

**Table S1** Analytical method validation parameters that belong to the LC-MS/MS method

No	Analytes	RT <sup>a</sup>	M.I. ( <i>m/z</i> ) <sup>b</sup>	F.I. ( <i>m/z</i> ) <sup>c</sup>	Ion. mode	Equation	<i>r</i> <sup>2</sup>	RSD% <sup>e</sup>		Linearity Range (mg/L)	LOD/LO <i>Q</i> (µg/L) <sup>f</sup>	Recovery (%)		U <sup>g</sup>	G r. N o
								Interday	Intraday			Interday	Intraday		
1	Quinic acid	3.0	190.8	93	Neg	y=-0.0129989+2.97989x	0.99	0.69	0.51	0.1-5	25.7/33.3	1.0011	1.0083	0.0372	1
2	Fumaric acid	3.9	115.2	40.9	Neg	y=-0.0817862+1.03467x	0.99	1.05	1.02	1-50	135.7/167.9	0.9963	1.0016	0.0091	1
3	Aconitic acid	4.0	172.8	129	Neg	y=-0.7014530+32.9994x	0.97	2.07	0.93	0.1-5	16.4/31.4	0.9968	1.0068	0.0247	1
4	Gallic acid	4.4	168.8	79	Neg	y=0.0547697+20.8152x	0.99	1.6	0.81	0.1-5	13.2/17.0	1.001	0.9947	0.0112	1
5	Epigallocatechin	6.7	304.8	219	Neg	y=-0.00494986+0.0483704x	0.99	1.22	0.73	1-50	237.5/265.9	0.9969	1.004	0.0184	3
6	Protocatechuic acid	6.8	152.8	108	Neg	y=0.211373+12.8622x	0.95	1.43	0.76	0.1-5	21.9/38.6	0.9972	1.0055	0.035	1
7	Catechin	7.4	288.8	203.1	Neg	y=-0.00370053+0.431369x	0.99	2.14	1.08	0.2-10	55.0/78.0	1.0024	1.0045	0.0221	3
8	Gentisic acid	8.3	152.8	109	Neg	y=-0.0238983+12.1494x	0.99	1.81	1.22	0.1-5	18.5/28.2	0.9963	1.0077	0.0167	1
9	Chlorogenic acid	8.4	353	85	Neg	y=0.289983+36.3926x	0.99	2.15	1.52	0.1-5	13.1/17.6	1	1.0023	0.0213	1
10	Protocatechuic aldehyde	8.5	137.2	92	Neg	y=0.257085+25.4657x	0.99	2.08	0.57	0.1-5	15.4/22.2	1.0002	0.9988	0.0396	1
11	Tannic acid	9.2	182.8	78	Neg	y=0.0126307+26.9263x	0.99	2.4	1.16	0.05-2.5	15.3/22.7	0.997	0.995	0.019	1
12	Epigallocatechin gallate	9.4	457	305.1	Neg	y=-0.0380744+1.61233x	0.99	1.3	0.63	0.2-10	61.0/86.0	0.9981	1.0079	0.0147	3
13	1,5-dicaffeoylquinic acid	9.8	515	191	Neg	y=-0.0164044+16.6535x	0.99	2.42	1.48	0.1-5	5.8/9.4	0.9983	0.9997	0.0306	1
14	4-OH Benzoic acid	10.5	137.2	65	Neg	y=-0.0240747+5.06492x	0.99	1.24	0.97	0.2-10	68.4/88.1	1.0032	1.0068	0.0237	1
15	Epicatechin	11.6	289	203	Neg	y=-0.0172078+0.0833424x	0.99	1.47	0.62	1-50	139.6/161.6	1.0013	1.0012	0.0221	3

16	Vanillic acid	11.8	166.8	108	Neg	$y = -0.0480183 + 0.779564x$	0.99	1.92	0.76	1-50	141.9/164.9	1.0022	0.9998	0.0145	1
17	Caffeic acid	12.1	179	134	Neg	$y = 0.120319 + 95.4610x$	0.99	1.11	1.25	0.05-2.5	7.7/9.5	1.0015	1.0042	0.0152	1
18	Syringic acid	12.6	196.8	166.9	Neg	$y = -0.0458599 + 0.663948x$	0.99	1.18	1.09	1-50	82.3/104.5	1.0006	1.0072	0.0129	1
19	Vanillin	13.9	153.1	125	Poz	$y = 0.00185898 + 20.7382x$	0.99	1.1	0.85	0.1-5	24.5/30.4	1.0009	0.9967	0.0122	1
20	Syringic aldehyde	14.6	181	151.1	Neg	$y = -0.0128684 + 7.90153x$	0.99	2.51	0.77	0.4-20	19.7/28.0	1.0001	0.9964	0.0215	1
21	Daidzin	15.2	417.1	199	Poz	$y = 9.45747 + 152.338x$	0.99	2.25	1.32	0.05-2.5	7.0/9.5	0.9955	1.0017	0.0202	2
22	Epicatechin gallate	15.5	441	289	Neg	$y = -0.0142216 + 1.06768x$	0.99	1.63	1.28	0.1-5	19.5/28.5	0.9984	0.9946	0.0229	3
23	Piceid	17.2	391	135/106.9	Poz	$y = 0.00772525 + 25.4181x$	0.99	1.94	1.16	0.05-2.5	13.8/17.8	1.0042	0.9979	0.0199	1
24	p-Coumaric acid	17.8	163	93	Neg	$y = 0.0249034 + 18.5180x$	0.99	1.92	1.43	0.1-5	25.9/34.9	1.0049	1.0001	0.0194	1
25	Ferulic acid-D3-ISH	18.8	196.2	152.1	Neg	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	0.017	1
26	Ferulic acid	18.8	192.8	149	Neg	$y = -0.0735254 + 1.34476x$	0.99	1.44	0.53	1-50	11.8/15.6	0.9951	0.9976	0.0181	1
27	Sinapic acid	18.9	222.8	193	Neg	$y = -0.0929932 + 0.836324x$	0.99	1.45	0.52	0.2-10	65.2/82.3	1.0031	1.0037	0.0317	1
28	Coumarin	20.9	146.9	103.1	Poz	$y = 0.0633397 + 136.508x$	0.99	2.11	1.54	0.05-2.5	214.2/247.3	0.995	0.9958	0.0383	1
29	Salicylic acid	21.8	137.2	65	Neg	$y = 0.239287 + 153.659x$	0.99	1.48	1.18	0.05-2.5	6.0/8.3	0.995	0.9998	0.0158	1
30	Cynaroside	23.7	447	284	Neg	$y = 0.280246 + 6.13360x$	0.99	1.56	1.12	0.05-2.5	12.1/16.0	1.0072	1.0002	0.0366	2
31	Miquelianin	24.1	477	150.9	Neg	$y = -0.00991585 + 5.50334x$	0.99	1.31	0.95	0.1-5	10.6/14.7	0.9934	0.9965	0.022	2
32	Rutin-D3-ISH	25.5	612.2	304.1	Neg	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	2
33	Rutin	25.6	608.9	301	Neg	$y = -0.0771907 + 2.89868x$	0.99	1.38	1.09	0.1-5	15.7/22.7	0.9977	1.0033	0.0247	2
34	isoquercitrin	25.	463	271	Neg	$y = -$	0.99	2.13	0.78	0.1-5	8.7/13.5	1.0057	0.9963	0.022	2

		6				$0.111120+4.10546x$	8								
35	Hesperidin	25.8	611.2	449	Poz	$y=0.139055+13.2785x$	0.999	1.84	1.35	0.1-5	19.0/26.0	0.9967	1.0043	0.0335	2
36	o-Coumaric acid	26.1	162.8	93	Neg	$y=0.00837193+11.2147x$	0.999	2.11	1.46	0.1-5	31.8/40.4	1.0044	0.9986	0.0147	1
37	Genistin	26.3	431	239	Neg	$y=1.65808+7.57459x$	0.991	2.01	1.28	0.1-5	14.9/21.7	1.0062	1.0047	0.0083	2
38	Rosmarinic acid	26.6	359	197	Neg	$y=-0.0117238+8.04377x$	0.999	1.24	0.86	0.1-5	16.2/21.2	1.0056	1.0002	0.013	1
39	Ellagic acid	27.6	301	284	Neg	$y=0.00877034+0.663741x$	0.999	1.57	1.23	0.4-20	56.9/71.0	1.0005	1.0048	0.0364	1
40	Cosmosiin	28.2	431	269	Neg	$y=-0.708662+8.62498x$	0.998	1.65	1.3	0.1-5	6.3/9.2	0.994	0.9973	0.0083	2
41	Quercitrin	29.8	447	301	Neg	$y=-0.00153274+3.20368x$	0.999	2.24	1.16	0.1-5	4.8/6.4	0.996	0.9978	0.0268	2
42	Astragalin	30.4	447	255	Neg	$y=0.00825333+3.51189x$	0.999	2.08	1.72	0.1-5	6.6/8.2	0.9968	0.9957	0.0114	2
43	Nicotiflorin	30.6	592.9	255.0/284.0	Neg	$y=0.00499333+2.62351x$	0.999	1.48	1.23	0.05-2.5	11.9/16.7	0.9954	1.0044	0.0108	2
44	Fisetin	30.6	285	163	Neg	$y=0.0365705+8.09472x$	0.999	1.75	1.19	0.1-5	10.1/12.7	0.998	1.0042	0.0231	3
45	Daidzein	34	253	223	Neg	$y=-0.0329252+6.23004x$	0.999	2.18	1.73	0.1-5	9.8/11.6	0.9926	0.9963	0.037	3
46	Quercetin-D3-ISH	35.6	304	275.9	Neg	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	3
47	Quercetin	35.7	301	272.9	Neg	$y=+0.00597342+3.39417x$	0.999	1.89	1.38	0.1-5	15.5/19.0	0.9967	0.9971	0.0175	3
48	Naringenin	35.9	270.9	119	Neg	$y=-0.00393403+14.6424x$	0.999	2.34	1.69	0.1-5	2.6/3.9	1.0062	1.002	0.0392	3
49	Hesperetin	36.7	301	136.0/286.0	Neg	$y=+0.0442350+6.07160x$	0.999	2.47	2.13	0.1-5	7.1/9.1	0.9998	0.9963	0.0321	3
50	Luteolin	36.7	284.8	151.0/175.0	Neg	$y=-0.0541723+30.7422x$	0.999	1.67	1.28	0.05-2.5	2.6/4.1	0.9952	1.0029	0.0313	3
51	Genistein	36.9	269	135	Neg	$y=-0.00507501+12.1933x$	0.999	1.48	1.19	0.05-2.5	3.7/5.3	1.0069	1.0012	0.0337	3
52	Kaempferol	37.9	285	239	Neg	$y=-0.00459557+3.13754x$	0.999	1.49	1.26	0.05-2.5	10.2/15.4	0.9992	0.999	0.0212	3
53	Apigenin	38.	268.	151.0/14	Neg	$y=0.119018+34.8730x$	0.99	1.17	0.96	0.05-	1.3/2.0	0.9985	1.0003	0.017	3

		2	8	9.0				8		2.5			8		
54	Amentoflavone	39.7	537	417	Neg	$y=0.727280+33.3658x$	0.99	1.35	1.12	0.05-2.5	2.8/5.1	0.9991	1.0044	0.034	3
55	Chrysin	40.5	252.8	145.0/119.0	Neg	$y=-0.0777300+18.8873x$	0.99	1.46	1.21	0.05-2.5	1.5/2.8	0.9922	1.005	0.032	3
56	Acacetin	40.7	283	239	Neg	$y=-0.559818+163.062x$	0.99	1.67	1.28	0.02-1	1.5/2.5	0.9949	1.0011	0.036	3

<sup>a</sup>R.T.: Retention time, <sup>b</sup>MI (*m/z*): Molecular ions of the standard analytes (*m/z* ratio), <sup>c</sup>FI (*m/z*): Fragment ions <sup>d</sup>*r*<sup>2</sup>: Coefficient of determination, <sup>e</sup>RSD: Relative standard deviation, <sup>f</sup>LOD/LOQ ( $\mu\text{g/L}$ ): Limit of detection/quantification, <sup>g</sup>U (%): percent relative uncertainty at 95% confidence level ( $k = 2$ ), <sup>h</sup>IS: Internal standard, <sup>i</sup>Gr. No: Represents grouping of internal standards, these numbers indicate which IS stands for which phenolic compound.