

Supplementary Material

Brevifolincarboxylic acid			Castalagin			Ellagic acid			Gallic acid		
Real	Predicted		Real	Predicted		Real	Predicted		Real	Predicted	
	1	2		1	2		1	2		1	2
1	40.0%	10.0%	1	40.0%	10.0%	1	55.6%	0%	1	22.2%	22.2%
2	10.0%	40.0%	2	10.0%	40.0%	2	22.2%	22.2%	2	0%	55.6%
Total percentage of correct predictions		80.0%	Total percentage of correct predictions		80.0%	Total percentage of correct predictions		77.8%	Total percentage of correct predictions		77.8%

Latifolicinin C acid			Protocatechuic acid			Protocatechuic aldehyde			Aesculetin		
Real	Predicted		Real	Predicted		Real	Predicted		Real	Predicted	
	1	2		1	2		1	2		1	2
1	57.1%	0%	1	33.3%	11.1%	1	10.0%	30.0%	1	40.0%	20.0%
2	0%	42.9%	2	11.1%	44.5%	2	0%	60.0%	2	0%	40.0%
Total percentage of correct predictions		100%	Total percentage of correct predictions		77.8%	Total percentage of correct predictions		70.0%	Total percentage of correct predictions		80.0%

Figure S1. Confusion matrices considering only the validation set for the chemical parameters under study. Legend: 1- group with values higher than average; 2- group with values below than average.

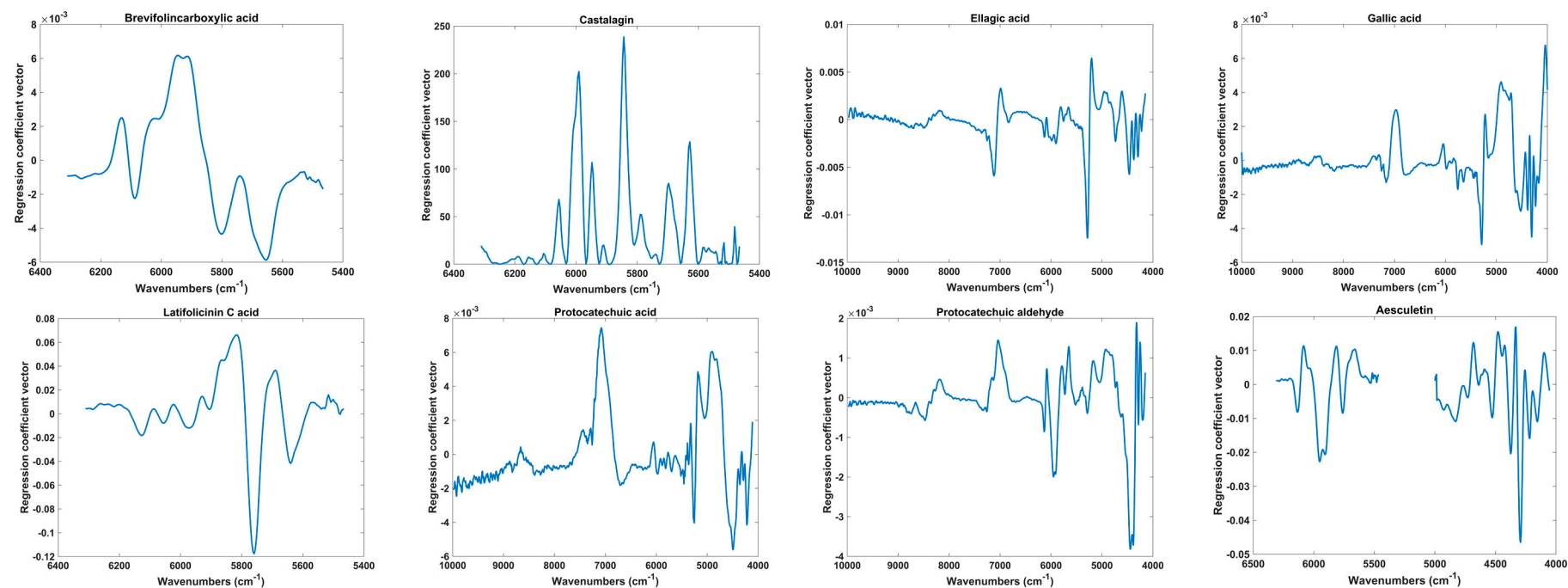
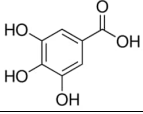
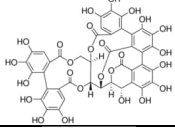
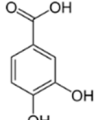
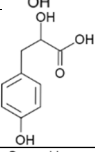
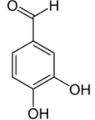
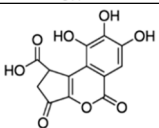
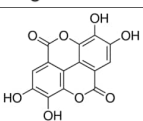
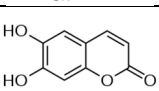


Figure S2. Regression coefficient vectors of the PLS-DA models for the discrimination of samples with high and low amounts of brevifolincarboxylic acid, castalagin, ellagic acid, gallic acid, latifolicinin C acid, protocatechuic acid, protocatechuic aldehyde and aesculetin.

Table S1. Chemical structures and physicochemical properties of the standards [6].

Compound	Structure	Molecular weigh	Exact mass	pKa	logP	IC ₅₀ (DPPH)
Gallic acid (1)		188.13	170.02152	4.21	0.70	8.14 ± 0.26 μM [27]
Castalagin (2)		934.64	934.07123	7.14	2.03	15 μM equiv. Trolox [28]
Protocatechuic acid (3)		154.12	154.02661	4.26	0.86	147.3 ± 3.6 μM [29]
Latifolicinin C acid (4)		182.17	182.05791	*	*	*
Protocatechuic aldehyde (5)		138.12	138.03169	7.46	1.08	74.2 ± 1.2 μM [29]
Brevifolincarboxylic acid (6)		292.2	292.02192	2.91	0.41	4.6 μM [30]
Ellagic acid (7)		302.19	302.00627	5.54	0.24	4.60 ± 0.15 μM [27]
Aesculetin (8)		178.14	178.02661	7.91	0.98	25.18 μM [31]

* unreported data. **pKa** and **logP** predicted by Chemaxon for castalagin, protocatechuic aldehyde, brevifolincarboxylic acid, aesculetin and reported in PubChem for gallic acid, protocatechuic acid and ellagic acid.