

SUPPORTING INFORMATION MATERIALS

File 1. Loadings (Correlation Coefficients between The Original Variables and The Principal Components) of The Three PCs (PC1, PC2 and PC3) for Each *Citrus* Juice Samples.

Variables	PC1	PC2	PC3
Naringenin-7- <i>O</i> -rutinoside-4'- <i>O</i> -glucoside	-0.007	0.062	0.015
Naringenin-7- <i>O</i> -neohesperidoside-4'- <i>O</i> -glucoside	-0.050	-0.041	0.041
Naringenin- <i>O</i> -hexosylhexoside	-0.050	-0.041	0.040
Naringenin-7- <i>O</i> -neohesperidoside	-0.049	-0.040	0.040
Hesperetin-7- <i>O</i> -neohesperidoside	-0.050	-0.041	0.041
Isosakuranetin-7- <i>O</i> -neohesperidoside	-0.050	-0.041	0.041
Apigenin-6- <i>C</i> -hexoside- <i>O</i> -hexoside	-0.050	-0.041	0.040
Kaempferol-3- <i>O</i> -ramnosylhexoside-7- <i>O</i> -hexoside	0.006	0.049	0.120
Isoramnetin-3- <i>O</i> -hexoside-7- <i>O</i> -ramnosylhexoside	0.007	0.062	0.000
Tamarixetin-3- <i>O</i> -ramnosylhexoside-7- <i>O</i> -hexoside	-0.017	0.016	0.139
Quercetin-3- <i>O</i> -rhamnoside-7- <i>O</i> -ramnosylhexoside	0.007	0.069	0.052
Kaempferol-3- <i>O</i> -rhamnosylhexoside-7- <i>O</i> -rhamnoside	0.005	0.042	0.123
Isorhamnetin-3- <i>O</i> -rhamnoside-7- <i>O</i> -ramnosylhexoside	0.008	0.070	0.049
Quercetin-3- <i>O</i> -rutinoside	0.049	-0.030	0.072
Tamarixetin -3- <i>O</i> -ramnosylhexoside	0.004	0.035	0.119
Kaempferol-3- <i>O</i> -rutinoside	0.005	0.039	0.126
Scopoletin- <i>O</i> -hexoside	-0.049	-0.041	0.040

*In bold, values higher than ≥ 0.049

File 2. Loadings of The Three PCs (PC1, PC2 and PC3) for Each *Citrus* Juice Samples, Considering only The Variables which Concentration were Near or Higher than 10 mg/L at Least in One of Four Species of Studied *Citrus* Juices.

Variables	PC1	PC2	PC3
Eriodictyol-7- <i>O</i> -rutinoside-4'- <i>O</i> -glucoside	-0.123	-0.114	-0.105
Naringenin-7- <i>O</i> -rutinoside-4'- <i>O</i> -glucoside	0.056	0.126	-0.258
Eriodictyol-7- <i>O</i> -rutinoside	-0.124	-0.109	-0.109
Naringenin-7- <i>O</i> -rutinoside	0.113	-0.059	-0.253
Naringenin-7- <i>O</i> -neohesperidoside	0.091	-0.182	-0.062
Hesperetin-7- <i>O</i> -rutinoside	-0.062	0.149	-0.178
Hesperetin-7- <i>O</i> -neohesperidoside	0.092	-0.183	-0.057
Isosakuranetin-7- <i>O</i> -rutinoside	0.011	0.150	-0.292
Isosakuranetin-7- <i>O</i> -neohesperidoside	0.091	-0.182	-0.060
Apigenin-6,8-di- <i>C</i> -glucoside	0.061	0.040	-0.390
Diosmetin-6,8-di- <i>C</i> -glucoside	-0.123	-0.106	-0.088
Luteolin-7- <i>O</i> -rutinoside	-0.116	-0.080	-0.115
Diosmetin-6- <i>C</i> -glucoside	-0.110	-0.102	-0.121
Quercetin-3- <i>O</i> -rutinoside	-0.123	-0.068	-0.133
<i>O</i> -hexósido of ferulic acid	0.098	-0.149	-0.049

File 3. Loadings of The Three PCs (PC1, PC2, PC3 and PC4) for Sweet Orange and Tangerine Juice Samples, Considering Only The Variables which Concentration were Near or Higher than 10 mg/L at Least in One of Four Species of Studied *Citrus* Juices.

Variables	PC1	PC2	PC3	PC4
Naringenin-7-O-rutinoside-4'-O-glucoside	-0.185	0.206	-0.084	0.247
Eriodictyol-7-O-rutinoside	-0.089	0.181	-0.177	-0.277
Naringenin-7-O-rutinoside	-0.248	0.090	0.108	0.015
Hesperetin-7-O-rutinoside	-0.167	-0.024	-0.038	-0.648
Isosakuranetin-7-O-rutinoside	-0.233	-0.134	0.001	-0.066
Apigenin-6,8-di-C-glucoside	-0.224	0.011	-0.230	0.433
Diosmetin-6,8-di-C-glucoside	0.034	-0.291	0.013	0.004
Luteolin-7-O-rutinoside	-0.120	-0.273	-0.023	-0.092
Diosmetin-6-C-glucoside	-0.116	-0.210	0.171	0.325
Quercetin-3-O-rutinoside	-0.089	0.046	0.566	-0.254
O-hexoside of ferulic acid-	0.009	0.096	0.510	0.257

File 4. PC1 Loadings and Total X and Y Variance for Each Factor and Explained Variance of The Polyphenols in Each One of Factors.

	PLS				PCR				
	PC1	PC2	PC3	PC4	PC1 Loadings	PC1	PC2	PC3	PC1 Loadings
ExpYCal(tot) (PCs)	92.040	93.135	93.721	95.417	---	91.666	91.765	92.542	---
ExpXCal(tot) (PCs)	60.608	72.876	89.235	92.942	---	60.625	81.990	91.413	---
Naringenin-7- <i>O</i> -rutinoside-4'- <i>O</i> -glucoside	42.523	64.959	93.708	95.916	-0.253	43.836	94.885	95.901	-0.256
Eriodictyol-7- <i>O</i> -rutinoside	58.654	63.604	63.686	63.686	-0.297	59.257	59.852	64.374	-0.298
Naringenin-7- <i>O</i> -rutinoside	43.634	87.918	97.563	97.689	0.256	41.906	79.843	97.156	0.251
Naringenin-7- <i>O</i> -neohesperidoside	93.524	97.177	97.279	97.574	0.375	92.795	94.333	97.482	0.373
Hesperetin-7- <i>O</i> -rutinoside	49.222	51.936	75.506	99.634	-0.272	49.455	68.733	94.858	-0.272
Hesperetin-7- <i>O</i> -neohesperidoside	95.731	98.804	98.805	98.807	0.379	95.063	96.063	98.609	0.378
Isosakuranetin-7- <i>O</i> -rutinoside	54.698	77.929	92.432	95.336	-0.287	55.865	57.168	94.113	-0.289
Isosakuranetin-7- <i>O</i> -neohesperidoside	93.517	96.986	96.988	96.999	0.375	92.819	93.924	96.809	0.373
Apigenin-6,8-di- <i>C</i> -glucoside	4.048	31.054	93.172	95.261	-0.080	4.525	94.541	94.779	-0.082
Quercetin-3- <i>O</i> -rutinoside	55.623	55.739	95.440	97.047	-0.289	55.929	86.918	94.907	-0.290
<i>O</i> -hexoside of ferulic acid-	75.518	75.527	77.004	84.409	0.337	75.421	75.628	76.556	0.336