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Article

Chemometric characterization of strawberries and blueberries according to their phenolic profile: combined effect of cultivar and cultivation system

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Content

Table S1. Presence of each identified compound in integrated and organic strawberry and blueberry fruit samples.

Table S2. Presence of each identified compound in integrated and organic strawberry and blueberry leaf samples.

Figure S1. Proposed fragmentation pathway of compound 37.

29	Procyanidin dimer B type isomer 3	+	+	+	+	+	+	+	+	+	+	+	+
30	Methyl 3-caffeoylquininate	-	-	-	-	-	-	-	-	-	-	-	-
31	Caffeic acid	+	+	+	+	+	+	+	+	+	+	+	+
32	Epicatechin	+	+	+	+	+	+	-	-	-	-	-	-
33	5-Caffeoylquinic acid isomer	+	+	+	+	+	+	-	-	-	-	-	-
34	Syringic acid	+	+	+	+	+	+	-	-	-	-	-	-
35	Caffeoylshikimic acid	+	+	+	+	+	+	-	-	-	-	-	-
36	Myricetin 3- <i>O</i> -rutinoside	-	-	-	-	-	-	-	-	-	-	-	-
37	Quercetin 3- <i>O</i> -hexoside-7- <i>O</i> -hexuronide	-	-	-	-	-	-	-	-	-	-	-	-
38	Myricetin 3- <i>O</i> -hexoside	+	+	+	+	+	+	-	-	-	-	-	-
39	Methyl 4-caffeoylquininate	-	-	-	-	-	-	-	-	-	-	-	-
40	Ellagic acid pentoside	-	-	-	-	-	-	+	+	+	+	+	+
41	Methyl 3- <i>p</i> -coumaroylquininate	-	-	-	-	-	-	-	-	-	-	-	-
42	Ellagic acid rhamnoside	-	-	-	-	-	-	+	+	+	+	+	+
43	Apigenin 8- <i>C</i> -glucoside	+	+	+	+	+	+	-	-	-	-	-	-
44	Methyl 5-caffeoylquininate isomer 1	+	+	+	+	+	+	+	+	+	+	+	+
45	Coumaric acid hexoside isomer 3	-	-	-	-	-	-	+	+	+	+	+	+
46	Quercetin 3- <i>O</i> -rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
47	Myricetin 3- <i>O</i> -pentoside	+	+	+	+	+	+	-	-	-	-	-	-
48	<i>p</i> -Coumaric acid	+	+	+	+	+	+	+	+	+	+	+	+
49	Quercetin 3- <i>O</i> -galactoside	+	+	+	+	+	+	+	+	+	+	+	+
50	Methyl 5-caffeoylquininate isomer 2	+	+	+	+	+	+	-	-	-	-	-	-
51	Ellagic acid	-	-	-	-	-	-	+	+	+	+	+	+
52	Kaempferol 7- <i>O</i> -rutinoside	+	+	+	+	+	+	+	+	+	+	+	+
53	Quercetin 3- <i>O</i> -rhamnosyl-hexuronide	-	-	-	-	-	-	-	-	-	-	-	-
54	Vanillic acid	+	+	+	+	+	+	+	+	+	+	+	+
55	Isorhamnetin 3- <i>O</i> -rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
56	Quercetin 3- <i>O</i> -pentoside	+	+	+	+	+	+	-	-	-	-	-	-
57	Sinapic acid	+	+	+	+	+	+	-	-	-	-	-	-
58	Ferulic acid	+	+	+	+	+	+	+	+	+	+	+	+
59	Methyl 5- <i>p</i> -coumaroylquininate isomer 1	-	-	-	-	-	-	-	-	-	-	-	-
60	Kaempferol 3- <i>O</i> -glucoside	+	+	+	+	+	+	+	+	+	+	+	+
61	Syringetin 3- <i>O</i> -hexoside	+	+	+	+	+	+	-	-	-	-	-	-

62	Isorhamnetin 3- <i>O</i> -hexoside	+	+	+	+	+	+	-	-	-	-	-	-
63	Quercetin 3- <i>O</i> -acetyl-hexoside isomer 1	+	+	+	+	+	+	-	-	-	-	-	-
64	Isorhamnetin 3- <i>O</i> -hexuronide	+	+	+	+	+	+	+	+	+	+	+	+
65	Dicaffeoylquinic acid isomer 1	+	+	-	+	+	-	-	-	-	-	-	-
66	Methyl 5- <i>p</i> -coumaroylquinic acid isomer 2	-	-	-	-	-	-	-	-	-	-	-	-
67	Quercetin 3- <i>O</i> -acetyl-hexoside isomer 2	+	+	+	+	+	+	-	-	-	-	-	-
68	Quercetin 3- <i>O</i> -methyl-malonyl-hexoside	+	+	+	+	+	+	-	-	-	-	-	-
69	Quercetin 7- <i>O</i> -hexuronide	+	+	+	+	+	+	+	+	+	+	+	+
70	Isorhamnetin 3- <i>O</i> -pentoside	+	+	+	+	+	+	-	-	-	-	-	-
71	Quercetin 3- <i>O</i> -malonyl-hexoside	+	+	+	+	+	+	+	+	+	+	+	+
72	Dicaffeoylquinic acid isomer 2	+	+	-	+	+	-	-	-	-	-	-	-
73	Kaempferol 7- <i>O</i> -hexuronide	-	-	-	-	-	-	+	+	+	+	+	+
74	Isorhamnetin 3- <i>O</i> -malonyl-rutinoside	+	-	-	+	-	-	-	-	-	-	-	-
75	Myricetin	-	-	-	+	+	+	-	-	-	-	-	-
76	Methyl 3,4-dicaffeoylquinic acid	+	-	-	+	-	-	-	-	-	-	-	-
77	Kaempferol 3- <i>O</i> -hexuronide methyl ether	+	+	+	+	+	+	+	+	+	+	+	+
78	Kaempferol 3- <i>O</i> -malonyl-hexoside	+	-	-	+	-	-	+	+	+	+	+	+
79	Methyl caffeate	+	+	+	+	+	+	+	+	+	+	+	+
80	Methyl 3,5-dicaffeoylquinic acid	+	+	-	+	+	-	-	-	-	-	-	-
81	Feruloyl-coumaroylquinic acid isomer 1	+	-	-	+	-	-	-	-	-	-	-	-
82	Methyl 4,5-dicaffeoylquinic acid	+	+	-	+	+	-	-	-	-	-	-	-
83	Kaempferol 3- <i>O-p</i> -coumaroyl-hexoside	-	-	-	-	-	-	+	+	+	+	+	+
84	<i>cis, trans</i> -Abscisic acid	+	+	+	+	+	+	+	+	+	+	+	+
85	Feruloyl-coumaroylquinic acid isomer 2	+	+	-	+	+	-	-	-	-	-	-	-
86	Quercetin	+	+	+	+	+	+	+	+	+	+	+	+
87	Feruloyl-coumaroylquinic acid isomer 3	-	-	-	-	-	-	-	-	-	-	-	-
88	Cinnamic acid	+	+	+	+	+	+	+	+	+	+	+	+
89	Naringenin	+	+	+	+	+	+	-	-	-	-	-	-
90	Kaempferol	-	-	-	+	+	+	+	+	+	+	+	+
91	Syringetin	-	-	-	+	+	+	-	-	-	-	-	-
92	Isorhamnetin	-	-	-	+	+	+	-	-	-	-	-	-
93	Pinocembrin	-	-	-	-	-	-	-	-	-	-	-	-

+ stands for detected; - stands for not detected.

Table S2. Presence of each identified compound in integrated and organic strawberry and blueberry leaf samples.

No	Compound name	Blueberry-leaf						Strawberry-leaf					
		Integrated			Organic			Integrated			Organic		
		Bluecrop	Duke	Nui	Bluecrop	Duke	Nui	Alba	Fayette	Clery	Alba	Fayette	Clery
1	Gallic acid hexoside isomer 1	+	+	+	+	+	+	+	+	+	+	+	+
2	Dihydroxybenzoic acid hexoside isomer 1	+	+	+	+	+	+	+	+	+	+	+	+
3	Gallic acid hexoside isomer 2	+	+	+	+	+	+	+	+	+	+	+	+
4	Prodelphinidin dimer B type	+	+	+	+	+	+	-	-	-	-	-	-
5	Caffeoyltartaric acid	-	-	-	-	-	-	+	+	+	+	+	+
6	Chlorogenic acid hexoside isomer 1	+	+	+	+	+	+	+	+	+	+	+	+
7	Gallocatechin	+	+	+	+	+	+	-	-	-	-	-	-
8	Dihydroxybenzoic acid hexosyl-pentoside	+	+	+	+	+	+	+	+	+	+	+	+
9	Gallic acid hexoside isomer 3	+	+	+	+	+	+	+	+	+	+	+	+
10	Chlorogenic acid hexoside isomer 2	+	+	+	+	+	+	+	+	+	+	+	+
11	Caffeic acid hexoside isomer 1	+	+	+	+	+	+	-	-	-	-	-	-
12	Dihydroxybenzoic acid pentoside	+	+	+	+	+	+	+	+	+	+	+	+
13	3-O-Caffeoylquinic acid isomer 1	+	+	+	+	+	+	-	-	-	-	-	-
14	Hydroxybenzoic acid hexoside	-	-	-	-	-	-	+	+	+	+	+	+
15	3-O-Caffeoylquinic acid isomer 2	+	+	+	+	+	+	-	-	-	-	-	-
16	Procyanidin dimer B type isomer 1	+	+	+	+	+	+	+	+	+	+	+	+
17	Aesculin	+	+	+	+	+	+	+	+	+	+	+	+
18	Caffeic acid hexoside isomer 2	+	+	+	+	+	+	+	+	+	+	+	+
19	Coumaric acid hexoside isomer 1	+	+	+	+	+	+	+	+	+	+	+	+
20	Procyanidin dimer B type isomer 2	-	-	-	-	-	-	-	-	-	-	-	-
21	5-O-Caffeoylquinic acid	+	+	+	+	+	+	+	+	+	+	+	+
22	Epigallocatechin	-	-	-	-	-	-	-	-	-	-	-	-
23	Dihydroxybenzoic acid hexoside isomer 2	-	-	-	-	-	-	+	+	+	+	+	+
24	Quercetin 3-O-hexoside-7-O-hexuronide	-	-	-	-	-	-	+	+	+	+	+	+
25	Catechin	+	+	+	+	+	+	+	+	+	+	+	+
26	<i>p</i> -Hydroxybenzoic acid	+	+	+	+	+	+	+	+	+	+	+	+
27	Coumaric acid hexoside isomer 2	-	-	-	-	-	-	+	+	+	+	+	+
28	4-O-Caffeoylquinic acid	+	+	+	+	+	+	-	-	-	-	-	-

29	Procyanidin dimer B type isomer 3	-	-	-	-	-	-	-	-	-	-	-	-
30	Methyl 3-caffeoylquininate	+	+	+	+	+	+	-	-	-	-	-	-
31	Caffeic acid	+	+	+	+	+	+	+	+	+	+	+	+
32	Epicatechin	-	-	-	-	-	-	-	-	-	-	-	-
33	5-Caffeoylquinic acid isomer	+	+	+	+	+	+	+	+	+	+	+	+
34	Syringic acid	-	-	-	-	-	-	+	+	+	+	+	+
35	Caffeoylshikimic acid	+	+	+	+	+	+	+	+	+	+	+	+
36	Myricetin 3- <i>O</i> -rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
37	Quercetin 3- <i>O</i> -hexosyl-hexuronide	-	-	-	-	-	-	+	+	+	+	+	+
38	Myricetin 3- <i>O</i> -hexoside	+	+	+	+	+	+	-	-	-	-	-	-
39	Methyl 4-caffeoylquininate	+	+	+	+	+	+	-	-	-	-	-	-
40	Ellagic acid pentoside	-	-	-	-	-	-	+	+	+	+	+	+
41	Methyl 3- <i>p</i> -coumaroylquininate	+	+	+	+	+	+	-	-	-	-	-	-
42	Ellagic acid rhamnoside	-	-	-	-	-	-	+	+	+	+	+	+
43	Apigenin 8- <i>C</i> -glucoside	+	+	+	+	+	+	-	-	-	-	-	-
44	Methyl 5-caffeoylquininate isomer 1	+	+	+	+	+	+	+	+	+	+	+	+
45	Coumaric acid hexoside isomer 3	-	-	-	-	-	-	+	+	+	+	+	+
46	Quercetin 3- <i>O</i> -rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
47	Myricetin 3- <i>O</i> -pentoside	+	+	+	+	+	+	-	-	-	-	-	-
48	<i>p</i> -Coumaric acid	+	+	+	+	+	+	+	+	+	+	+	+
49	Quercetin 3- <i>O</i> -galactoside	+	+	+	+	+	+	+	+	+	+	+	+
50	Methyl 5-caffeoylquininate isomer 2	+	+	+	+	+	+	-	-	-	-	-	-
51	Ellagic acid	-	-	-	-	-	-	+	+	+	+	+	+
52	Kaempferol 7- <i>O</i> -rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
53	Quercetin 3- <i>O</i> -rhamnosyl-hexuronide	-	-	-	-	-	-	+	+	+	+	+	+
54	Vanillic acid	+	+	+	+	+	+	+	+	+	+	+	+
55	Isorhamnetin 3- <i>O</i> -rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
56	Quercetin 3- <i>O</i> -pentoside	+	+	+	+	+	+	+	+	+	+	+	+
57	Sinapic acid	+	+	+	+	+	+	+	+	+	+	+	+
58	Ferulic acid	+	+	+	+	+	+	+	+	+	+	+	+
59	Methyl 5- <i>p</i> -coumaroylquininate isomer 1	+	+	+	+	+	+	-	-	-	-	-	-
60	Kaempferol 3- <i>O</i> -glucoside	+	+	+	+	+	+	+	+	+	+	+	+
61	Syringetin 3- <i>O</i> -hexoside	+	+	-	+	+	+	-	-	-	-	-	-

62	Isorhamnetin 3- <i>O</i> -hexoside	+	+	+	+	+	+	-	-	-	-	-	-
63	Quercetin 3- <i>O</i> -acetyl-hexoside isomer 1	+	+	+	+	+	+	-	-	-	-	-	-
64	Isorhamnetin 3- <i>O</i> -hexuronide	+	+	+	+	+	+	+	+	+	+	+	+
65	Dicaffeoylquinic acid isomer 1	+	+	-	+	+	-	-	-	-	-	-	-
66	Methyl 5- <i>p</i> -coumaroylquininate isomer 2	+	+	+	+	+	+	-	-	-	-	-	-
67	Quercetin 3- <i>O</i> -acetyl-hexoside isomer 2	+	+	+	+	+	+	-	-	-	-	-	-
68	Quercetin 3- <i>O</i> -methyl-malonyl-hexoside	+	+	+	+	+	+	-	-	-	-	-	-
69	Quercetin 7- <i>O</i> -hexuronide	+	+	+	+	+	+	+	+	+	+	+	+
70	Isorhamnetin 3- <i>O</i> -pentoside	-	+	-	-	+	-	-	-	-	-	-	-
71	Quercetin 3- <i>O</i> -malonyl-hexoside	+	+	+	+	+	+	-	-	-	-	-	-
72	Dicaffeoylquinic acid isomer 2	+	+	-	+	+	-	-	-	-	-	-	-
73	Kaempferol 7- <i>O</i> -hexuronide	-	-	-	-	-	-	+	+	+	+	+	+
74	Isorhamnetin 3- <i>O</i> -malonyl-rutinoside	+	+	-	+	+	-	-	-	-	-	-	-
75	Myricetin	+	+	+	+	+	+	-	-	-	-	-	-
76	Methyl 3,4-dicaffeoylquininate	+	-	-	+	-	-	-	-	-	-	-	-
77	Kaempferol 3- <i>O</i> -hexuronide methyl ether	-	-	-	-	-	-	+	+	+	+	+	+
78	Kaempferol 3- <i>O</i> -malonyl-hexoside	+	+	+	+	+	+	-	-	-	-	-	-
79	Methyl caffeate	+	+	+	+	+	+	+	+	+	+	+	+
80	Methyl 3,5-dicaffeoylquininate	+	+	-	+	+	-	-	-	-	-	-	-
81	Feruloyl-coumaroylquinic acid isomer 1	+	-	-	+	-	-	-	-	-	-	-	-
82	Methyl 4,5-dicaffeoylquininate	+	+	-	+	+	-	-	-	-	-	-	-
83	Kaempferol 3- <i>O-p</i> -coumaroyl-hexoside	-	-	-	-	-	-	+	+	+	+	+	+
84	<i>cis, trans</i> -Abscisic acid	-	-	-	-	-	-	-	-	-	-	-	-
85	Feruloyl-coumaroylquinic acid isomer 2	+	+	-	+	+	-	-	-	-	-	-	-
86	Quercetin	+	+	+	+	+	+	+	+	+	+	+	+
87	Feruloyl-coumaroylquinic acid isomer 3	+	+	-	+	+	-	-	-	-	-	-	-
88	Cinnamic acid	+	+	+	+	+	+	+	+	+	+	+	+
89	Naringenin	+	+	+	+	+	+	+	+	+	+	+	+
90	Kaempferol	+	+	+	+	+	+	+	+	+	+	+	+
91	Syringetin	-	-	-	-	-	-	-	-	-	-	-	-
92	Isorhamnetin	+	+	+	+	+	+	-	-	-	-	-	-
93	Pinocembrin	-	-	-	-	-	-	+	+	+	+	+	+

+ stands for detected: - stands for not detected.

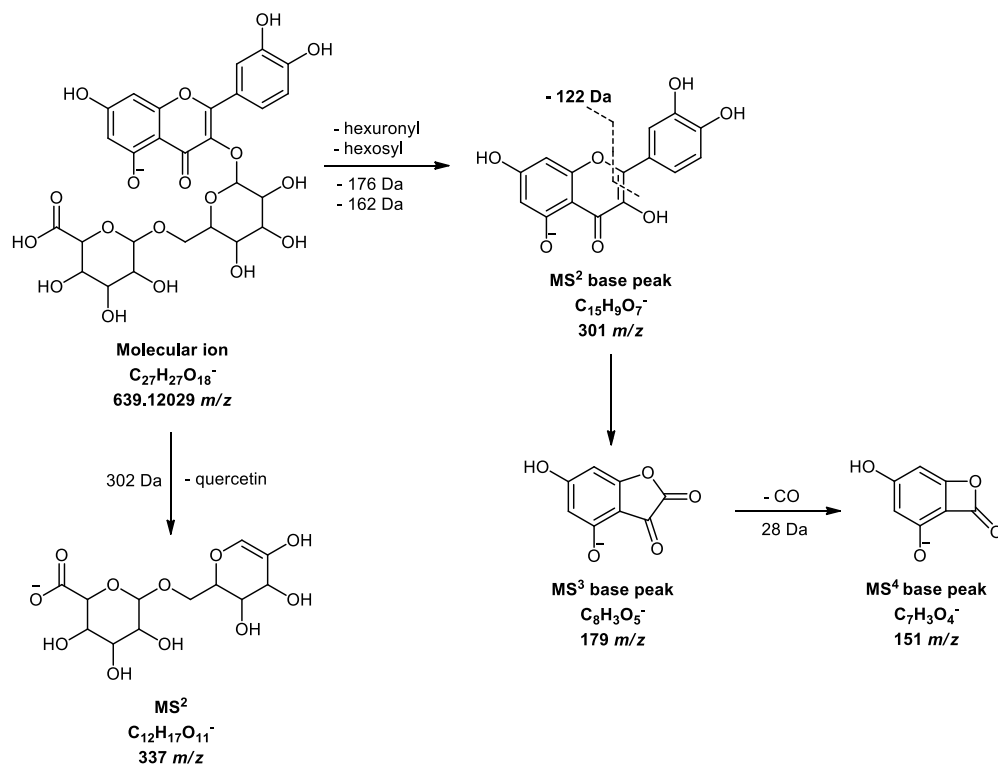


Figure S1. Proposed fragmentation pathway of compound 37.