Supplementary information

Supplementary Table 1. The annotation of peaks isolated from American Elderberry juices

Compounds	Formula	Adducts	Theoretical Mass	Observed Mass	Δm (ppm)	Activities	Ref
3-4, Dihydroxybenzoic acid	$C_7H_6O_4$	$[M-H]^-$	154.02661	154.027	1.5	Antioxidant, anti-inflammatory	[1]
3-Furoic acid	$C_5H_4O_3$	$[M-H]^-$	112.01605	112.017	4.3	Allosteric modulator	[2]
3-hydroxycoumarin	$C_9H_6O_3$	$[M+H]^+$	162.03169	162.031	-2.9	Anticancer, anti-inflammatory, antimicrobial	[3–5]
4-caffeoylquinic acid (cryptochlorogenic acid)	$C_{16}H_{18}O_9$	$[M+H]^+$	354.09508	354.095	1.2	Anti-inflammatory, antioxidant, antidiabetic	[6,7]
4-hydroxybenzaldehyde	$C_7H_6O_2$	$[M+H]^+$	122.03678	122.036	-5.0	Antioxidant, wound healing, vasculoprotective agent	[8,9]
5,7-Dihydroxychromone	$C_9H_6O_4$	$[M+H]^+$	178.02661	178.026	-2.4	Antioxidant, antidiabetic, anticancer	[10–12]
7,8-Dihydroxycoumarin (Daphnetin)	$C_9H_6O_4$	$[M+H]^+$	178.02661	178.026	-2.4	Neuroprotective, antioxidant, anti-inflammatory, anticancer	[13,14]
Allamandin	$C_{15}H_{16}O_7$	$[M+H]^+$	308.0896	308.089	-1.3	Antiviral, anticancer	[15–17]
Anethole	$C_{10}H_{12}O$	$[M+H]^+$	148.08882	148.088	-3.6	Antimicrobial, antioxidant, anti-inflammatory	[18,19]
Aurentiacin	$C_{18}H_{18}O_4$	$[M+H]^+$	298.12051	298.12	-1.0	Anti-inflamatory, antimicrobial	[20,21]
Betaine	$C_5H_{11}NO_2$	$[M+H]^+$	117.07898	117.078	-4.3	Antioxidant, anti-inflammatory	[22,23]
Burseran	$C_{22}H_{26}O_6$	$[M+Na]^+$	386.17294	386.173	-0.2	Anti-inflammatory, anticancer	[24–27]

Caffeic acid	$C_9H_8O_4$	$[M-H]^-$	180.04226	180.043	2.0	Antioxidant	[28]
Castanospermine	$C_8H_{15}NO_4$	$[M+H]^+$	189.10011	189.1	-2.3	Antivirus, anticancer	[29,30]
Catechin	$C_{15}H_{14}O_6$	$[M-H]^-$	290.07904	290.079	0.2	Antioxidant, anticancer, cardiovasculoprotective potency	[31,32]
Cearoin	$C_{14}H_{12}O_4$	$[M+H]^+$	244.07356	244.073	-0.9	Anticancer, anti-inflammatory, antimicrobial	[33–35]
Chlorogenic acid (5-caffeoylquinic acid)	$C_{16}H_{18}O_9$	$[M+H]^+$	354.09508	354.095	1.2	Antimicrobial, antidiabetic, antioxidant, anti-obesity, antihypertension	[36,37]
Chromone	$C_9H_6O_2$	$[M+H]^+$	146.03678	146.036	-3.1	Antiallergic, anti-inflammatory, antidiabetic, anticancer, and antimicrobial	[38,39]
Cinnamaldehyde	C_9H_8O	$[M+H]^+$	132.05751	132.057	-3.8	Antimicrobial, antidiabetic, antioxidant	[40,41]
Citric acid	$C_6H_8O_7$	$[M-H]^-$	192.027	192.027	0.6	Antioxidant, anti-inflammation	[42,43]
Cotinine	$C_{10}H_{12}N_2O$	$[M+H]^+$	176.09496	176.094	-4.9	Neuroprotective	[44]
Coumarin	$C_9H_6O_2$	$[M+H]^+$	146.03678	146.036	-3.1	Anticancer, anti-inflammatory, antimicrobial	[3,4]
Cuminaldehyde	$C_{10}H_{12}O$	$[M+H]^+$	148.08882	148.088	-3.6	Antimicrobial, antioxidant, anticancer	[45,46]
Cyanidin 3-O-galactoside	$C_{21}H_{21}O_{11}$	$[M+]^+$	449.10839	449.108	1.4	Antioxidant, anti-inflammatory, anticancer	[47]
Cyanidin 3-O-glucoside	$C_{21}H_{21}O_{11}$	$[M+H]^+$	449.10839	449.109	2.1	Antioxidant, anti-inflammatory	[48–50]

Cyanidin 3-O-rutinoside	C27H31O15	[M+]+	595.1663	595.166	0.0	Antioxidant, anti-inflammatory	48,50
Cyanidin 3-O-sambubioside	C26H29O15	[M+]+	581.15065	581.15	1.9	Anticancer, antihypertension, antioxidant, antimicrobial	51,52
Cyanidin 3-O-sophoroside	C27H31O16	[M+]+	611.16121	611.161	0.2	Anticancer, antioxidant	53,54
Cyanidin 3,5-O-diglucoside	C27H31O16	[M+]+	611.16121	611.161	0.2	Antioxidant, anti-inflammatory, skin hydration effect	55,56
Dehydrozingerone	C11H12O3	[M+H] +	192.07864	192.078	-3.7	Antioxidant, anti-inflammatory, antidepressant, antimicrobial, antidiabetic, anticancer	57–60
Delphinidin 3-O-rutinoside (tulipanin)	C27H31O16	[M+H] +	611.16121	611.16	1.2	Antioxidant, anticancer	61,62
Dimethadione	C5H7NO3	[M+NH4] +	129.04259	129.042	-2.4	Antiepileptic	63
Epiafzelechin trimethyl ether	C18H20O5	[M+H] +	316.13107	316.131	-0.8	Anticancer	64
Epicatechin	C15H14O6	[M-H] -	290.07904	290.079	1.3	Antioxidant, anti-inflammatory, neuroprotective agent	65–67
Estragole	C10H12O	[M+H] +	148.08882	148.088	-3.6	Antioxidant, anticancer	68
Ethyl p-coumarate	C11H12O3	[M+H] +	192.07864	192.078	-3.7	Antifungal, antioxidant	69,70
Ferulic acid	C10H10O4	[M+H] +	194.05791	194.057	4.3	Antioxidant, anti-inflammatory, anticancer, antimicrobial	71,72
Gallic acid	C7H6O5	[M+NH4] +	170.02152	170.021	2.1	Antioxidant, anti-inflammatory, anticancer, antimicrobial, antiviral	73

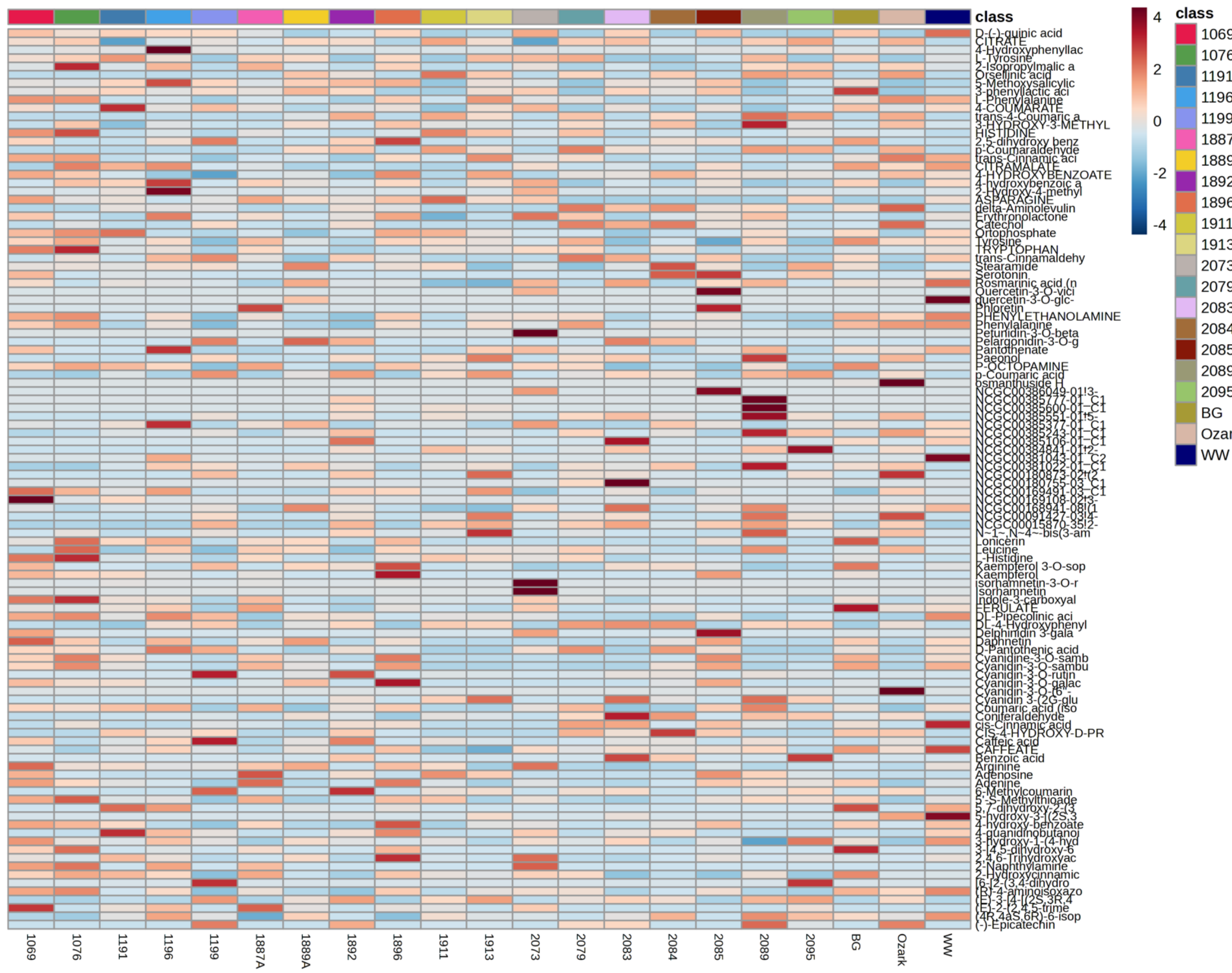
Gastrodin	C13H18O7	[M+Na]+	286.10525	286.105	-0.6	Neuroprotective, antidiabetic, anti-inflammatory	74,75
Herniarin	C10H8O3	[M+H]+	176.04734	176.047	-2.7	Anticancer, anti-inflammatory, neuroprotective	76,76
Hymechrome	C10H8O3	[M+H]+	176.04734	176.047	-2.7	Anticancer	77
Hyperoside (Quercetin 3-galactoside)	C21H20O12	[M-H]-	464.09548	464.096	0.5	Anticancer, anti-inflammatory, antibacterial, antiviral, antidepressant	78
Indoleacrylic acid	C11H9NO2	[M+H]+	187.06333	187.063	-2.4	Anti-inflammatory	79
Isohopeaphenol	C56H42O12	[M+K]+	906.26763	905.265	-1106.6	Antioxidant, antimicrobial, antiviral	80–82
Isorhamnetin	C16H12O7	[M+H]+	316.0583	316.058	0.9	Anticancer, antioxidant	83,84
Isorhamnetin 3-rutinoside (Narcissin)	C28H32O16	[M-H]-	624.16903	624.169	0.2	Antiviral, antioxidant, antimicrobial, anticancer	85–87
Isorhamnetin-3-glucoside	C22H22O12	[M-H]-	478.11113	478.111	0.5	Anti-inflammatory	88
Kaempferol	C15H10O6	[M-H]-	286.04774	286.048	1.2	Antimicrobial, antioxidant	89,90
Kaempferol 3-glucoside (astragalin)	C21H20O11	[M-H]-	448.10056	448.101	1.5	Anti-inflammatory, antioxidant, antidiabetic, anticancer, cardioprotective agent, cosmetic use	91
Kaempferol 3-O-rutinoside	C27H30O15	[M+H]+	594.15847	594.158	0.2	Antioxidant	92,93
Kinetin riboside	C15H17N5O5	[M+NH4]+	347.12296	347.122	-3.4	Anticancer	94,95
Kuwanon L	C35H30O11	[M+H]+	626.17881	626.175	-6.0	Antiviral, anti-inflammatory, antimicrobial	96–98

L-tyrosine	C9H11NO3	$[M+H]^+$	181.07389	181.074	-1.9	Antidepressant, antioxidant	99,100
L-Valine	C5H11NO2	$[M+H]^+$	117.07898	117.078	-4.3	Amino acid	101
Lucenin 2	C27H30O16	$[M+H]^+$	610.15338	610.154	0.3	Anti-inflammatory, antioxidant	102
Luteolin	C15H10O6	$[M-H]^-$	286.04774	286.048	1.2	Anticancer, antiviral	103–106
Monocerin	C16H20O6	$[M+H]^+$	308.12599	308.125	-3.3	Antimicrobial	107
Moroctic acid (stearidonic acid)	C18H28O2	$[M+NH4]^+$	276.20892	276.209	-0.5	Anti-inflammatory, anticancer, anti-acne	108–110
Myricetin (Myricitin)	C15H10O8	$[M-H]^-$	318.03757	318.038	2.0	Anticancer, anti-inflammatory, antidiabetic, cardio-cerebrovascular protection agent, anti-neurodegenerative	111
Myristicin	C11H12O3	$[M+H]^+$	192.07864	192.078	-3.7	Anticancer, antimicrobial, anti-inflammatory, antioxidant	112–114
Naringenin	C15H12O5	$[M-H]^-$	272.06847	272.069	2.3	Anticancer, antioxidant, anti-inflammatory, antidiabetic, neuroprotective agent	115,116
Neochlorogenic acid (3-caffeoylquinic acid)	C16H18O9	$[M+H]^+$	354.09508	354.095	0.5	Antioxidant, antifungal, anti-inflammatory and anticarcinogenic effects	117,118
Niacin (Vit B3)	C6H5NO2	$[M+H]^+$	123.03203	123.032	-3.9	Anti-dyslipidemic, anti-inflammatory	119,120
Niacinamide	C6H6N2O	$[M+H]^+$	122.04801	122.048	-3.2	Anti-acne, antiaging and skin improvement effect	121,122
Nutlin-3	C30H30Cl2N4O4	$[M+K]^+$	580.16441	579.165	-1723.1	Anticancer	123,124

p-Coumaric acid	C9H8O3	$[M-H]^{-}$	164.04734	164.048	3.0	Antimicrobial, antioxidant, anticancer	125–127
p-Cymene	C10H14	$[M+H]^{+}$	134.10955	134.109	-2.7	Antioxidant, anti-inflammatory, anticancer, antimicrobial	128–131
Palmitoyl glycine	C18H35NO3	$[M+Na]^{+}$	313.26169	313.262	-0.5	Anti-inflammatory	132
Pelargonidin 3-O-glucoside	C21H21O10	$[M+]^{+}$	433.11347	433.113	0.7	Anti-inflammatory, antioxidant	133–135
Peonidin 3-O-glucoside	C22H23ClO11	$[M+H]^{+}$	498.09289	498.094	1.6	Anti-inflammatory, antioxidant, anticancer	136,137
Picolinic acid	C6H5NO2	$[M+H]^{+}$	123.03203	123.032	-3.9	Anticancer, antiviral	138–140
Pyroglutamic acid	C5H7NO3	$[M+H]^{+}$	129.04259	129.042	-3.1	Antimicrobial, anti-inflammatory, neurogenic activities	141,142
Quercetin	C15H10O7	$[M-H]^{-}$	302.04265	302.043	0.9	Antioxidant, anti-inflammatory, anticancer	43,143–145
Quercetin-3-b-D-glucoside (isoquercetin)	C21H20O12	$[M-H]^{-}$	464.09548	464.096	0.9	Antioxidant, anti-inflammatory, neuroprotective	146–148
r-Viniferin	C56H42O12	$[M+K]^{+}$	906.26763	905.265	-1106.6	Antioxidant, anti-inflammatory, antimicrobial, anticancer	149–151
Rutin	C27H30O17	$[M-H]^{-}$	610.15338	610.153	0.1	Anticancer, antioxidant, anti-inflammatory	43,146,152,153
Salicin	C13H18O7	$[M+Na]^{+}$	286.10525	286.105	-0.6	Anticancer, antioxidant	154–156
Salicylaldehyde	C7H6O2	$[M+H]^{+}$	122.03678	122.036	-5.0	Antimicrobial	157
Salidroside	C14H20O7	$[M+Na]^{+}$	300.1209	300.12	-1.5	Anticancer, anti-inflammation, antioxidant, antivirus, antiaging, neuroprotective	158–160

Spermine	C10H26N4	$[M+H]^+$	202.21575	202.215	-2.6	Antioxidant, anticancer, antiaging	29,161,162
Tamarixetin	C16H12O7	$[M+H]^+$	316.0583	316.058	-0.9	Anticancer, anti-inflammatory, anti-oxidation, organ protection, prevention of obesity	163–165
Tropolone	C7H6O2	$[M+H]^+$	122.03678	122.036	-5.0	Anticancer, antimicrobial	166,167
Vanilloloside	C14H20O8	$[M-H]^-$	316.11582	316.116	0.3	Antimicrobial, antioxidant, anticancer	168–170
Vitisin C	C56H42O12	$[M+K]^+$	906.26763	905.265	-1106.6	Neuroprotective, antioxidant	148,171

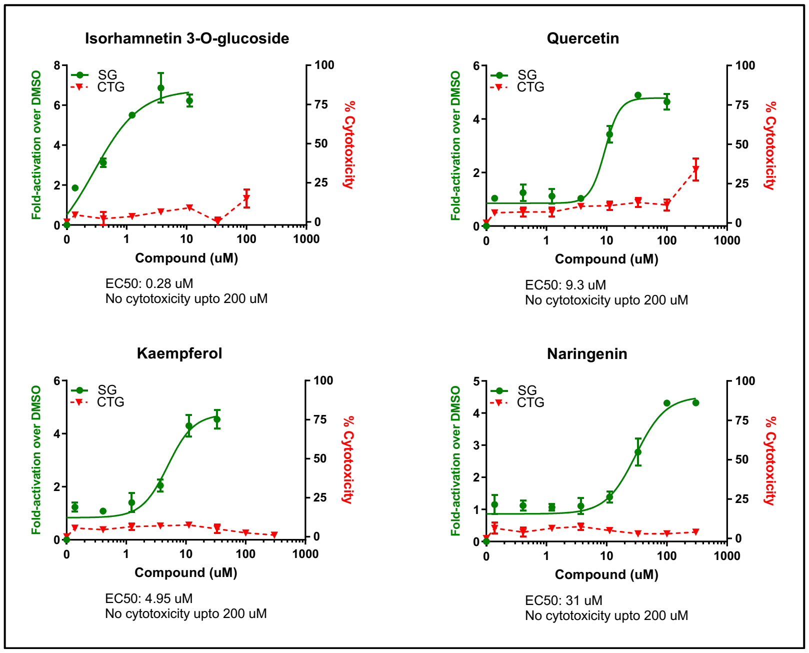
Procedures employed for the identification or putative identification[172] are comparisons with MS spectral data or accurate mass in the METLIN library.



Supplementary Figure 1. The heatmap relative intensity of 108 putatively identified compounds in the juices of 21 American elderberry genotypes.

Supplementary Table 2. K-means clustering result.

Cluster	Members
Cluster 1	1191 , 1191.1 , 1191.2 , 1196 , 1196.1 , 1196.2 , 1199 , 1199.1 , 1199.2 , 1889A , 1889A.1 , 1889A.2 , 1892 , 1892.1 , 1892.2 , 1911 , 1911.1 , 1911.2 , 1913 , 1913.1 , 1913.2 , 2073 , 2073.1 , 2073.2 , 2079 , 2079.1 , 2079.2 , 2083 , 2083.1 , 2083.2 , 2084 , 2084.1 , 2084.2 , 2085.1 , 2089 , 2089.1 , 2089.2 , 2095 , 2095.1 , 2095.2
Cluster 2	Ozark , Ozark.1 , Ozark.2
Cluster 3	1069 , 1069.1 , 1069.2 , 1076 , 1076.1 , 1076.2 , 1887A , 1887A.1 , 1887A.2 , 1896 , 1896.1 , 1896.2 , 2085 , 2085.2 , BG , BG.1 , BG.2 , WW , WW.1 , WW.2

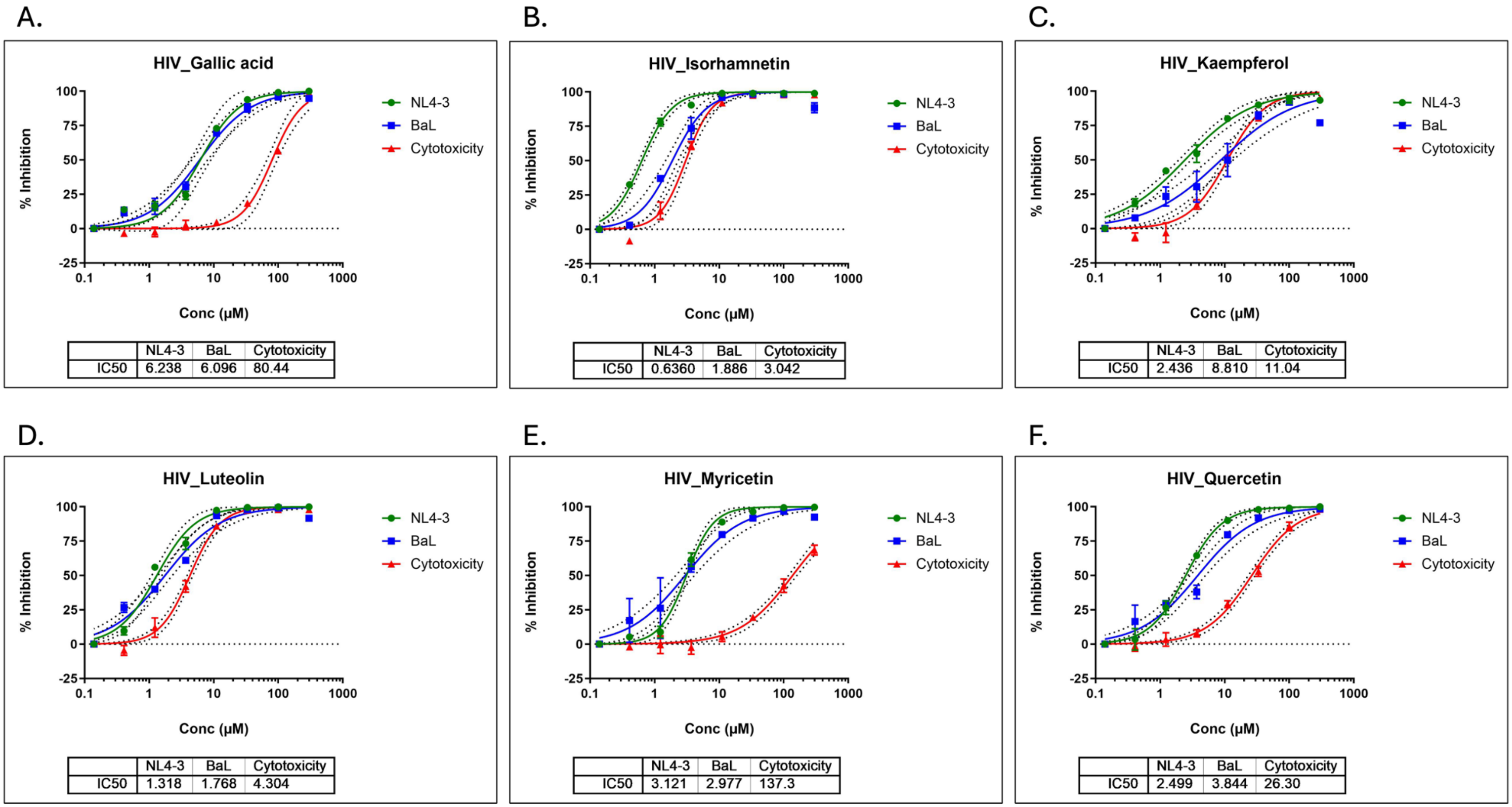


Supplementary Figure 2. Representative American elderberry compound cytotoxicity in ARE assay in HepG2 cell line (n=2).

Supplementary Table 3. IC_{50} concentration of AE putative compounds against HIV strains NL4-2 and BaL

No.	Compound name	NL4-3		BaL	
		Mean	SD	Mean	SD
1	Caffeic acid	97.14	13.97	>100	0.00
2	4-caffeoylquinic acid (cryptochlorogenic acid)	>100	0.00	>100	0.00
3	Catechin hydrate	NI	NI	NI	NI
4	Chlorogenic acid (5-caffeoylquinic acid)	NI	NI	NI	NI
5	p-Coumaric acid	NI	NI	NI	NI
6	Cyanidin 3,5-*O*-diglucoside	NI	NI	NI	NI
7	Cyanidin 3-*O*-galactoside	55.95	3.57	>100	0.00
8	Cyanidin 3-*O*-glucoside	65.77	11.68	>100	0.00
9	Cyanidin 3-*O*-rutinoside	>100	0.00	>100	0.00
10	Cyanidin 3-*O*-sambubioside	51.28	2.10	>100	0.00
11	Cyanidin 3-*O*-sophoroside	53.31	5.10	87.37	2.88
12	Delphinidin 3-*O*-rutinoside	34.92	1.25	97.52	9.13
13	3-4, Dihydroxybenzoic acid	NI	NI	NI	NI
14	(-)-Epicatechin	NI	NI	NI	NI
15	Ferulic acid	NI	NI	NI	NI
16	Gallic acid	6.24	0.12	6.24	0.12
17	Hyperoside (Quercetin 3-galactoside)	NI	NI	NI	NI
18	Isorhamnetin	0.64	0.01	2.22	0.69
19	Isorhamnetin 3-rutinoside	NI	NI	NI	NI
20	Kaempferol	2.45	0.28	8.73	0.70
21	Kaempferol 3-glucoside	NI	NI	NI	NI
22	Kaempferol 3-*O*-rutinoside	NI	NI	NI	NI
23	Luteolin	1.32	0.05	1.77	0.02
24	Myricetin	3.11	0.12	2.97	1.39
25	Naringenin	NI	NI	NI	NI
26	Neochlorogenic acid (3-caffeoylquinic acid)	NI	NI	NI	NI
27	Pelargonidin 3-*O*-glucoside	NI	NI	NI	NI
28	Peonidin 3-*O*-glucoside	NI	NI	NI	NI
29	Quercetin	2.49	0.24	3.84	0.56
30	Quercetin-3-β-D-glucoside (hirsutrin)	>100	0.00	>100	0.00
31	Rutin (Quercetin-3-rutinoside)	NI	NI	NI	NI
32	Isorhamnetin 3-*O*-glucoside	NI	NI	NI	NI

*NI = No inhibition.
**Compounds with an IC_{50} concentration greater than 100μM were found to have no inhibitory on the growth of *S. aureus* (n=2).



Supplementary Figure 3. Antiviral activity of American elderberry compounds against HIV strains NL4-3 and BaL (n=2).

Supplementary Table 4. The IC_{50} concentration of American elderberry putative compounds against *S. aureus*

No.	Compounds	IC_{50} (µM)	SD
1	Caffeic acid	NI	NI
2	4-caffeoylquinic acid (cryptochlorogenic acid)	NI	NI
3	Catechin hydrate	NI	NI
4	Chlorogenic acid (5-caffeoylquinic acid)	NI	NI
5	p-Coumaric acid	NI	NI
6	Cyanidin 3,5-*O*-diglucoside	NI	NI
7	Cyanidin 3-*O*-galactoside	21.95	0.37
8	Cyanidin 3-*O*-glucoside	10.27	0.52
9	Cyanidin 3-*O*-rutinoside	8.44	0.01
10	Cyanidin 3-*O*-sambubioside	16.78	0.92
11	Cyanidin 3-*O*-sophoroside	32.36	9.19
12	Delphinidin 3-*O*-rutinoside	22.00	2.66
13	3-4, Dihydroxybenzoic zcid	NI	NI
14	(-)-Epicatechin	NI	NI
15	Ferulic acid	NI	NI
16	Gallic acid	NI	NI
17	Hyperoside (Quercetin 3-galactoside)	NI	NI
18	Isorhamnetin	NI	NI
19	Isorhamnetin 3-rutinoside	NI	NI
20	Kaempferol	NI	NI
21	Kaempferol 3-glucoside	NI	NI
22	Kaempferol 3-*O*-rutinoside	NI	NI
23	Luteolin	NI	NI
24	Myricetin	NI	NI
25	Naringenin	NI	NI
26	Neochlorogenic acid (3-caffeoylquinic acid)	NI	NI
27	Pelargonidin 3-*O*-glucoside	46.45	5.78
28	Peonidin 3-*O*-glucoside	28.65	2.25
29	Quercetin	>100	0.00
30	Quercetin-3-β-D-glucoside (hirsutrin)	NI	NI
31	Rutin (Quercetin-3-rutinoside)	NI	NI
32	Isorhamnetin 3-*O*-glucoside	NI	NI
33	Vancomycin (Control +)	2.16	0.42

*NI = No inhibition.

**Compounds with an IC_{50} concentration greater than 100µM were found to have no inhibitory on the growth of *S. aureus* (n=2).

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