Supplementary material

Article

Optimization of Extraction Conditions for Phenolic Compounds from Potato Tubers: LC-MS Phenolic Profile as a powerful Tool to Assess the Genotypes, Vegetation Period, and Production Systems of Potato

Aleksandra Dramićanin [1,*], Nikola Horvacki [2], Uroš Gašić [3,*] and Dušanka Milojković-Opsenica [1]

[1] Department of Analytical Chemistry, Center of Excellence for Molecular Food Sciences, Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, P.O. Box 51, 11158 Belgrade, Serbia
[2] Innovation Centre of the Faculty of Chemistry Ltd., Studentski trg 12-16, 11158 Belgrade, Serbia
[3] Department of Plant Physiology, Institute for Biological Research "Siniša Stanković"—National Institute of the Republic of Serbia, University of Belgrade, Bulevar despota Stefana 142, 11108 Belgrade, Serbia
* Correspondence: akosovic@chem.bg.ac.rs (A.D.); uros.gasic@ibiss.bg.ac.rs (U.G.)

Content

Table S1. Total phenolic content (g GAE/kg) and radical scavenging activity (mmol TE/kg) in extracts of potato samples from five different extraction methods. C, I, O – type of production system (C – conventional, I – integral, O – organic), M, F, L, J – potato variety (M – Marabel, F – Red Fantasy, L – Laura, J – Jelly), III – third year of production.

Table S2. Content of phenolic compounds (mg/kg) in potato samples extracted with 80% methanol (Extraction 1) and a mixture of acetone-water (70:30, *v*/*v*) (Extraction 3). C, I, O – type of production (C – conventional, I – integral, O – organic), M, F, L, J – potato variety (M – Marabel, F – Red Fantasy, L – Laura, J – Jelly), protocatechuic acid – ProA, 5-O-caffeoylquinic acid – CQA, *p*-hydroxybenzoic acid – *p*-HbA, caffeic acid – CA, p-coumaric acid – *p*-CoA, quercetin-3-O-glucoside – Q3G, naringin – Nar, quercetin-3-O-rhamnoside – Q3R, kaempferol – Kae and ferulic acid – FerA.

Table S3. The number of principal components and the percentage of variance they explain.

Table S4. Results of the comparative *t*-test; protocatechuic acid – ProA, 5-O-caffeoylquinic acid – CQA, *p*-hydroxybenzoic acid – *p*-HbA, caffeic acid – CA, *p*-coumaric acid – *p*-CoA, quercetin-3-O-glucoside – Q3G, naringin – Nar, quercetin-3-O-rhamnoside – Q3R, kaempferol – Kae and ferulic acid – FerA. Bold values indicate the presence of a statistically significant difference between extractions.

Table S5. Total phenolic content (g GAE/kg) and antioxidant capacity (mmol TE/kg) in the peel and bulk of four potato varieties (M – Marabel, F - Red Fantasy, L – Laura, J – Jelly) from three types of production systems (C – conventional, I – integral, O – organic production) and three production years (I, II, and III).

Table S6. Peak areas of phenolic compounds identified in the bulk and peel of four potato varieties from three types of production using UHPLC-LTQ Orbitrap MS/MS (in excel).

Figure S1. Total phenolic content (g GAE/kg) and antioxidant capacity (mmol TE/kg) in samples of bulk and peel from four potato varieties (M – Marabel, F – Red Fantasy, L – Laura, J – Jelly) from three types of production (C – conventional, I – integral, O – organic production) presented for individual production years (I, II, and III) and as a three-year average content.

Table S1. Total phenolic content (g GAE/kg) and radical scavenging activity (mmol TE/kg) in extracts of potato samples from five different extraction methods. C, I, O – type of production system (C – conventional, I – integral, O – organic), M, F, L, J – potato variety (M – Marabel, F – Red Fantasy, L – Laura, J – Jelly), III – third year of production.

Sample No.	Sample label	Type of production / Variety	TPC (g GAE/kg)					RSA (mmol TE/kg)				
			Type of extraction					Type of extraction				
			1	2	3	4	5	1	2	3	4	5
1	1/III	CM	4.76	3.15	3.37	2.90	2.54	17.97	11.28	20.84	10.43	8.33
2	2/III	CM	4.14	2.86	3.57	2.74	2.13	11.70	10.64	19.76	10.00	10.37
3	5/ III	IM	2.72	1.77	2.57	1.77	1.56	8.93	6.80	13.69	8.67	6.63
4	6/ III	IM	2.77	1.72	2.82	2.21	1.51	18.63	6.88	15.25	10.09	7.86
5	9/ III	OM	3.43	2.46	3.55	2.50	1.81	23.97	9.32	17.95	10.84	9.94
6	10/ III	OM	2.76	3.21	3.64	2.09	1.68	19.18	4.93	13.45	9.90	8.32
7	13/ III	CF	4.41	3.55	4.69	3.02	3.23	27.51	15.09	24.01	11.99	15.26
8	14/ III	CF	4.60	3.35	4.54	3.09	3.73	26.81	14.15	24.27	12.66	19.18
9	17/ III	IF	3.88	2.61	4.53	2.77	2.88	28.87	10.49	20.19	11.09	13.07
10	18/ III	IF	4.80	3.65	3.89	3.52	3.33	19.51	15.51	25.89	16.03	17.42
11	21/ III	OF	4.89	3.00	4.28	2.92	3.63	24.78	12.23	25.24	12.38	19.48
12	22/ III	OF	5.21	3.99	4.56	2.73	4.93	28.86	15.32	26.42	14.06	14.67
13	25/ III	CL	4.33	3.15	2.95	3.09	2.92	19.87	14.21	20.32	10.04	16.25
14	28/ III	CL	4.63	3.50	3.18	3.28	4.17	23.69	16.57	30.65	13.77	22.21
15	31/ III	IL	4.90	4.27	4.53	3.60	4.01	31.05	19.76	12.59	14.75	25.63
16	32/ III	IL	4.69	3.56	3.43	3.25	3.76	18.19	17.09	16.15	14.32	20.91
17	33/ III	OL	5.58	4.38	3.79	3.57	4.62	24.24	19.22	14.73	16.23	25.94
18	35/ III	OL	5.04	4.45	3.79	3.34	4.40	26.97	20.10	28.40	14.55	24.65
19	37/ III	CJ	1.88	1.44	1.27	1.64	1.37	8.01	4.74	10.38	6.90	8.23
20	38/ III	CJ	2.06	1.61	1.68	1.63	1.56	10.35	5.40	11.17	5.57	9.11
21	42/ III	IJ	1.82	1.44	2.09	1.28	1.23	12.42	5.52	9.76	6.56	6.75
22	43/ III	IJ	1.92	1.60	1.88	1.48	1.39	9.69	5.59	10.35	6.76	7.73
23	46/ III	OJ	2.87	2.20	2.70	2.02	1.55	15.04	8.29	11.95	7.16	7.27
24	47/ III	OJ	1.73	1.33	2.53	2.21	0.77	15.90	3.65	6.63	3.34	3.36

Table S2. Content of phenolic compounds (mg/kg) in potato samples extracted with 80% methanol (Extraction 1) and a mixture of acetone-water (70:30, *v*/*v*) (Extraction 3). C, I, O – type of production (C – conventional, I – integral, O – organic), M, F, L, J – potato variety (M – Marabel, F – Red Fantasy, L – Laura, J – Jelly), protocatechuic acid – ProA, 5-O-caffeoylquinic acid – CQA, *p*-hydroxybenzoic acid – *p*-HbA, caffeic acid – CA, p-coumaric acid – *p*-CoA, quercetin-3-O-glucoside – Q3G, naringin – Nar, quercetin-3-O-rhamnoside – Q3R, kaempferol – Kae and ferulic acid – FerA.

Sample No.	Sample label	Type of production /Variety	Type of extraction	ProA	CQAs	*p*-HbA	CA	Rutin	*p*-CoA	Q3G	FerA	Nar	Q3R	Kae
1	1/III	CM	Extraction 1 (80% metanol)	1.16	87.14	0.31	55.84	0.80	0.77	0.16	1.76	0.70	0.11	0.47
2	2/III	CM		1.42	93.20	0.33	62.46	0.25	0.81	0.23	1.26	0.35	0.13	0.48
3	5/ III	IM		1.21	76.09	0.51	60.19	2.03	0.86	0.19	1.59	0.49	0.08	0.47
4	6/ III	IM		1.09	73.89	0.34	51.82	3.64	0.91	0.16	2.18	0.83	0.10	0.45
5	9/ III	OM		0.91	73.47	0.34	41.60	0.67	0.68	0.13	2.42	0.68	0.06	0.50
6	10/ III	OM		0.95	72.38	0.27	43.22	0.33	0.79	0.15	2.29	0.37	0.07	0.51
7	13/ III	CF		1.09	68.51	0.29	52.57	1.85	0.92	0.13	2.01	0.24	0.08	0.56
8	14/ III	CF		0.89	85.58	0.17	71.17	0.39	0.89	0.14	2.56	0.48	0.04	0.61
9	17/ III	IF		1.07	59.28	0.21	65.66	0.42	1.21	0.08	1.86	0.60	0.05	0.60
10	18/ III	IF		1.38	76.39	0.14	73.86	0.23	0.77	0.14	1.29	0.69	0.06	0.64
11	21/ III	OF		1.14	63.48	0.25	68.36	1.80	0.78	0.13	1.49	0.62	0.05	0.61
12	22/ III	OF		1.21	83.15	0.22	74.08	3.26	0.70	0.11	1.41	0.78	0.03	0.60
13	25/ III	CL		0.74	57.80	0.35	47.61	0.50	0.70	0.12	2.31	1.07	0.10	0.72
14	28/ III	CL		0.87	72.92	0.33	49.79	2.34	0.90	0.13	1.87	0.65	0.20	0.72
15	31/ III	IL		1.01	78.79	0.27	60.45	0.64	0.65	0.15	1.85	0.58	0.12	0.62
16	32/ III	IL		0.89	76.79	0.36	48.38	0.46	0.65	0.12	1.82	0.65	0.09	0.65
17	33/ III	OL		0.90	97.40	0.26	55.99	3.18	0.73	0.10	2.49	0.71	0.06	0.54
18	35/ III	OL		0.87	81.29	0.26	51.19	1.58	0.56	0.11	1.53	0.91	0.08	0.58
19	37/ III	CJ		1.09	83.60	0.65	45.39	0.55	0.55	0.12	2.02	0.65	0.08	0.55
20	38/ III	CJ		1.32	80.87	0.56	56.07	0.99	0.64	0.08	2.13	0.23	0.08	0.41
21	42/ III	IJ		1.02	108.75	0.29	50.79	4.49	0.83	0.15	2.85	0.54	0.05	0.51
22	43/ III	IJ		1.14	88.40	0.48	57.17	1.81	0.62	0.12	1.83	0.36	0.09	0.39
23	46/ III	OJ		0.67	33.46	0.34	42.34	0.18	0.26	0.10	2.71	0.31	0.07	0.39
24	47/ III	OJ		0.92	31.17	0.32	47.06	0.28	0.46	0.08	3.14	0.40	0.10	0.45

Table S2. Continued.

Sample No.	Sample label	Type of production /Variety	Type of extraction	ProA	CQA	*p*-HbA	CA	Rutin	*p*-CoA	Q3G	FerA	Nar	Q3R	Kae
25	1/III	CM	Extraction 3 (acetone-water mixture (70:30, v/v))	0.86	25.95	0.61	29.73	19.00	0.06	0.38	0.48	0.57	0.24	0.39
26	2/III	CM		0.81	23.76	0.47	35.30	6.59	0.08	0.75	0.37	0.44	0.51	0.38
27	5/ III	IM		0.76	26.76	0.30	26.43	0.93	0.05	0.56	0.17	0.27	0.36	0.39
28	6/ III	IM		1.12	34.39	0.21	28.30	2.01	0.07	0.37	0.19	0.58	0.23	0.49
29	9/ III	OM		0.80	26.35	0.36	31.65	2.02	0.13	0.58	0.26	0.53	0.41	0.37
30	10/ III	OM		0.57	34.85	0.29	19.80	4.94	0.21	0.31	0.13	0.09	0.19	0.37
31	13/ III	CF		1.45	47.12	0.40	29.00	1.33	0.66	0.21	0.99	0.28	0.12	0.38
32	14/ III	CF		0.79	25.32	0.26	30.81	7.78	0.07	0.14	0.42	0.51	0.09	0.41
33	17/ III	IF		0.80	65.93	0.25	32.79	0.41	0.71	0.21	1.08	0.17	0.11	0.43
34	18/ III	IF		0.67	23.64	0.39	38.49	7.07	0.16	0.10	0.40	0.29	0.05	0.38
35	21/ III	OF		1.07	33.85	0.17	38.15	1.96	0.12	0.14	0.21	0.17	0.14	0.38
36	22/ III	OF		0.75	30.01	0.26	33.49	1.16	0.26	0.07	0.20	0.12	0.08	0.38
37	25/ III	CL		0.64	24.37	0.21	35.54	2.14	0.14	0.14	0.30	0.09	0.14	0.36
38	28/ III	CL		0.61	27.69	0.12	30.50	4.07	0.18	0.14	0.13	0.24	0.13	0.37
39	31/ III	IL		0.97	19.75	0.23	26.27	0.20	0.15	0.07	1.25	0.48	0.08	0.40
40	32/ III	IL		0.83	28.93	0.29	27.17	0.13	0.26	0.07	1.56	0.37	0.10	0.37
41	33/ III	OL		1.42	17.08	0.23	24.29	0.17	0.26	0.08	1.57	0.38	0.11	0.39
42	35/ III	OL		1.30	15.03	0.22	21.66	0.15	0.08	0.06	1.42	0.41	0.09	0.39
43	37/ III	CJ		1.28	24.49	0.32	27.69	0.22	0.11	0.13	1.22	0.44	0.09	0.42
44	38/ III	CJ		0.94	32.88	0.18	31.84	0.18	0.08	0.09	2.14	0.61	0.10	0.44
45	42/ III	IJ		1.70	17.93	0.26	28.49	0.20	0.31	0.12	1.73	0.32	0.11	0.43
46	43/ III	IJ		1.64	16.33	0.25	24.57	0.18	0.38	0.12	1.84	0.33	0.12	0.38
47	46/ III	OJ		0.56	2.06	0.44	12.94	0.18	0.13	0.11	0.67	0.25	0.07	0.41
48	47/ III	OJ		0.83	1.29	0.39	7.55	0.22	0.19	0.12	0.50	0.31	0.08	0.37

Table S3. The number of principal components and the percentage of variance they explain.

Number of principal components	Values of the covariance matrix (X)	% Variance	Total % of variance
1	4.67e+000	42.46	42.46
2	2.01e+000	18.25	60.71
3	1.05e+000	9.57	70.28
4	1.01e+000	9.14	79.42

Table S4. Results of the comparative *t*-test; protocatechuic acid – ProA, 5-O-caffeoylquinic acid – CQA, *p*-hydroxybenzoic acid – *p*-HbA, caffeic acid – CA, *p*-coumaric acid – *p*-CoA, quercetin-3-O-glucoside – Q3G, naringin – Nar, quercetin-3-O-rhamnoside – Q3R, kaempferol – Kae and ferulic acid – FerA. Bold values indicate the presence of a statistically significant difference between extractions.

	ProA	CQA	*p*-HbA	CA	Rutin	*p*-CoA	Q3G	FerA	Nar	Q3R	Kae
t_{Stat}	0,85	**11,07**	1,40	**15,77**	0,85	**13,20**	**2,20**	**7,60**	**4,09**	**3,01**	**6,61**

*$t_{Critical\ two\ tail}$ = 2,07

Table S5. Total phenolic content (g GAE/kg) and antioxidant capacity (mmol TE/kg) in the peel and bulk of four potato varieties (M – Marabel, F - Red Fantasy, L – Laura, J – Jelly) from three types of production systems (C – conventional, I – integral, O – organic production) and three production years (I, II, and III).

			TPC (g GAE/kg)						RSA (mmol TE/kg)					
			I		II		III		I		II		III	
Sample No.	Sample label	Type of production/ Variety	bulk	peel	bulk	peel	bulk	peel	bulk	peel	bulk	peel	bulk	peel
1	1	CM	2.78	3.37	0.93	3.90	2.78	4.76	2.75	18.66	3.01	20.24	3.73	17.97
2	2	CM	2.16	3.57	1.01	3.42	2.16	4.14	3.49	16.94	2.73	18.99	4.90	11.70
3	5	IM	1.15	2.57	0.92	2.61	1.15	2.72	3.34	12.96	3.29	25.80	4.41	8.93
4	6	IM	0.79	2.82	0.83	3.05	0.99	2.77	2.16	15.71	3.76	23.43	3.21	18.63
5	9	OM	1.48	3.55	0.94	4.17	1.48	3.43	2.99	19.84	2.38	21.27	5.88	23.97
6	10	OM	1.00	2.94	1.26	4.62	1.00	2.76	4.91	21.11	2.76	18.74	3.16	19.18
7	13	CF	1.41	4.09	1.48	4.46	1.41	4.41	4.22	26.02	4.47	25.29	3.21	27.51
8	14	CF	1.28	3.54	1.75	4.59	1.28	4.60	2.75	34.21	5.32	23.23	3.21	26.81
9	17	IF	1.64	4.53	1.94	5.93	1.64	3.88	3.68	22.77	5.72	24.55	3.76	28.87
10	18	IF	1.54	3.89	1.96	6.14	1.54	4.80	4.27	12.05	4.67	33.14	2.83	19.51
11	21	OF	1.84	4.28	0.99	4.81	1.84	4.89	2.21	26.50	3.19	28.24	4.14	24.78
12	22	OF	1.78	4.56	1.37	4.44	1.78	5.21	2.90	22.96	2.43	37.57	3.76	28.86
13	25	CL	2.04	2.95	1.89	5.04	2.04	4.33	4.29	18.18	3.54	25.28	2.78	19.87
14	28	CL	1.93	3.18	2.02	4.91	1.93	4.63	4.83	17.30	4.96	24.55	3.92	23.69
15	31	IL	1.54	4.53	1.88	4.85	1.54	4.90	3.86	17.30	3.83	21.11	2.83	31.05
16	32	IL	1.66	3.73	1.75	4.63	1.66	4.69	3.16	15.24	4.91	22.10	2.42	18.19
17	33	OL	1.71	3.79	1.46	7.49	1.71	5.58	3.76	25.19	2.99	21.12	3.10	24.24
18	35	OL	1.02	3.79	1.59	7.45	1.32	5.04	3.01	25.58	3.58	25.68	2.45	26.97
19	37	CJ	0.78	1.27	1.85	3.56	0.68	1.88	6.19	17.18	3.36	11.54	1.63	8.01
20	38	CJ	0.84	1.68	1.95	3.41	0.84	2.06	2.60	13.16	6.85	11.72	2.40	10.35
21	42	IJ	1.28	2.09	1.36	3.02	1.28	1.82	3.19	9.53	4.09	14.86	2.89	12.42
22	43	IJ	0.90	1.78	1.05	3.61	0.90	1.92	2.26	19.64	4.74	39.49	2.56	9.69
23	46	OJ	0.95	2.70	0.46	2.88	0.95	2.87	1.42	16.69	3.59	13.01	3.59	15.04
24	47	OJ	0.77	2.53	0.48	2.62	0.77	1.73	1.72	13.99	7.10	12.81	2.07	15.90

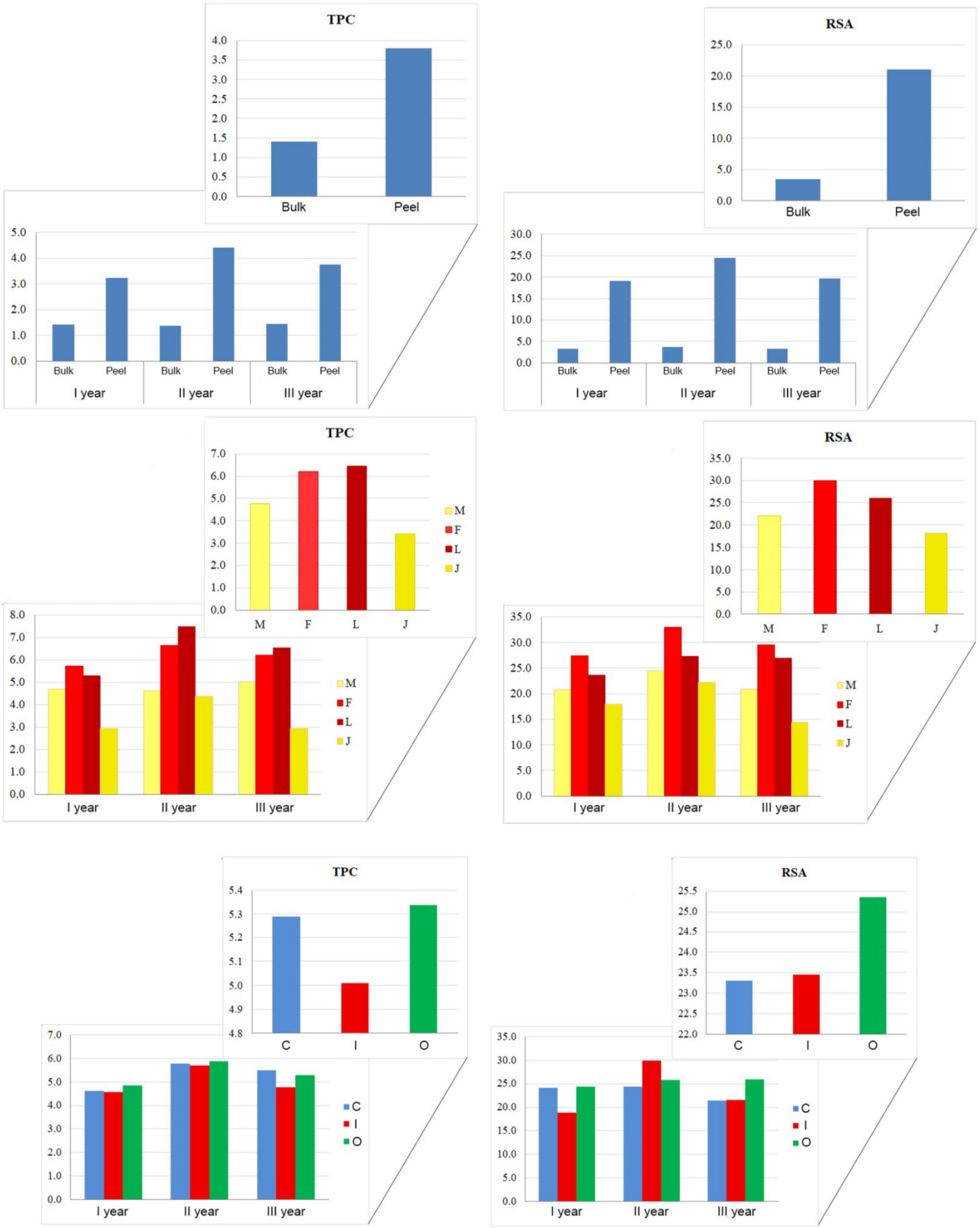


Figure S1. Total phenolic content (g GAE/kg) and antioxidant capacity (mmol TE/kg) in samples of bulk and peel from four potato varieties (M – Marabel, F – Red Fantasy, L – Laura, J – Jelly) from three types of production (C – conventional, I – integral, O – organic production) presented for individual production years (I, II, and III) and as a three-year average content.