

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> -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.

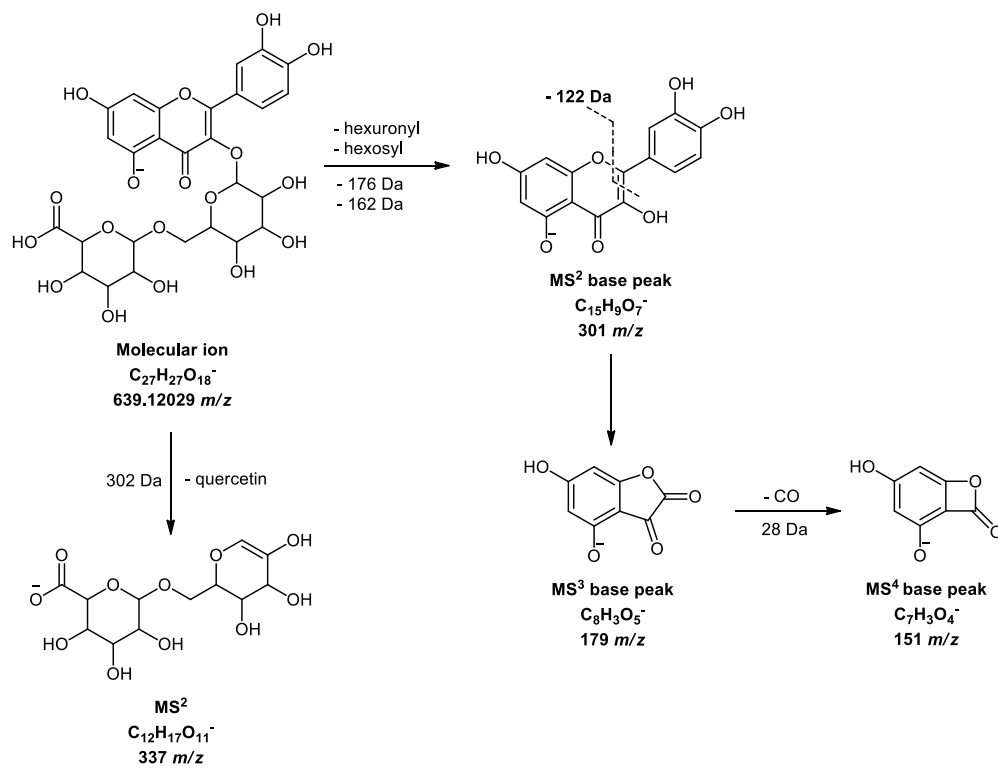
Table S2. Presence of each identified compound in integrated and organic strawberry and blueberry leaf samples.

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-O-rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
37	Quercetin 3-O-hexosyl-hexuronide	-	-	-	-	-	-	+	+	+	+	+	+
38	Myricetin 3-O-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-O-rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
47	Myricetin 3-O-pentoside	+	+	+	+	+	+	-	-	-	-	-	-
48	<i>p</i> -Coumaric acid	+	+	+	+	+	+	+	+	+	+	+	+
49	Quercetin 3-O-galactoside	+	+	+	+	+	+	+	+	+	+	+	+
50	Methyl 5-caffeoylquininate isomer 2	+	+	+	+	+	+	-	-	-	-	-	-
51	Ellagic acid	-	-	-	-	-	-	+	+	+	+	+	+
52	Kaempferol 7-O-rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
53	Quercetin 3-O-rhamnosyl-hexuronide	-	-	-	-	-	-	+	+	+	+	+	+
54	Vanillic acid	+	+	+	+	+	+	+	+	+	+	+	+
55	Isorhamnetin 3-O-rutinoside	+	+	+	+	+	+	-	-	-	-	-	-
56	Quercetin 3-O-pentoside	+	+	+	+	+	+	+	+	+	+	+	+
57	Sinapic acid	+	+	+	+	+	+	+	+	+	+	+	+
58	Ferulic acid	+	+	+	+	+	+	+	+	+	+	+	+
59	Methyl 5- <i>p</i> -coumaroylquininate isomer 1	+	+	+	+	+	+	-	-	-	-	-	-
60	Kaempferol 3-O-glucoside	+	+	+	+	+	+	+	+	+	+	+	+
61	Syringetin 3-O-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.