sk(co)_{SRa}$; non-organic shell apple extract: $Sk(sh)_{MK}$; non-organic core apple extract: $Sk(co)_{MK}$). p -level values lower than 0.05 are bolded.

	$Sk(sh)_{SRa}$	$Sk(co)_{SRa}$	$Sk(sh)_{SRb}$	$Sk(sh)_{MK}$	$Sk(co)_{MK}$
$Sk(sh)_{SRa}$		0.012772	0.999924	0.000277	0.000735
$Sk(co)_{SRa}$			0.011632	0.000397	0.014135
$Sk(sh)_{SRb}$				0.000276	0.000698
$Sk(sh)_{MK}$					0.002299
$Sk(co)_{MK}$					

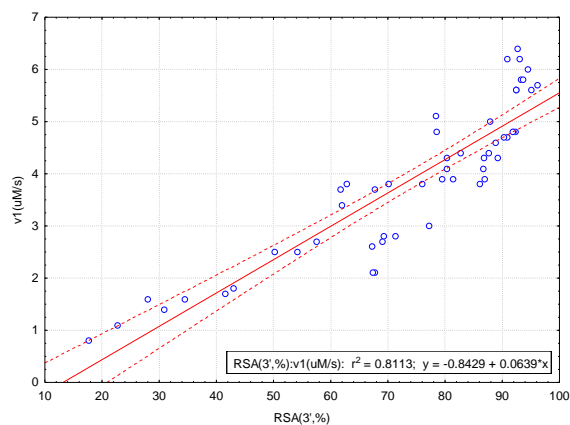
3. Correlations and principal component analysis (PCA) of the antioxidant activity and DPPH \cdot kinetics of apple extracts



$$\bar{v}_1 = -0.38(\pm 0.08) + 0.068(\pm 0.001) \cdot \text{RSA}(1')$$

$$n = 54, r^2 = 0.982, F = 2855, s = 0.20, p < 0.00001$$

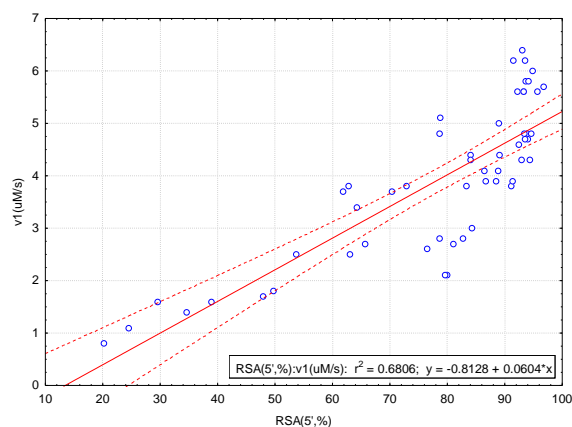
(a)



$$\bar{v}_1 = -0.84(\pm 0.33) + 0.064(\pm 0.004) \cdot \text{RSA}(3')$$

$$n = 54, r^2 = 0.901, F = 224, s = 0.64, p < 0.00001$$

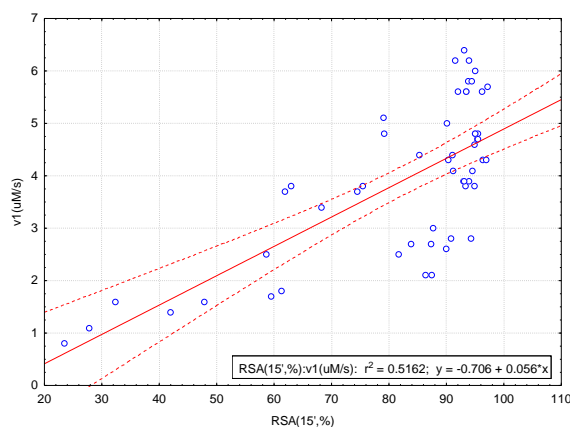
(b)



$$\bar{v}_1 = -0.81(\pm 0.46) + 0.060(\pm 0.006) \cdot \text{RSA}(5')$$

$$n = 54, r^2 = 0.825, F = 111, s = 0.84, p < 0.00001$$

(c)



$$\bar{v}_1 = -0.71(\pm 0.64) + 0.056(\pm 0.008) \cdot \text{RSA}(15')$$

$$n = 54, r^2 = 0.718, F = 55, s = 1.03, p < 0.00001$$

(d)

Figure S7. Correlations between mean DPPH \cdot reaction rate for the first time range of 0–30 s, \bar{v}_1 , and antioxidant activity, RSA, at various times for all apple extracts. (a) RSA at 1 min; (b) RSA at 3 min; (c) RSA at 5 min; (d) RSA at 15 min.

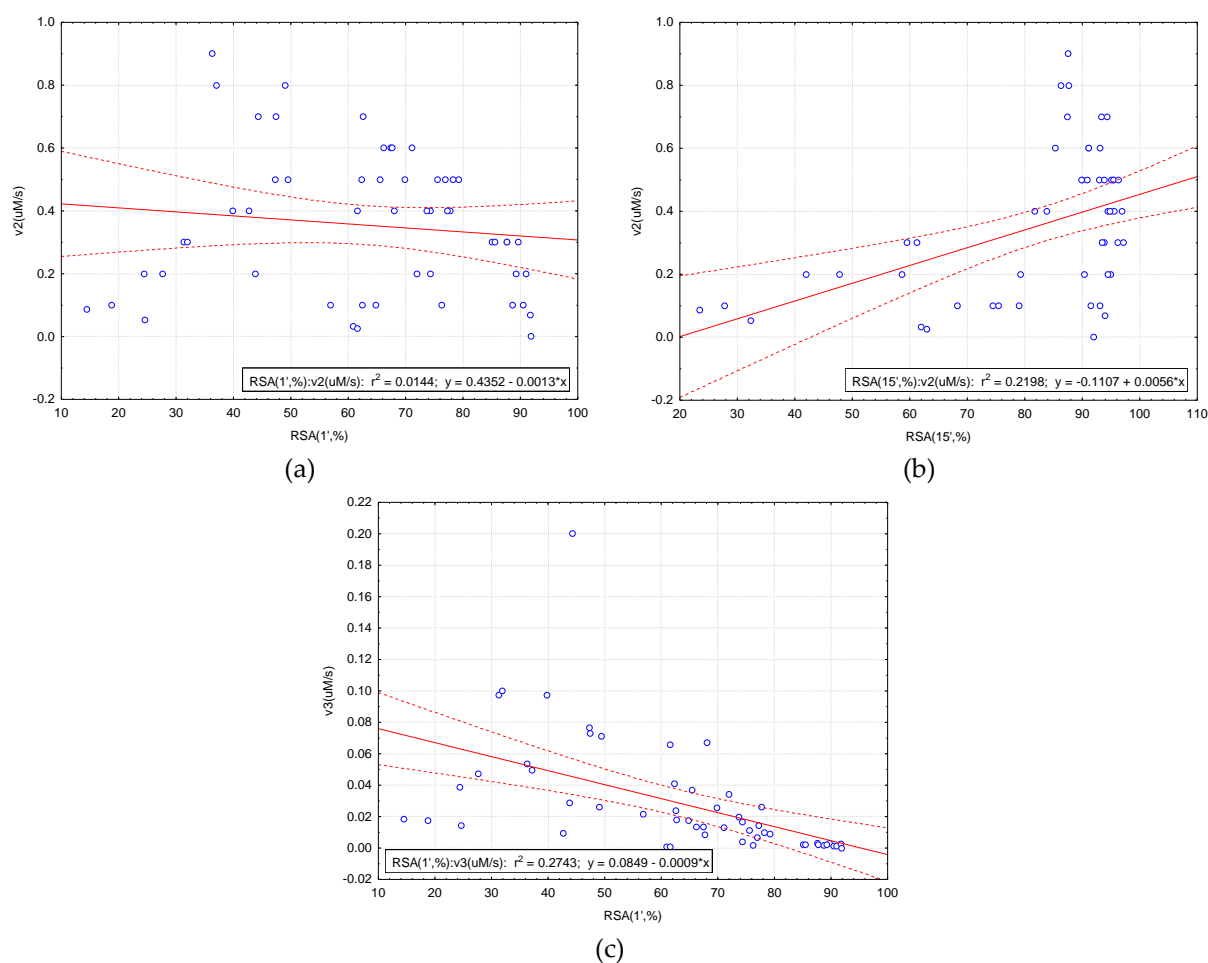


Figure S8. Representative dependences between the mean DPPH· reaction rates for the second and third time ranges of 30–180 s and 180–900 s (\bar{v}_2 and \bar{v}_3), and antioxidant activity, RSA, at various times for all apple extracts. These correlations are not statistically significant. (a) \bar{v}_2 vs. RSA at 1 min; (b) \bar{v}_2 vs. RSA at 15 min; (c) \bar{v}_3 vs. RSA at 1 min.

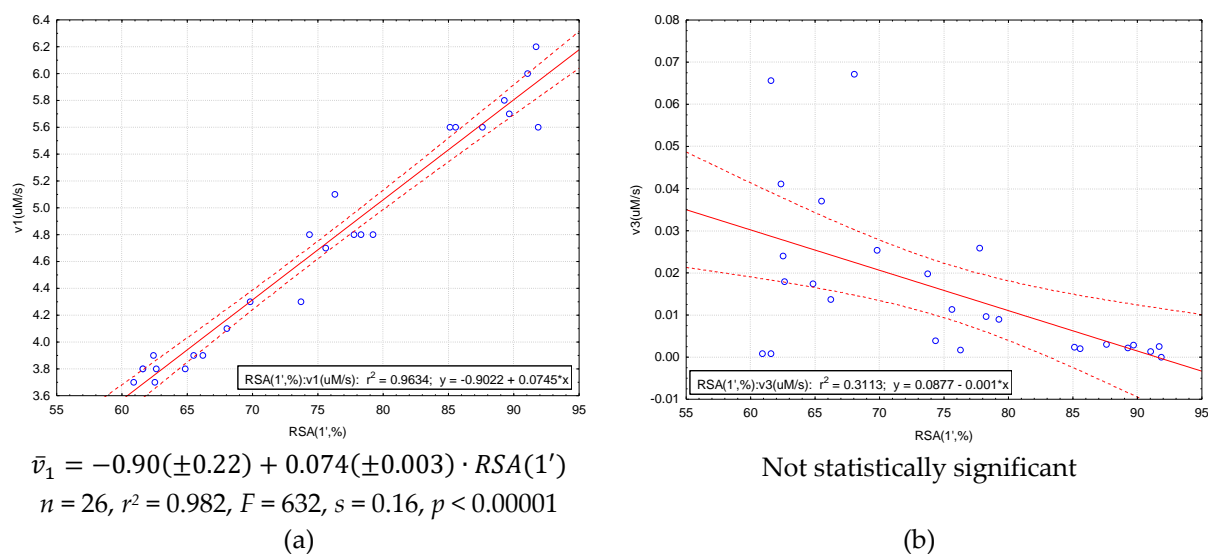


Figure S9. Representative correlations between mean DPPH· reaction rates for the first and third time ranges (0–30 s and 180–900 s, \bar{v}_1 and \bar{v}_3), and antioxidant activity, RSA, at various times for all organic apple extracts. (a) \bar{v}_1 vs. RSA at 1 min; (a) \bar{v}_3 vs. RSA at 1 min.

Linear correlation between antioxidant and DPPH· kinetic parameters and classical analysis parameters for all apple core samples (Eqs. S1-S4)

$$RSA(3') = -103.5(\pm 88.8) + 31.02(\pm 16.83) \cdot pH \quad (S1)$$

$$n = 26, r = 0.352, F = 3.4, s = 25.6, p < 0.08$$

$$RSA(5') = -112.5(\pm 88.9) + 33.62(\pm 16.85) \cdot pH \quad (S2)$$

$$n = 26, r = 0.377, F = 4.0, s = 25.6, p < 0.06$$

$$RSA(15') = -112.3(\pm 83.4) + 34.84(\pm 15.81) \cdot pH \quad (S3)$$

$$n = 26, r = 0.410, F = 4.9, s = 24.05, p < 0.04$$

$$\bar{v}_1 = -1.65(\pm 0.68) + 0.38(\pm 0.13) \cdot pH \quad (S4)$$

$$n = 26, r = 0.516, F = 8.7, s = 0.20, p < 0.007$$

Linear correlation between antioxidant and DPPH· kinetic parameters and classical analysis parameters for organic apple core samples (Eqs. S5-S9)

$$RSA(1') = 21.78(\pm 7.77) + 3.40(\pm 0.60) \cdot Sugar_content \quad (S5)$$

$$n = 12, r = 0.880, F = 34.5, s = 2.93, p < 0.0002$$

$$RSA(3') = 16.97 + 4.81(\pm 1.42) \cdot Sugar_content \quad (S6)$$

$$n = 12, r = 0.732, F = 11.5, s = 7.2, p < 0.007$$

$$RSA(5') = 15.69 + 5.25(\pm 1.70) \cdot Sugar_content \quad (S7)$$

$$n = 12, r = 0.698, F = 9.5, s = 8.6, p < 0.01$$

$$RSA(15') = 18.64 + 5.30(\pm 2.00) \cdot Sugar_content \quad (S8)$$

$$n = 12, r = 0.642, F = 7.0, s = 10.1, p < 0.025$$

$$\bar{v}_1 = 1.14(\pm 0.40) + 0.221(\pm 0.030) \cdot Sugar_content \quad (S9)$$

$$n = 12, r = 0.920, F = 54.8, s = 0.15, p < 0.00002$$

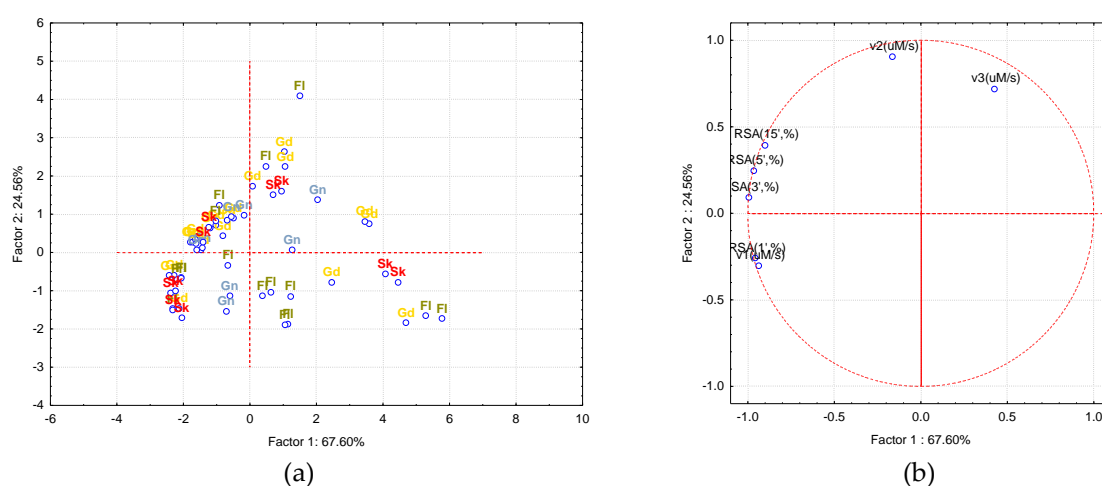


Figure S10. PCA results for the antioxidant activity and DPPH· kinetics data of all organic and non-organic apple extracts by variety (“Golden Delicious” – “Gd”, orange, “Florina” – “Fl”, green, “Generos” – “Gn”, turquoise, “Starkrimson” – “Sk”, red): (a) PC_2 versus PC_1 scores plot; (b) PC_2 versus PC_1 loadings plot.

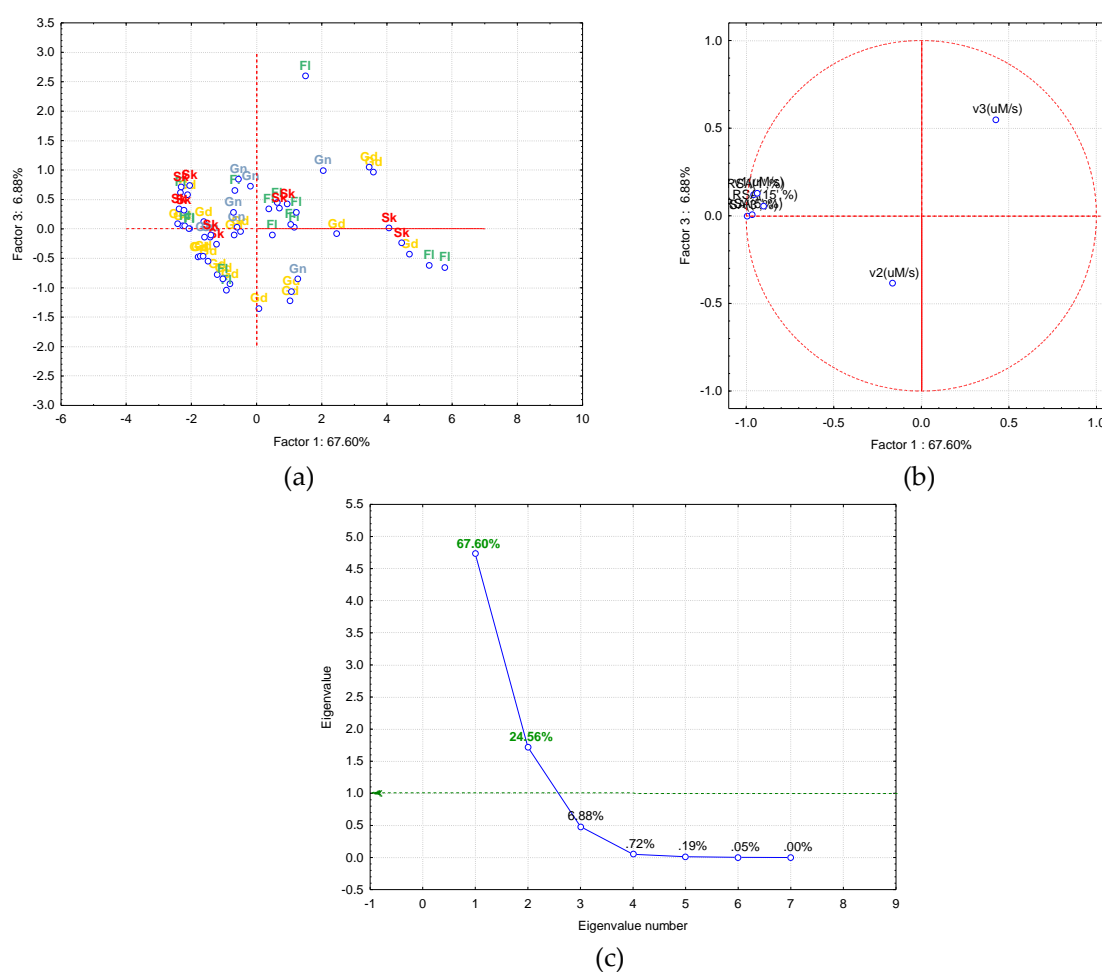


Figure S11. PCA results for the antioxidant activity and DPPH· kinetics data of all organic and non-organic apple extracts by variety (“Golden Delicious” – “Gd”, orange, “Florina” – “Fl”, green, “Generos” – “Gn”, turquoise, “Starkrimson” – “Sk”, red): (a) PC_3 versus PC_1 scores plot; (b) PC_3 versus PC_1 loadings plot; (c) eigenvalues of the correlation matrix.

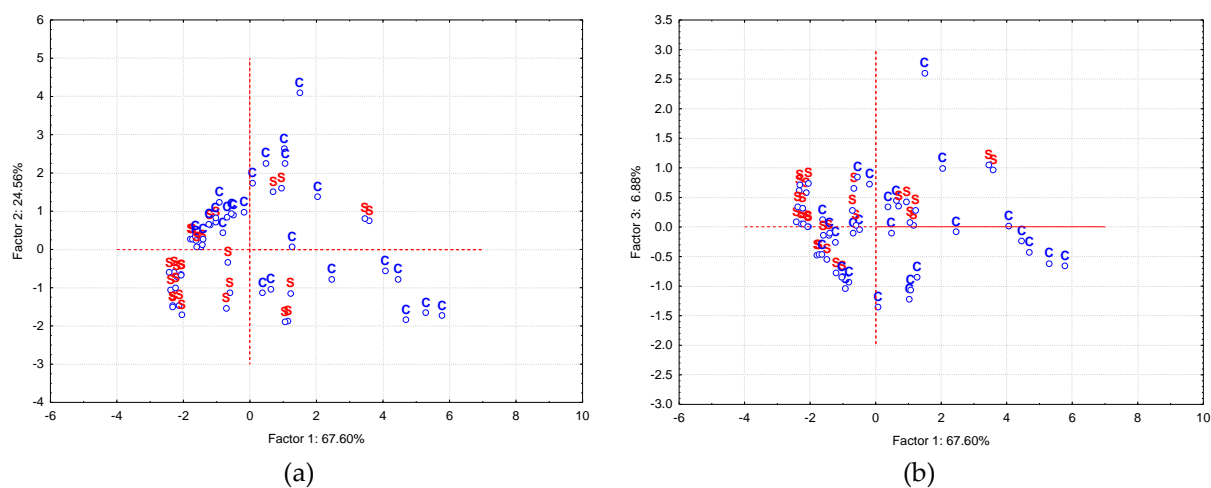
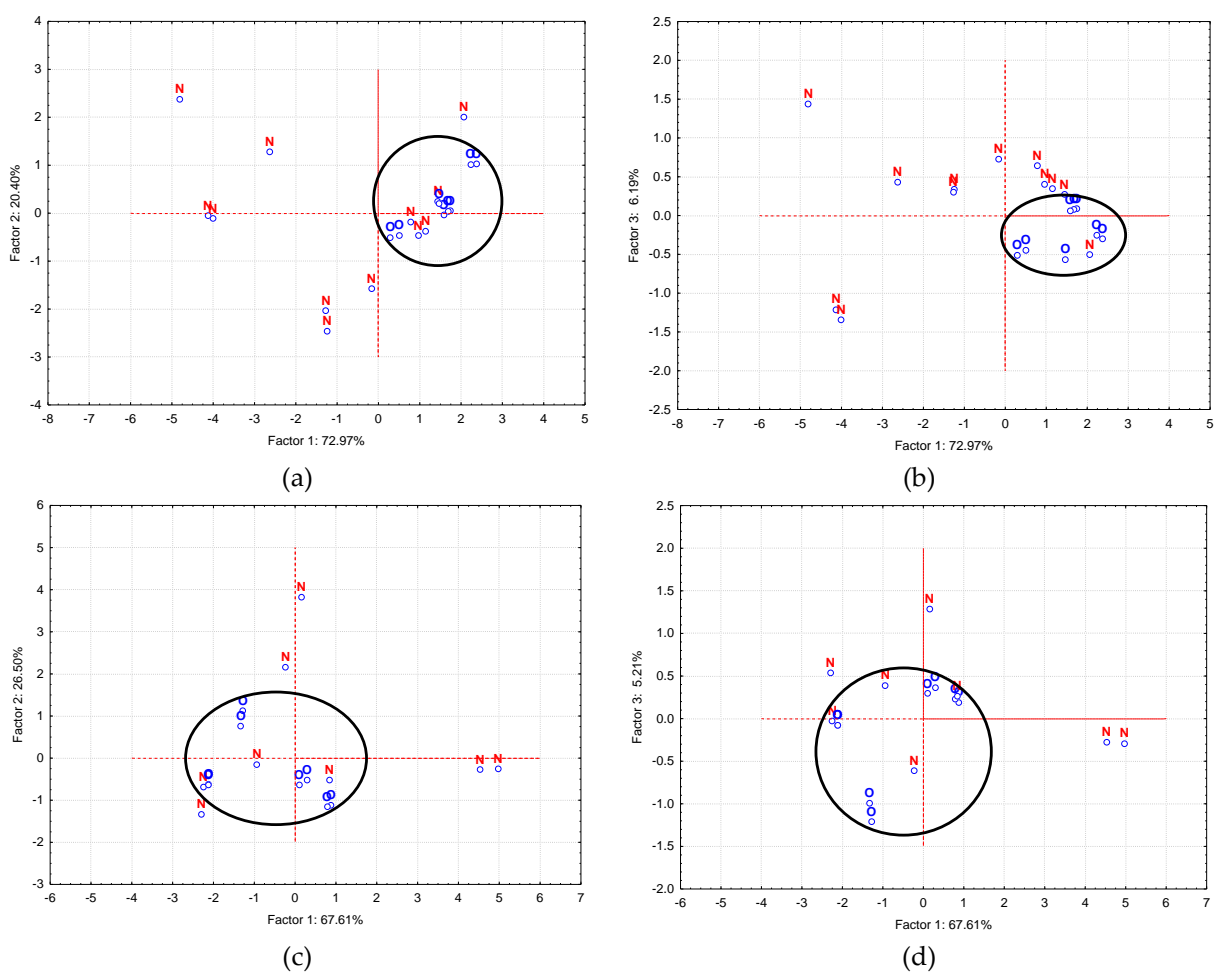


Figure S12. PCA results for the antioxidant activity and DPPH· kinetics data of all organic and non-organic apple extracts by the fruit part (shell – “S”, red, and core – “C”, blue): (a) PC_2 versus PC_1 scores plot; (b) PC_3 versus PC_1 scores plot.



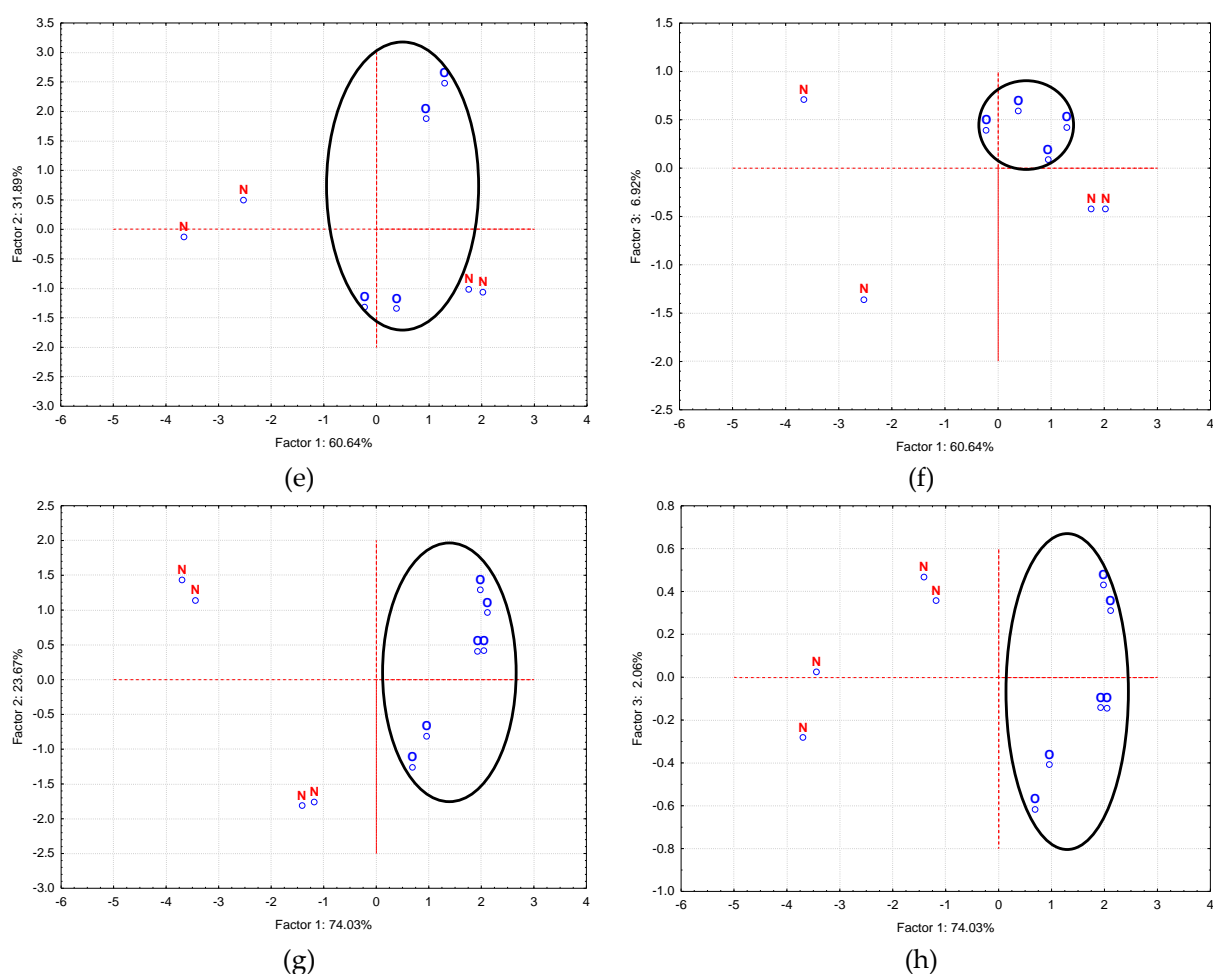
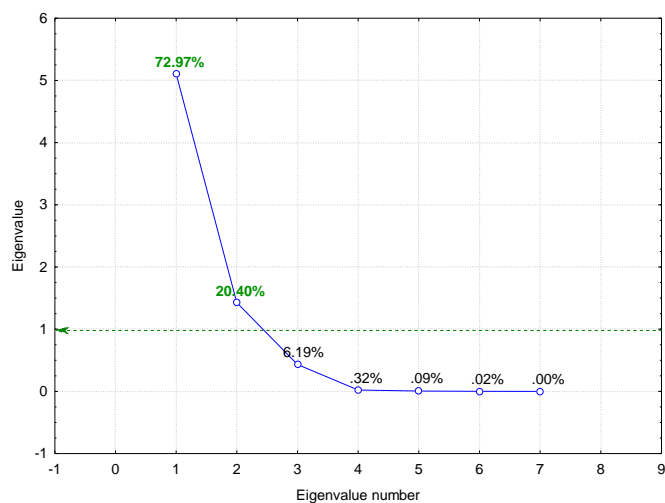
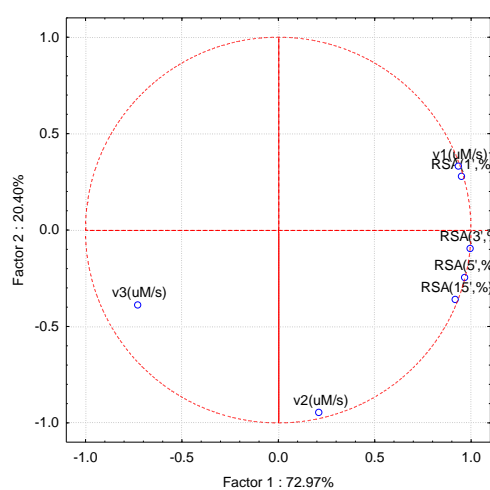
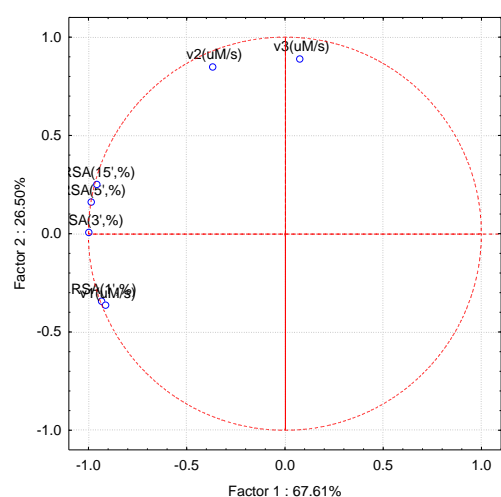
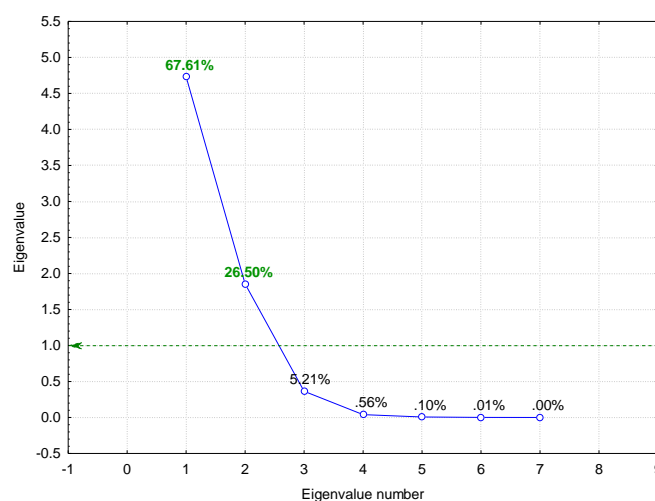


Figure S13. PCA results for the antioxidant activity and DPPH· kinetics data of organic (“O” - blue) and non-organic (“N” - red) apple extracts: (a) PC_2 versus PC_1 scores plot for “Golden Delicious” apple variety; (b) PC_3 versus PC_1 scores plot for “Golden Delicious” apple variety; (c) PC_2 versus PC_1 scores plot for “Florina” apple variety; (d) PC_3 versus PC_1 scores plot for “Florina” apple variety; (e) PC_2 versus PC_1 scores plot for “Generos” apple variety; (f) PC_3 versus PC_1 scores plot for “Generos” apple variety; (g) PC_2 versus PC_1 scores plot for “Starkrimson” apple variety; (h) PC_3 versus PC_1 scores plot for “Starkrimson” apple variety.

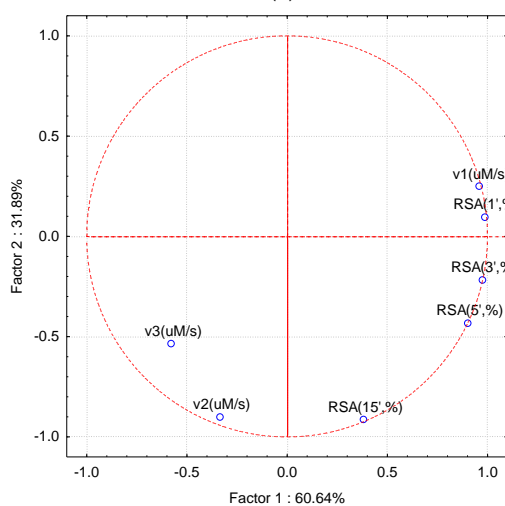




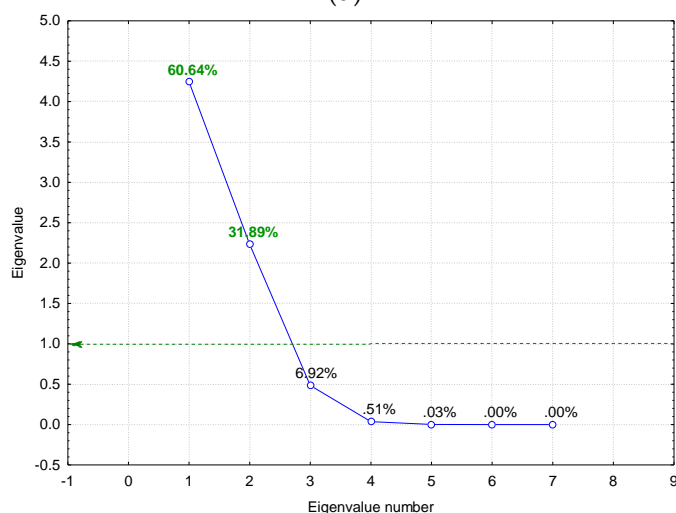
(c)



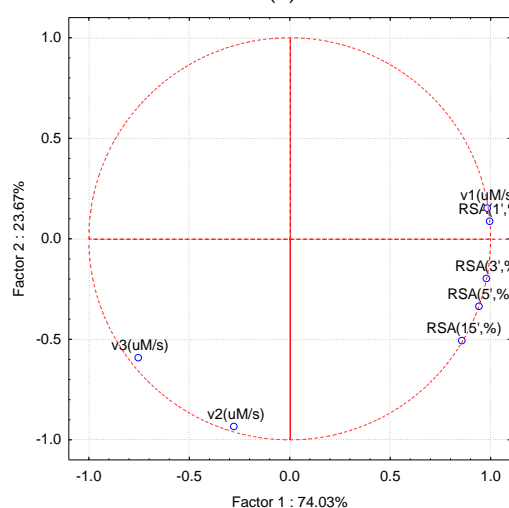
(d)



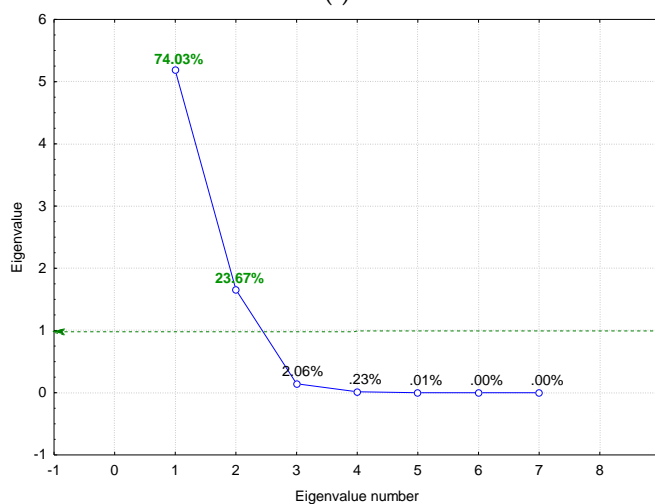
(e)



(f)



(g)



(h)

Figure S14. PCA results for the antioxidant activity and DPPH \cdot kinetics data of organic and non-organic apple extracts: (a) PC_2 versus PC_1 loadings plot for "Golden Delicious" apple variety; (b) eigenvalues of the correlation matrix for "Golden Delicious" apple variety; (c) PC_2 versus PC_1 loadings plot for "Florina" apple variety; (d) eigenvalues of the correlation matrix for "Florina" apple variety; (e) PC_2 versus PC_1 loadings plot for "Generos" apple variety; (f) eigenvalues of the correlation matrix for "Generos" apple variety; (g) PC_2 versus PC_1 loadings plot for "Starkrimson" apple variety; (h) eigenvalues of the correlation matrix for "Starkrimson" apple variety.