

Supplementary material for the article:

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Table S1

Validation data on phenolics quantified in almond samples in negative ionization mode with mean expected retention time (t_R , min), mass of parent ion (m/z), masses of product ions (m/z) with specified collision energy (eV), correlation coefficient, limit of detection (LOD), limit of quantification (LOQ), recovery, relative standard deviation (RSD), as determined using UHPLC-DAD MS/MS analysis.

N ^o	Phenolic compound (mg/kg)	t_R , min	Parent Ion, m/z	Product Ion, m/z (Collision Energy, eV)	R^2	LOD, mg/L	LOQ, mg/L	Recovery (%)	RSD (%)
Hydroxybenzoic acid derivatives									
20	Protocatechuic acid	4.18	153.013	108.09 (23); 109.10 (14)	0.9962	0.13	0.42	85	3.40
21	<i>p</i> -Hydroxybenzoic acid	5.20	137.057	93.19 (19); 108.33 (22)	0.9931	0.19	0.64	100	4.05
22	Ellagic acid	6.57	300.980	284.00 (32); 300.04 (30)	0.9949	0.10	0.35	59	1.43
23	Vanillic acid	6.65	167.034	108.00 (21); 153.00 (15)	0.9945	0.20	0.68	86	3.61
Hydroxycinnamic acid derivatives									
24	Aesculin	4.86	339.080	133.09 (44); 177.06 (25)	0.9971	0.11	0.37	82	4.95
25	Chlorogenic acid	5.15	353.103	191.28 (25)	0.9998	0.03	0.11	112	1.21
26	Aesculetin	5.52	176.911	133.08 (21); 162.06(19)	0.9962	0.12	0.41	104	1.12
27	Caffeic acid	5.64	179.004	134.00 (13); 135.00 (16)	0.9967	0.12	0.41	111	0.88

28	<i>p</i>-Coumaric acid	6.39	163.031	93.12 (39); 119.09 (16)	0.9931	0.18	0.61	114	1.58
29	Ferulic acid	6.75	193.057	134.00 (18); 178.00 (15)	0.9919	0.16	0.55	98	3.45
30	Sinapic acid	6.76	223.082	149.21 (36)	0.9941	0.14	0.48	102	0.86
31	Coniferyl aldehyde	7.51	177.060	97.00 (14); 162.00 (17)	0.9972	0.11	0.37	87	2.73
Dihydrochalcones									
32	Phlorizin	7.17	435.149	167.16 (34); 273.16 (20)	0.9961	0.16	0.54	79	2.92
33	Phloretin	8.75	273.066	123.23 (26); 167.20 (19)	0.9995	0.03	0.11	86	4.72
Stilbenoids									
34	Resveratrol	7.77	227.060	143.18 (22); 185.04 (22)	0.9983	0.10	0.33	89	2.67
Flavonoids and derivatives									
35	Catechin	5.29	289.094	203.00 (23); 245.03 (31)	0.9937	0.18	0.60	108	1.50
36	Rutin	6.23	609.197	299.98 (42); 301.20 (32)	0.9980	0.11	0.37	82	1.09
37	Hyperoside	6.40	463.002	271.01 (44); 300.02 (29)	0.9975	0.09	0.29	106	0.67
38	Cynaroside	6.48	447.000	284.01 (40); 285.03 (27)	0.9977	0.08	0.27	96	1.54
39	Naringin	6.74	579.241	151.42 (43); 217.26 (33)	0.9992	0.05	0.16	99	2.06
40	Astragalin	6.75	477.088	255.03 (43); 284.03 (29)	0.9999	0.01	0.03	88	3.75
41	Luteolin	8.17	285.035	133.05 (30); 150.95 (24)	0.9946	0.21	0.68	102	0.70
42	Apigenin	8.91	269.032	117.24 (43); 149.00 (24)	0.9971	0.09	0.31	89	3.29

43	Naringenin	8.92	271.036	119.10 (25); 151.07 (19)	0.9961	0.16	0.54	103	2.66
44	Kaempferol	9.02	285.074	211.00 (32); 227.00 (32)	0.9978	0.12	0.41	90	4.43
45	Chrysin	10.72	253.054	119.00 (36); 143.00 (30)	0.9908	0.20	0.66	98	1.65
46	Pinocembrin	10.83	255.081	150.93 (25); 213.04 (25)	0.9976	0.09	0.31	93	0.91
47	Galangin	10.86	269.037	169.00 (32); 171.00 (32)	0.9970	0.13	0.43	109	2.65
