



1 *Supplementary materials*

2 ***Fragaria viridis* Fruit Metabolites: Variation of**  
3 **LC-MS Profile and Antioxidant Potential during**  
4 **Ripening and Storage**

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11 **Content**

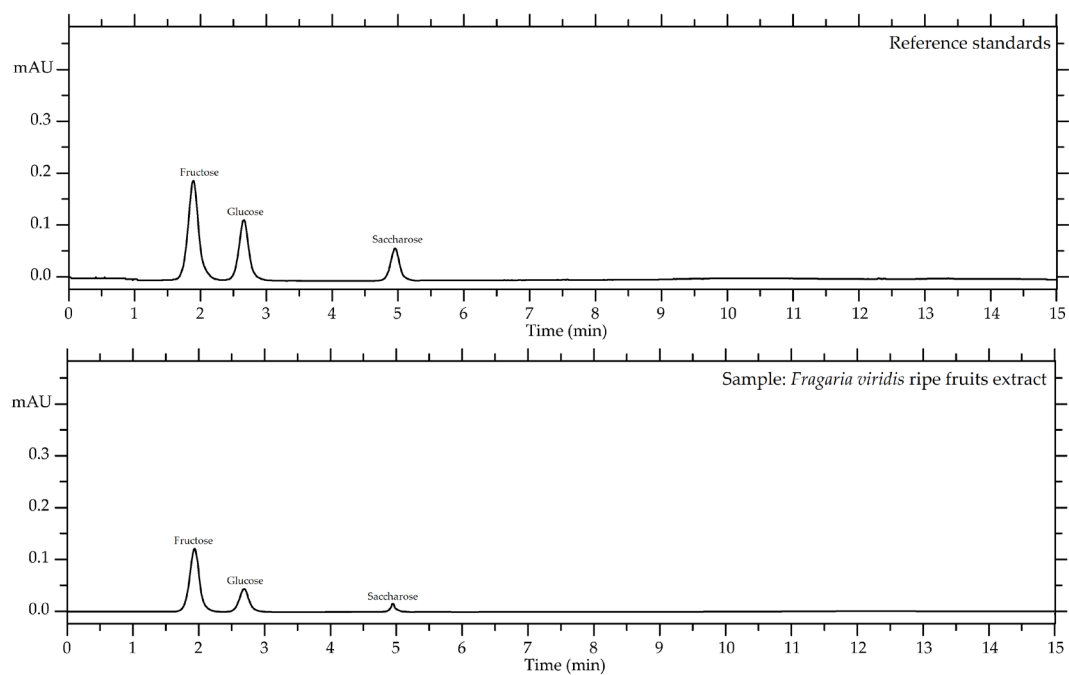
12 **Figure S1.** High-Performance Liquid Chromatography with Diode Array Detection chromatogram of free  
13 sugars in *F. viridis* ripe fruits.

14 **Figure S2.** High-Performance Liquid Chromatography with Electrospray Ionization Triple Quadrupole Mass  
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17 **Table S1.** Reference standards used for the qualitative and quantitative analysis by HPLC-DAD-ESI-tQ-MS  
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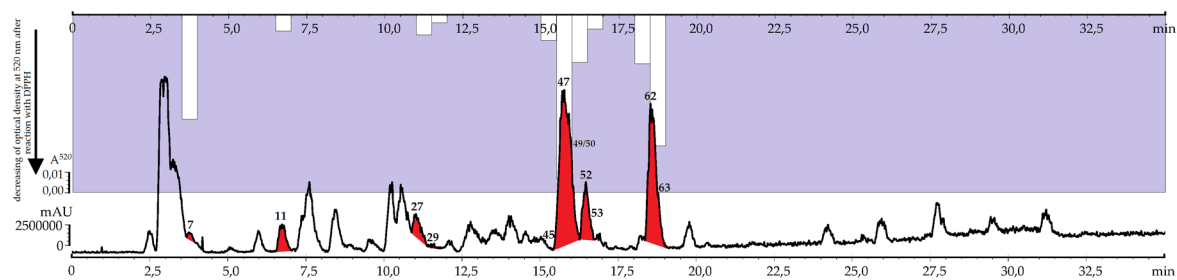
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**Figure S1.** High-Performance Liquid Chromatography with Diode Array Detection (HPLC-DAD) chromatogram (detector wavelength 190 nm) of free sugars in *F. viridis* ripe fruits.

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**Figure S2.** High-Performance Liquid Chromatography with Electrospray Ionization Triple Quadrupole Mass Spectrometric Detection (HPLC-ESI-tQ-MS) chromatogram (Total Ion Chromatogram or TIC mode, negative ionization) of *F. viridis* ripe fruits extract coupled with spectrophotometric DPPH radical scavenging assay.

31 **Table S1.** Reference standards used for the qualitative and quantitative analysis by  
 32 HPLC-DAD-ESI-tQ-MS assays.

No <sup>a</sup>	Compound	Standard <sup>a</sup>	Purity, (≥) %	Manufacturer (Cat. no) <sup>b</sup>
1	Hexosyl-hexose	Sucrose <sup>B</sup>	99	Sigma (S7903)
2	Hexose	Fructose <sup>A,B</sup>	99	Sigma (47739)
3	Citric acid	Citric acid <sup>A,B</sup>	99	Sigma (251275)
4	Malic acid	Malic acid <sup>A,B</sup>	99	Sigma (W265501)
5	Tartaric acid	Tartaric acid <sup>A,B</sup>	99	Sigma (W304401)
6	Fumaric acid	Fumaric acid <sup>A,B</sup>	99	Sigma (47910)
7	Ascorbic acid	Ascorbic acid <sup>A,B</sup>	99	Sigma (255564)
8	Oxalic acid	Oxalic acid <sup>A,B</sup>	99	Sigma (658537)
9	1- <i>O</i> -Galloyl glucose	1- <i>O</i> -Galloyl glucose <sup>A,B</sup>	90	Sigma (69288)
10	Gallic acid	Gallic acid <sup>A,B</sup>	97	Sigma (C7384)
11	Pedunculagin	Pedunculagin <sup>A,B</sup>	95	Toronto (P354070)
12	Umbelliferone	Umbelliferone <sup>A,B</sup>	99	Sigma (H24003)
13	4- <i>O</i> -Caffeoylquinic acid	4- <i>O</i> -Caffeoylquinic acid <sup>A,B</sup>	98	Sigma (65969)
14	Strictinin	Strictinin <sup>A,B</sup>	98	Funakoshi (NH026102)
15	5- <i>O</i> -Caffeoylquinic acid	5- <i>O</i> -Caffeoylquinic acid <sup>A,B</sup>	95	Sigma (C3878)
16	Strictinin isomer	Strictinin <sup>B</sup>	98	Funakoshi (NH026102)
17	3- <i>O</i> -Caffeoylquinic acid	3- <i>O</i> -Caffeoylquinic acid <sup>A,B</sup>	98	Sigma (94419)
18	Pedunculagin isomer	Pedunculagin <sup>B</sup>	95	Toronto (P354070)
19	Procyanidin B2	Procyanidin B2 <sup>A,B</sup>	90	Sigma (PHL89552)
20	Cyanidin 3- <i>O</i> -sophoroside	Cyanidin 3- <i>O</i> -sophoroside <sup>A,B</sup>	85	Sigma (42739)
21	Procyanidin B4	Procyanidin B4 <sup>A,B</sup>	98	ChemFaces (CFN91171)
22	Pelargonidin di- <i>O</i> -hexoside	Pelargonidin 3- <i>O</i> -rutinoside <sup>B</sup>	98	ChemFaces (CFN92133)
23	Catechin	Catechin <sup>A,B</sup>	95	Sigma (PHL89172)
24	<i>p</i> -Coumaric acid <i>O</i> -hexoside	<i>p</i> -Coumaric acid 4- <i>O</i> -glucoside <sup>B</sup>	95	Carbosynth (MC71595)
25	<i>p</i> -Coumaric acid 4- <i>O</i> -glucoside	<i>p</i> -Coumaric acid 4- <i>O</i> -glucoside <sup>A,B</sup>	95	Carbosynth (MC71595)
26	Cyanidin 3- <i>O</i> -rutinoside	Cyanidin 3- <i>O</i> -rutinoside <sup>A,B</sup>	90	Sigma (PHL80577)
27	Cyanidin 3- <i>O</i> -glucoside	Cyanidin 3- <i>O</i> -glucoside <sup>A,B</sup>	98	Sigma (94099)
28	Pelargonidin 3- <i>O</i> -rutinoside	Pelargonidin 3- <i>O</i> -rutinoside <sup>A,B</sup>	98	ChemFaces (CFN92133)
29	Pelargonidin 3- <i>O</i> -glucoside	Pelargonidin 3- <i>O</i> -glucoside <sup>A,B</sup>	98	ChemFaces (CFN92134)
30	Castalagin isomer	Castalagin <sup>B</sup>	95	Sigma (61221)
31	Procyanidin C2	Procyanidin C2 <sup>A,B</sup>	95	TransMIT (C6201-P045)
32	Cyanidin <i>O-p</i> -coumaroyl- <i>O</i> -hexoside	Cyanidin 3- <i>O</i> -glucoside <sup>B</sup>	98	Sigma (94099)
33	Casuarictin isomer	Pedunculagin <sup>B</sup>	95	Toronto (P354070)
34	Castalagin isomer	Castalagin <sup>B</sup>	95	Sigma (61221)
35	Sanguiin H2	Sanguiin H2 <sup>A</sup> Pedunculagin <sup>B</sup>	92 95	[68] Toronto (P354070)
36	Procyanidin trimer	Procyanidin C2 <sup>B</sup>	95	TransMIT (C6201-P045)
37	Pelargonidin <i>O-p</i> -coumaroyl- <i>O</i> -hexoside	Pelargonidin 3- <i>O</i> -glucoside <sup>B</sup>	98	ChemFaces (CFN92134)
38	Cyanidin <i>O</i> -acetyl- <i>O</i> -hexoside	Cyanidin 3- <i>O</i> -glucoside <sup>B</sup>	98	Sigma (94099)
39	Quercetin 3- <i>O</i> -sophoroside	Quercetin 3- <i>O</i> -sophoroside <sup>A,B</sup>	98	ChemFaces (CFN90630)
40	Casuarictin isomer	Pedunculagin <sup>B</sup>	95	Toronto (P354070)
41	Ellagic acid <i>O</i> -pentoside	Ellagic acid <sup>B</sup>	98	ChemFaces (CFN98716)
42	Sanguiin H10	Sanguiin H10 <sup>A</sup> Pedunculagin <sup>B</sup>	92 95	[68] Toronto (P354070)
43	Ellagic acid <i>O</i> -desoxyhexoside	Ellagic acid <sup>B</sup>	98	ChemFaces (CFN98716)
44	Sanguiin H2 isomer	Sanguiin H2 <sup>A</sup> Pedunculagin <sup>B</sup>	92 95	[68] Toronto (P354070)
45	Quercetin 3- <i>O</i> -rutinoside	Rutin	95	Sigma (R2303)
46	Sanguiin H6 isomer	Sanguiin H6 <sup>A</sup> Pedunculagin <sup>B</sup>	92 95	[68] Toronto (P354070)

Table S1. Continuation

No <sup>a</sup>	Compound	Standard <sup>a</sup>	Purity, (≥) %	Manufacturer (Cat. no) <sup>b</sup>
47	Lambertianin C	Lambertianin C <sup>A</sup>	92	[68]
		Pedunculagin <sup>B</sup>	95	Toronto (P354070)
48	Pelargonidin <i>O</i> -acetyl- <i>O</i> -hexoside	Pelargonidin 3- <i>O</i> -glucoside <sup>B</sup>	98	ChemFaces (CFN92134)
49	Quercetin 3- <i>O</i> -glucoside	Quercetin 3- <i>O</i> -glucoside <sup>A,B</sup>	98	Sigma (16654)
50	Quercetin 3- <i>O</i> -glucuronide	Quercetin 3- <i>O</i> -glucuronide <sup>A,B</sup>	90	Sigma (90733)
51	Agrimonic acid A	Agrimonic acid A <sup>A</sup>	90	[28]
		Agrimoniin <sup>B</sup>	95	[28]
52	Sanguin H6	Sanguin H6 <sup>A</sup>	92	[68]
		Pedunculagin <sup>B</sup>	95	Toronto (P354070)
53	Ellagic acid	Ellagic acid	98	ChemFaces (CFN98716)
54	Agrimonic acid B	Agrimonic acid B <sup>A</sup>	90	[28]
		Agrimoniin <sup>B</sup>	95	[28]
55	Quercetin 3- <i>O</i> -xyloside	Quercetin 3- <i>O</i> -xyloside <sup>A,B</sup>	97	Sigma (83390)
56	Quercetin 3- <i>O</i> -arabinoside	Quercetin 3- <i>O</i> -arabinoside <sup>A,B</sup>	95	Sigma (75759)
57	Kaempferol 3- <i>O</i> -rutinoside	Kaempferol 3- <i>O</i> -rutinoside <sup>A,B</sup>	98	Sigma (90242)
58	Kaempferol 3- <i>O</i> -glucoside	Kaempferol 3- <i>O</i> -glucoside <sup>A,B</sup>	97	Sigma (79851)
59	Kaempferol 3- <i>O</i> -glucuronide	Kaempferol 3- <i>O</i> -glucuronide <sup>A,B</sup>	98	ChemFaces (CFN90359)
60	Quercetin 3- <i>O</i> -(6''- <i>O</i> - <i>p</i> -coumaroyl)-glucoside	Helichryoside <sup>A,B</sup>	98	BioCrick (BCN9477)
61	Quercetin <i>O</i> - <i>p</i> -coumaroyl- <i>O</i> -hexoside	Helichryoside <sup>B</sup>	98	BioCrick (BCN9477)
62	Agrimoniin	Agrimoniin <sup>A,B</sup>	95	[28]
63	Fragariin A	Agrimoniin <sup>B</sup>	95	[28]
64	Quercetin <i>O</i> -malonyl- <i>O</i> -hexoside	Quercetin 3- <i>O</i> -(6''- <i>O</i> -malonyl)- glucoside <sup>B</sup>	85	Sigma (16733)
65	Quercetin 3- <i>O</i> -(6''- <i>O</i> -malonyl)-glucoside	Quercetin 3- <i>O</i> -(6''- <i>O</i> -malonyl)- glucoside <sup>A,B</sup>	85	Sigma (16733)
66	Kaempferol 3- <i>O</i> -(6''- <i>O</i> - <i>p</i> -coumaroyl)-glucoside	Tiliroside <sup>A,B</sup>	98	Sigma (79257)
67	1,2,3,4,6-Penta- <i>O</i> -galloylglucose	1,2,3,4,6-Penta- <i>O</i> -galloyl glucose <sup>A,B</sup>	96	Sigma (67548)
68	Kaempferol <i>O</i> -malonyl- <i>O</i> -hexoside	Kaempferol 3- <i>O</i> -(6''- <i>O</i> -malonyl)- glucoside <sup>B</sup>	95	BOC (81149-02-2)
69	Kaempferol 3- <i>O</i> -(6''- <i>O</i> -malonyl)-glucoside	Kaempferol 3- <i>O</i> -(6''- <i>O</i> -malonyl)- glucoside <sup>A,B</sup>	95	BOC (81149-02-2)
70	Quercetin 3- <i>O</i> -(2''- <i>O</i> -acetyl)-glucoside	Quercetin 3- <i>O</i> -(2''- <i>O</i> -acetyl)-glucoside <sup>A</sup>	92	[70]
		Quercetin 3- <i>O</i> -(6''- <i>O</i> -acetyl)-glucoside <sup>B</sup>	85	Extrasynthese (1099)
71	Quercetin 3- <i>O</i> -(6''- <i>O</i> -acetyl)-glucoside	Quercetin 3- <i>O</i> -(6''- <i>O</i> -acetyl)-glucoside <sup>A,B</sup>	85	Extrasynthese (1099)
72	Kaempferol <i>O</i> -acetyl- <i>O</i> -hexoside	Kaempferol 3- <i>O</i> -glucoside <sup>B</sup>	97	Sigma (79851)
73	Kaempferol <i>O</i> -acetyl- <i>O</i> -hexoside	Kaempferol 3- <i>O</i> -glucoside <sup>B</sup>	97	Sigma (79851)
74	Quercetin	Quercetin <sup>A,B</sup>	95	Sigma (Q4951)
75	Tormentic acid di- <i>O</i> -hexoside	Tormentic acid <sup>A,B</sup>	98	ChemFaces (CFN99434)
76	Kaempferol	Kaempferol <sup>A,B</sup>	99	Sigma (96353)
77	Pomolic acid di- <i>O</i> -hexoside	Pomolic acid <sup>B</sup>	98	ChemFaces (CFN99433)
78	Tormentic acid <i>O</i> -hexoside	Tormentic acid <sup>B</sup>	98	ChemFaces (CFN99434)
79	Quercetin 3- <i>O</i> -(2'',6''-di- <i>O</i> -acetyl)-glucoside	Quercetin 3- <i>O</i> -(2'',6''-di- <i>O</i> -acetyl)- glucoside	90	[70]
		Quercetin 3- <i>O</i> -(6''- <i>O</i> -acetyl)-glucoside <sup>B</sup>	85	Extrasynthese (1099)

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Table S1. Continuation

No <sup>a</sup>	Compound	Standard <sup>a</sup>	Purity, (≥) %	Manufacturer (Cat. no) <sup>b</sup>
80	Quercetin <i>O</i> -acetyl- <i>O</i> -malonyl- <i>O</i> -hexoside	Quercetin 3- <i>O</i> -(6''- <i>O</i> -malonyl)- glucoside <sup>B</sup>	85	Sigma (16733)
81	Tormentic acid	Tormentic acid <sup>A,B</sup>	98	ChemFaces (CFN99434)
82	Ellagic acid <i>O</i> -methyl ester- <i>O</i> -desoxyhexoside	Ellagic acid <sup>A,B</sup>	98	ChemFaces (CFN98716)
83	Pomolic acid <i>O</i> -hexoside	Pomolic acid <sup>A,B</sup>	98	ChemFaces (CFN99433)
84	Quercetin <i>O</i> -malonyl- <i>O</i> - <i>p</i> -coumaroyl- <i>O</i> -hexoside	Helichryoside <sup>B</sup>	98	BioCrick (BCN9477)
85	Quercetin <i>O</i> -malonyl- <i>O</i> - <i>p</i> -coumaroyl- <i>O</i> -hexoside	Helichryoside <sup>B</sup>	98	BioCrick (BCN9477)
86	Ellagic acid di- <i>O</i> -methyl ester- <i>O</i> -desoxyhexoside	Ellagic acid <sup>A,B</sup>	98	ChemFaces (CFN98716)
87	Kaempferol di- <i>O</i> -acetyl- <i>O</i> -hexoside	Kaempferol 3- <i>O</i> -glucoside <sup>B</sup>	97	Sigma (79851)
88	Quercetin <i>O</i> -acetyl- <i>O</i> - <i>p</i> -coumaroyl- <i>O</i> -hexoside	Helichryoside <sup>B</sup>	98	BioCrick (BCN9477)
89	Kaempferol <i>O</i> -acetyl- <i>O</i> -malonyl- <i>O</i> -hexoside	Kaempferol 3- <i>O</i> -(6''- <i>O</i> -malonyl)- glucoside <sup>B</sup>	95	BOC (81149-02-2)
90	Kaempferol <i>O</i> -malonyl- <i>O</i> - <i>p</i> -coumaroyl- <i>O</i> -hexoside	Tiliroside <sup>B</sup>	98	Sigma (79257)
91	Pomolic acid	Pomolic acid <sup>A,B</sup>	98	ChemFaces (CFN99433)
92	Kaempferol <i>O</i> -malonyl- <i>O</i> - <i>p</i> -coumaroyl- <i>O</i> -hexoside	Tiliroside <sup>B</sup>	98	Sigma (79257)
93	Kaempferol <i>O</i> -acetyl- <i>O</i> - <i>p</i> -coumaroyl- <i>O</i> -hexoside	Tiliroside <sup>B</sup>	98	Sigma (79257)
94	Quercetin di- <i>O</i> -acetyl- <i>O</i> - <i>p</i> -coumaroyl- <i>O</i> -hexoside	Helichryoside <sup>B</sup>	98	BioCrick (BCN9477)
95	Quercetin <i>O</i> -acetyl- <i>O</i> -malonyl- <i>O</i> - <i>p</i> -coumaroyl- <i>O</i> -hexoside	Helichryoside <sup>B</sup>	98	BioCrick (BCN9477)

35 <sup>a</sup> Standards were used in qualitative (<sup>A</sup>) or/and quantitative analysis (<sup>B</sup>). <sup>b</sup> Manufacturers list:  
36 BioCrick—BioCrick (Chengdu, Sichuan, PRC); BOC—BOC Sciences (Shirley, NY, USA);  
37 Carbosynth—Carbosynth Ltd. (Compton, UK); ChemFaces—ChemFaces (Wuhan, Hubei, PRC);  
38 Extrasynthese—Extrasynthese (Lyon, France); Funakoshi—Funakoshi Co. Ltd. (Tokyo, Japan);  
39 Sigma—Sigma-Aldrich (St. Louis, MO, USA); Toronto—Toronto Research Chemicals (North York, ON,  
40 Canada); TransMIT—TransMIT GmbH (Gießen, Germany).

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42 **Table S2.** Regression equations, correlation coefficients ( $r^2$ ), standard deviation ( $S_{yx}$ ), limits of  
 43 detection (LOD), limits of quantification (LOQ) and linear ranges for 48 reference standards.

Compound	Ionization <sup>a</sup>	CE <sup>b</sup> (eV)	Regression equation <sup>c</sup>		$r^2$	$S_{yx}$	LOD/ LOQ ( $\mu\text{g/mL}$ )	Linear range ( $\mu\text{g/mL}$ )
			$a$	$b \cdot 10^6$				
1,2,3,4,6-Penta- <i>O</i> -galloyl glucose	N	-25	2.4561	-0.0171	0.9979	12.33·10 <sup>-2</sup>	0.17/0.50	0.6–100.0
1- <i>O</i> -Galloyl glucose	N	-20	1.3586	-0.0663	0.9987	9.69·10 <sup>-2</sup>	0.24/0.71	0.8–100.0
3- <i>O</i> -Caffeoylquinic acid	N	-15	0.9320	-0.0523	0.9991	4.14·10 <sup>-2</sup>	0.15/0.44	0.5–100.0
4- <i>O</i> -Caffeoylquinic acid	N	-15	0.9217	-0.0437	0.9982	3.94·10 <sup>-2</sup>	0.14/0.43	0.5–100.0
5- <i>O</i> -Caffeoylquinic acid	N	-15	0.9406	-0.0497	0.9973	5.18·10 <sup>-2</sup>	0.18/0.55	0.6–100.0
Agrimoniin	N	-35	0.8214	-0.2716	0.9893	5.37·10 <sup>-2</sup>	0.22/0.65	0.7–100.0
Ascorbic acid	N	-10	0.9214	-0.0373	0.9997	2.10·10 <sup>-2</sup>	0.07/0.22	0.3–100.0
Castalagin	N	-35	0.9361	-0.4518	0.9870	9.35·10 <sup>-2</sup>	0.32/1.00	1.0–100.0
Catechin	N	-35	0.9562	-0.0521	0.9971	7.79·10 <sup>-2</sup>	0.27/0.82	0.9–100.0
Citric acid	N	-10	0.9518	-0.0267	0.9990	1.03·10 <sup>-2</sup>	0.03/0.10	0.1–100.0
Cyanidin 3- <i>O</i> -glucoside	N	-20	1.4267	-0.5637	0.9907	12.72·10 <sup>-2</sup>	0.29/0.89	0.9–100.0
Cyanidin 3- <i>O</i> -rutinoside	N	-20	1.6341	-0.4283	0.9900	15.02·10 <sup>-2</sup>	0.30/0.92	1.0–100.0
Cyanidin 3- <i>O</i> -sophoroside	N	-20	1.5963	-0.3518	0.9910	14.63·10 <sup>-2</sup>	0.30/0.92	1.0–100.0
Ellagic acid	N	-30	0.9114	-0.6312	0.9887	6.37·10 <sup>-2</sup>	0.23/0.70	0.7–100.0
Fructose	N	-10	1.5632	-0.0376	0.9983	5.14·10 <sup>-2</sup>	0.11/0.33	0.4–100.0
Fumaric acid	N	-10	0.8615	-0.0364	0.9982	2.03·10 <sup>-2</sup>	0.03/0.07	0.1–100.0
Gallic acid	N	-20	2.6538	-0.1376	0.9990	1.17·10 <sup>-2</sup>	0.01/0.04	0.1–100.0
Helichryoside	N	-30	2.0319	-0.3615	0.9811	10.09·10 <sup>-2</sup>	0.17/0.52	0.6–100.0
Kaempferol 3- <i>O</i> -(6''- <i>O</i> -malonyl)-glucoside	N	-30	2.3618	-0.5214	0.9873	11.35·10 <sup>-2</sup>	0.16/0.48	0.5–100.0
Kaempferol 3- <i>O</i> -glucoside	N	-20	2.0859	-0.9171	0.9980	6.18·10 <sup>-2</sup>	0.03/0.09	0.1–100.0
Kaempferol 3- <i>O</i> -glucuronide	N	-30	2.2126	-0.5160	0.9987	8.11·10 <sup>-2</sup>	0.12/0.37	0.4–100.0
Kaempferol 3- <i>O</i> -rutinoside	N	-30	1.9634	-0.4511	0.9952	9.18·10 <sup>-2</sup>	0.15/0.46	0.5–100.0
Kaempferol	N	-20	1.2416	-0.3615	0.9901	3.02·10 <sup>-2</sup>	0.08/0.24	0.3–100.0
Malic acid	N	-10	0.9911	-0.0379	0.9988	2.05·10 <sup>-2</sup>	0.07/0.21	0.3–100.0
Oxalic acid	N	-10	0.9804	-0.0210	0.9970	2.01·10 <sup>-2</sup>	0.06/0.21	0.3–100.0
<i>p</i> -Coumaric acid 4- <i>O</i> -glucoside	N	-20	1.4238	-0.0891	0.9901	7.33·10 <sup>-2</sup>	0.17/0.52	0.6–100.0
Pedunculagin	N	-35	0.6370	-0.4521	0.9872	6.11·10 <sup>-2</sup>	0.32/0.96	1.0–100.0
Pelargonidin 3- <i>O</i> -glucoside	N	-20	0.9634	-0.8634	0.9832	10.37·10 <sup>-2</sup>	0.36/1.07	1.1–100.0
Pelargonidin 3- <i>O</i> -rutinoside	N	-20	0.8237	-0.7310	0.9801	14.73·10 <sup>-2</sup>	0.59/1.79	2.0–100.0
Pomolic acid	N	-30	1.4784	-0.8634	0.9763	19.39·10 <sup>-2</sup>	0.43/1.31	1.5–100.0
Procyanidin B2	N	-25	1.3620	-0.0820	0.9961	9.91·10 <sup>-2</sup>	0.21/0.72	0.8–100.0
Procyanidin B4	N	-25	1.0634	-0.0933	0.9902	10.01·10 <sup>-2</sup>	0.31/0.94	1.0–100.0
Procyanidin C2	N	-25	1.4632	-0.0524	0.9953	8.12·10 <sup>-2</sup>	0.18/0.56	0.6–100.0
Quercetin 3- <i>O</i> -(6''- <i>O</i> -acetyl)-glucoside	N	-20	1.1103	-0.9217	0.9901	14.33·10 <sup>-2</sup>	0.42/1.29	1.5–100.0
Quercetin 3- <i>O</i> -(6''- <i>O</i> -malonyl)-glucoside	N	-20	1.2703	-0.7911	0.9814	15.26·10 <sup>-2</sup>	0.40/1.20	1.5–100.0
Quercetin 3- <i>O</i> -arabinoside	N	-20	1.4412	-0.6211	0.9930	11.25·10 <sup>-2</sup>	0.26/0.78	0.8–100.0
Quercetin 3- <i>O</i> -glucoside	N	-20	1.8267	-0.4160	0.9990	11.73·10 <sup>-2</sup>	0.21/0.67	0.7–100.0
Quercetin 3- <i>O</i> -glucuronide	N	-20	1.6705	-0.4374	0.9988	12.79·10 <sup>-2</sup>	0.25/0.77	0.8–100.0
Quercetin 3- <i>O</i> -sophoroside	N	-25	1.4001	-0.8214	0.9884	12.08·10 <sup>-2</sup>	0.29/0.86	1.0–100.0
Quercetin 3- <i>O</i> -xyloside	N	-20	1.5364	-0.3614	0.9927	10.07·10 <sup>-2</sup>	0.22/0.66	0.7–100.0
Quercetin	N	-15	1.1105	-0.3211	0.9937	4.18·10 <sup>-2</sup>	0.12/0.38	0.4–100.0
Rutin	N	-25	1.2716	-0.7389	0.9897	9.14·10 <sup>-2</sup>	0.23/0.72	0.8–100.0
Strictinin	N	-35	0.9634	-0.3518	0.9804	7.34·10 <sup>-2</sup>	0.25/0.76	0.8–100.0
Sucrose	N	-10	1.6278	-0.0428	0.9990	7.11·10 <sup>-2</sup>	0.14/0.44	0.5–100.0

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Table S2. Continuation

Compound	Ionization <sup>a</sup>	CE <sup>b</sup> (eV)	Regression equation <sup>c</sup>		$r^2$	$S_{yx}$	LOD/ LOQ ( $\mu\text{g/mL}$ )	Linear range ( $\mu\text{g/mL}$ )
			$a$	$b \cdot 10^6$				
Tartaric acid	N	-10	1.5330	-0.0863	0.9985	$4.15 \cdot 10^{-2}$	0.09/0.27	0.3–100.0
Tiliroside	N	-30	2.3312	-0.4563	0.9803	$14.92 \cdot 10^{-2}$	0.21/0.64	0.7–100.0
Tormentic acid	N	-30	1.2820	-0.9634	0.9697	$11.64 \cdot 10^{-2}$	0.30/0.91	1.0–100.0
Umbelliferone	N	-15	0.5697	-0.2634	0.9900	$4.33 \cdot 10^{-2}$	0.25/0.76	0.8–100.0

45 <sup>a</sup> Ionization mode : N—negative. <sup>b</sup> CE—collision energy. <sup>c</sup> Regression equation:  $y = a \cdot x + b$ .

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