

Supporting Information

Table 1S. Samples Employed in the Training (Calibration) and Test (Prediction and Validation) Sets for Partial Least Squares Regression.

% adulteration	Number of samples	Set
100	3	Calibration
50	5	Calibration
20	3	Calibration
12	3	Prediction and validation
7	3	Calibration
6	3	Prediction and validation
5	3	Calibration
2.5	3	Prediction and validation
2	3	Calibration
0	3	Calibration

Figure 2S. ExactFinder™ Report for the Cranberry Pharmaceutical Raw Extract Sample E3.

Found	Confirmed	Target Name	+/-	Area	RT (min)	Formula	Expected m/z	Measured m/z	Delta m/z (ppm)	Isotopic Pattern Score (%)	Num Isotopes Matched
●	1 of 1	D-(-)-Quinic acid	-	1.07E+10	1.01	C7H12O6	191.0561	191.0554	-3.54	90	4 of 4
●	1 of 1	Gallic acid	-	5.68E+08	1.55	C7H6O5	169.0142	169.0140	-1.51	100	4 of 4
●	1 of 1	Gentisic acid	-	4.74E+07	4.30	C7H6O4	153.0193	153.0191	-1.79	100	2 of 3
●	1 of 1	Chlorogenic acid	-	5.59E+08	3.85	C16H18O9	353.0878	353.0873	-1.49	100	5 of 5
●	1 of 1	Procyanidin B2	-	1.47E+08	2.61	C30H26O12	577.1351	577.1346	-0.88	100	5 of 5
●	1 of 1	Homogentisic acid	-	7.99E+06	2.09	C8H8O4	167.0350	167.0347	-1.70	100	2 of 3
●	1 of 1	Vanillic acid	-	5.14E+07	4.64	C8H8O4	167.0350	167.0346	-2.06	100	2 of 3
●	1 of 1	Caffeic acid	-	1.39E+09	4.66	C9H8O4	179.0350	179.0348	-0.82	100	5 of 5
●	1 of 1	(+)-catechin	-	5.53E+08	4.05	C16H14O6	289.0718	289.0713	-1.53	100	4 of 4
●	1 of 1	(-)-Epicatechin	-	2.22E+09	4.90	C16H14O6	289.0718	289.0714	-1.21	100	4 of 5
●	1 of 1	Procyanidin C1	-	7.10E+07	5.18	C45H38O18	865.1985	865.1970	-1.82	100	4 of 5
●	1 of 1	Vanillin	-	1.85E+07	5.86	C8H8O3	151.0401	151.0399	-0.80	100	2 of 2
●	1 of 1	p-coumaric acid	-	9.49E+08	5.87	C9H8O3	163.0401	163.0398	-1.86	100	4 of 5
●	1 of 1	Ellagic acid	-	2.65E+08	6.07	C14H6O8	300.9990	300.9984	-1.92	100	4 of 4
●	1 of 1	Ferulic acid	-	1.30E+07	6.32	C18H18O4	313.0506	313.0504	-1.36	100	2 of 2
●	1 of 1	Procyanidin A2	-	1.94E+09	6.40	C30H24O12	575.1195	575.1188	-1.26	100	5 of 6
●	1 of 1	Taxifolin	-	1.9E+08	6.38	C16H18O7	303.0510	303.0504	-2.12	100	3 of 4
●	1 of 1	Homoplantagin	-	4.17E+07	7.37	C22H22O11	461.1089	461.1082	-1.56	100	3 of 3
●	1 of 1	Quercitrin hydrate	-	1.82E+09	6.72	C24H20O11	447.0933	447.0925	-1.69	100	5 of 5
●	0 of 1	Polydatin	-	2.4E+06	7.03	C20H22O8	389.1242	389.1236	-1.45	82	2 of 3
●	1 of 1	Myricetin	-	6.63E+06	4.18	C16H10O8	317.0303	317.0296	-2.17	93	2 of 2
●	1 of 1	Nepetin-7-glucoside	-	1.25E+07	6.19	C22H22O12	477.1038	477.1033	-1.15	100	3 of 3
●	1 of 1	Syringaldehyde	-	4.10E+06	6.03	C9H10O4	181.0506	181.0504	-1.54	100	2 of 2
●	0 of 1	Homovanillic acid	-	8.96E+05	4.78	C9H10O4	181.0506	181.0504	-1.28	100	1 of 1
●	1 of 1	Veratric acid	-	2.6E+07	7.67	C9H10O4	181.0506	181.0505	-0.95	100	3 of 3
●	1 of 1	3,4-Dihydroxybenzaldehyd	-	1.19E+08	3.92	C7H6O3	137.0244	137.0240	-3.25	95	4 of 4
●	0 of 1	Rosmarinic acid	-	1.23E+06	6.90	C18H16O8	359.0772	359.0766	-1.79	100	1 of 1
●	1 of 1	Morin	-	3.10E+06	7.54	C16H10O7	301.0354	301.0351	-0.93	100	2 of 2
●	1 of 1	Kaempferol	-	3.39E+08	9.92	C16H10O6	285.0405	285.0399	-1.80	100	4 of 4
●	1 of 1	Fisetin	-	3.19E+06	7.14	C16H10O6	285.0405	285.0397	-2.77	94	2 of 2
●	1 of 1	Asiatic acid	-	6.27E+06	12.56	C30H48O5	487.3429	487.3422	-1.45	100	3 of 3