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Supplementary Materials

Chemical Fingerprinting Profile and Targeted Quantitative Analysis of Phenolic Compounds from Rooibos Tea (*Aspalathus linearis*) and Dietary Supplements Using UHPLC-PDA-MS

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	Name	Channel	R	R^2	Equation
1	Syringin	280.0 nm	0.999211	0.998424	Y = 2800 X + 823
2	Eriodictyol 1	280.0 nm	0.999198	0.998396	Y = 1760 X + 703
3	Eriodictyol 2	280.0 nm	0.999328	0.998656	Y = 1840 X + 538
4	Isoorientin	280.0 nm	0.999653	0.999306	Y = 2520 X – 1640
5	Orientin	280.0 nm	0.998531	0.997064	Y = 1790 X + 113
6	Aspalathin	280.0 nm	0.999529	0.999059	Y = 4620 X – 2300
7	Vitexin	280.0 nm	0.998984	0.997969	Y = 1500 X – 879
8	Bioquercetin	280.0 nm	0.994722	0.989471	Y = 1630 X + 6590
9	Hyperoside	280.0 nm	0.997803	0.995611	Y = 753 X – 1640
10	Isovitexin	280.0 nm	0.999337	0.998674	Y = 3970 X – 1120
11	Rutin	280.0 nm	0.998812	0.997625	Y = 1620 X – 475
12	Isoquercitrin	280.0 nm	0.998852	0.997705	Y = 1190 X – 1520
13	Nothofagin	280.0 nm	0.999291	0.998583	Y = 5760 X – 2530
14	Thermopsoside	280.0 nm	0.999190	0.998380	Y = 3450 X + 383

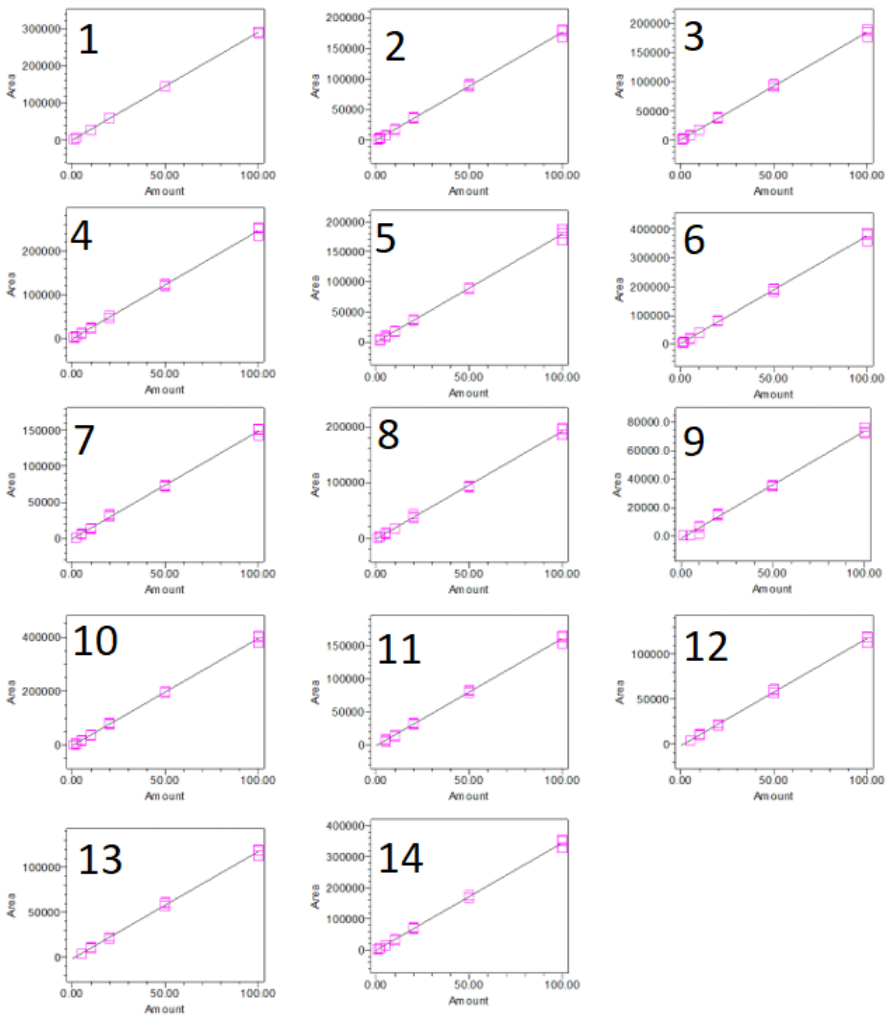
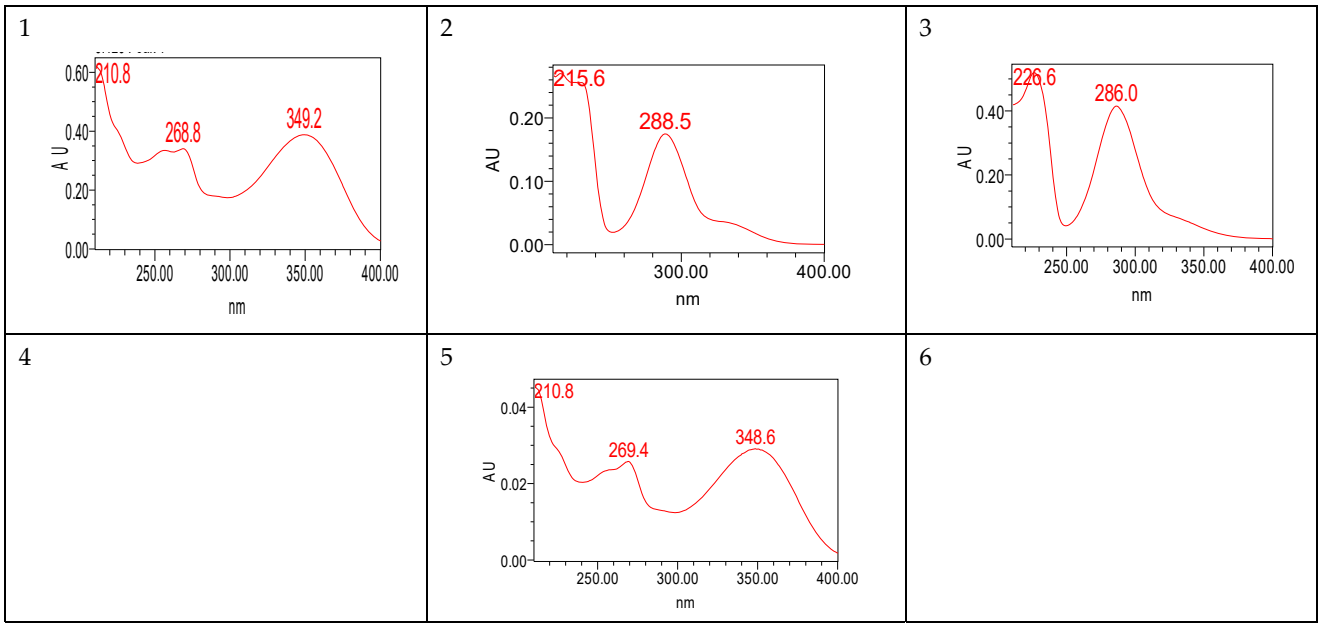


Figure S1. Calibration curves for compounds 1-14.



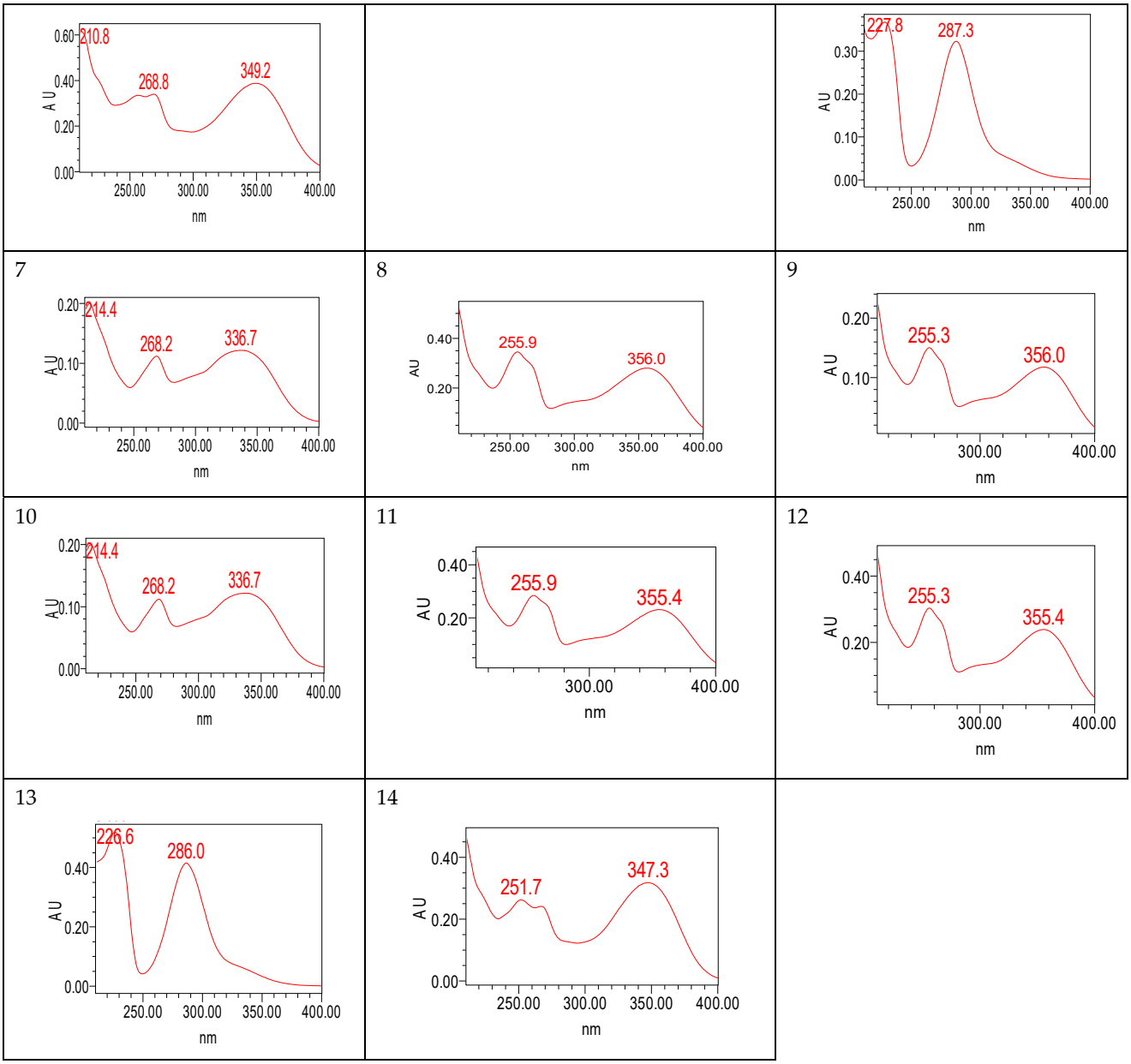


Figure S2. UV spectra for compounds 1-14.

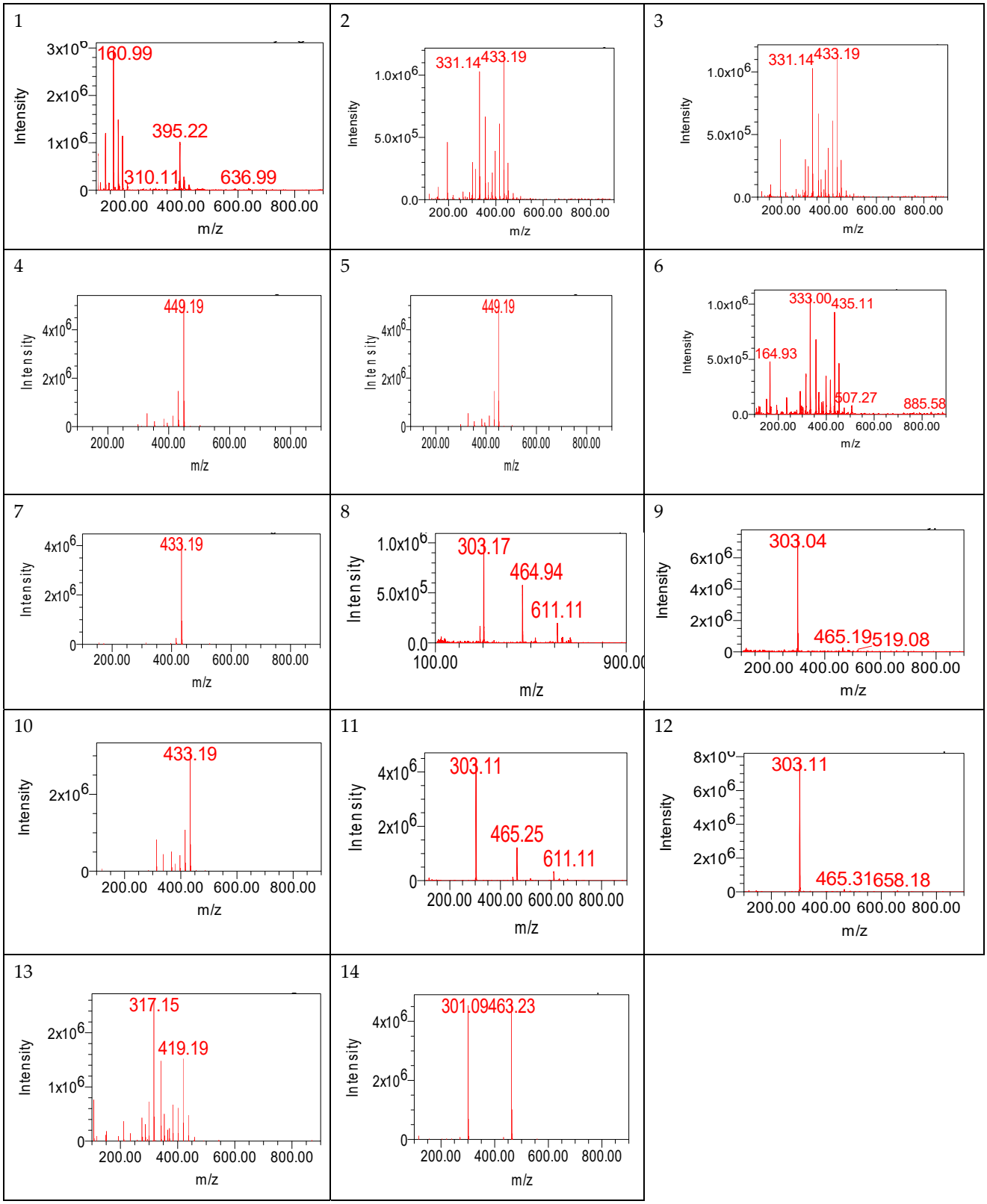


Figure S3. The positive mode of Mass spectra for compounds **1-14.**

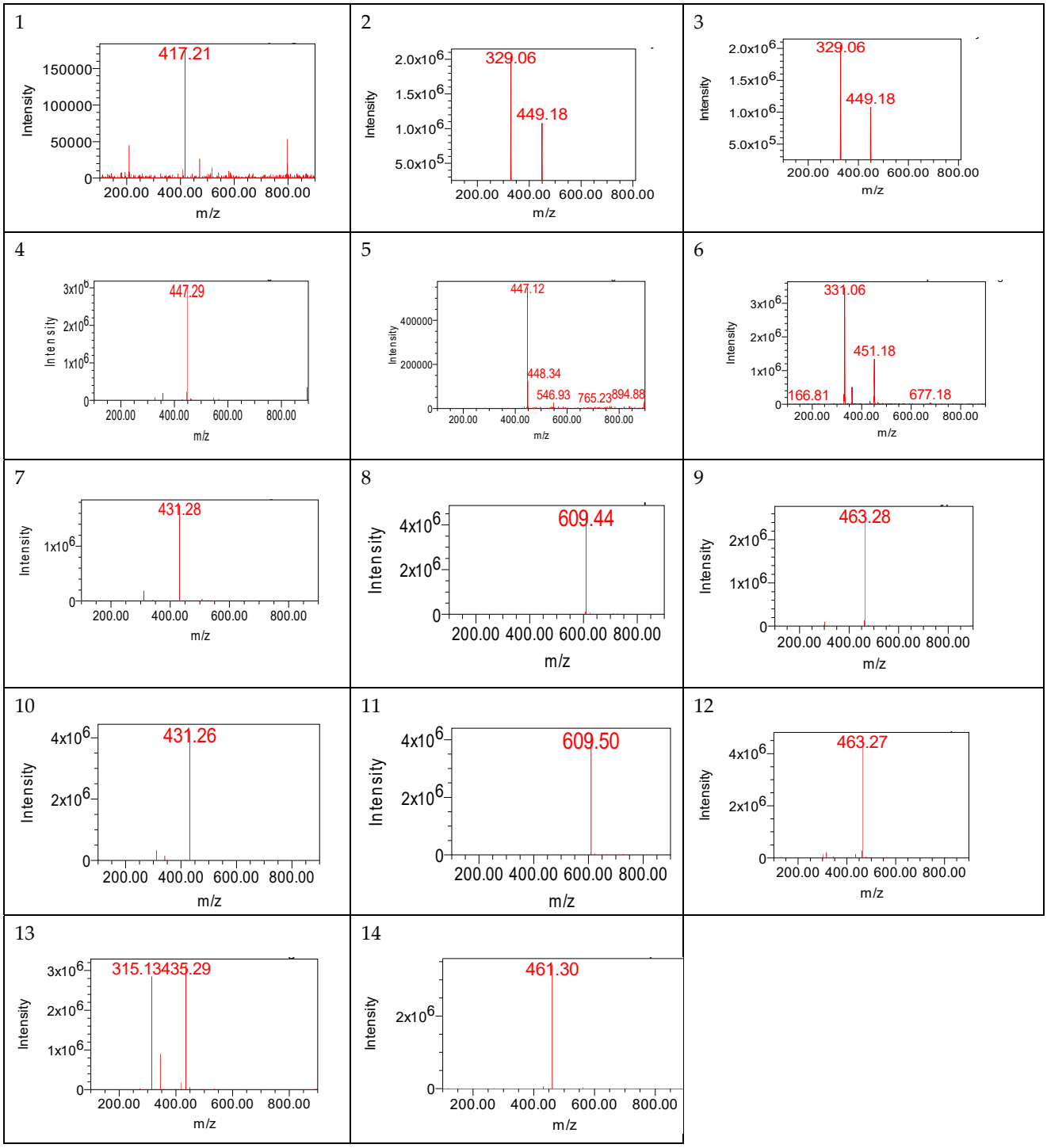
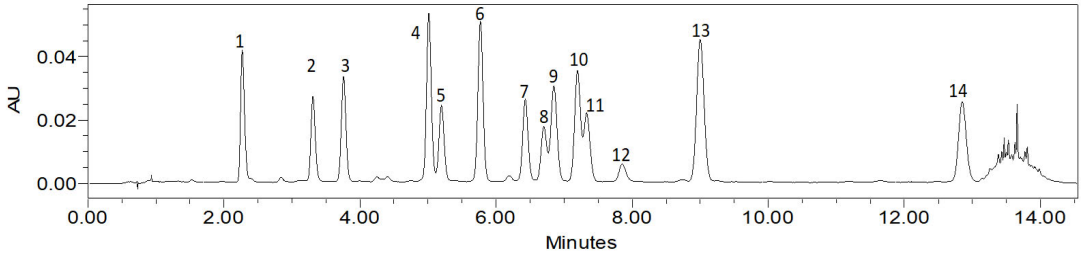


Figure S4. The negative mode of Mass spectra for compounds 1-14.

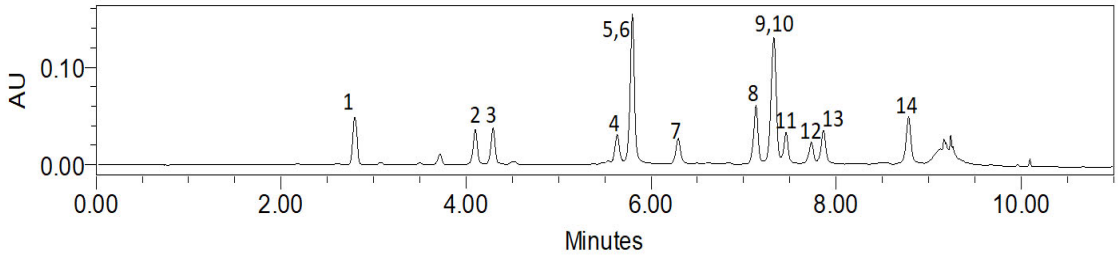
a) Column: HSS T3, 2.1 x 100 mm at 55 °C

Time (min)	Flow (mL/min)	% MeCN w/ 0.05% FA	% Water w/ 0.05% FA
0.00	0.35	12.0	88.0
5.00	0.35	16.0	84.0
10.00	0.35	18.0	82.0
12.00	0.35	20.0	80.0
13.00	0.35	50.0	50.0
14.00	0.35	100	0.0



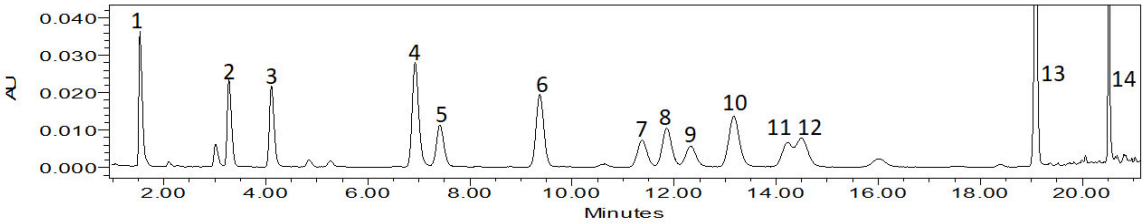
b) Column: Acquity UPLC BEH Shield RP18, 1.8 um, 2.1 x 100 mm at 45 °C

Time (min)	Flow (mL/min)	% MeCN w/ 0.05% FA	% Water w/ 0.05% FA
0.00	0.35	5.0	95.0
1.00	0.35	10.0	90.0
7.00	0.35	25.0	75.0
8.00	0.35	100.0	0.0



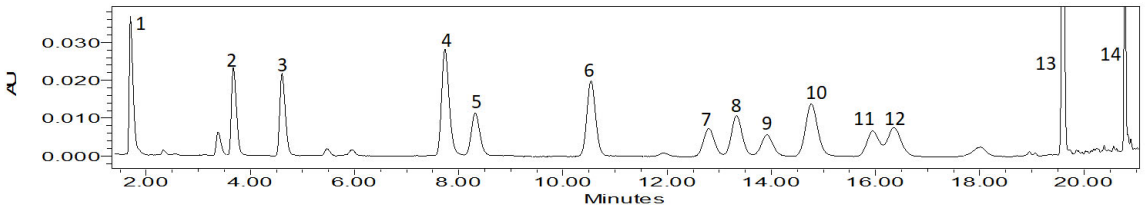
c) Column: Cortecs UPLC C18, 1.6 um, 2.1 x 100 mm at 30 °C

Time (min)	Flow (mL/min)	% MeCN w/ 0.05% FA	% Water w/ 0.05% FA
0.00	0.40	10.0	90.0
22.00	0.40	10.0	90.0
30.00	0.40	25.0	75.0
32.00	0.40	100.0	0.0



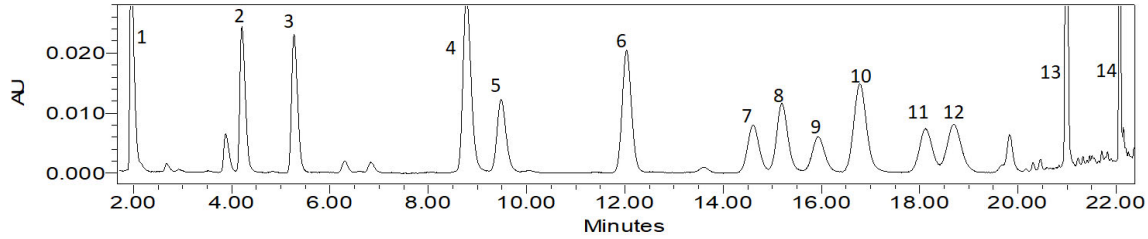
d) Column: Cortecs UPLC C18, 1.6 um, 2.1 x 100 mm at 30 °C

Time (min)	Flow (mL/min)	% MeCN w/ 0.05% FA	% Water w/ 0.05% FA
0.00	0.35	10.0	90.0
22.00	0.35	10.0	90.0
30.00	0.35	25.0	75.0
32.00	0.35	100.0	0.0



e) Column: Cortecs UPLC C18, 1.6 um, 2.1 x 100 mm at 30 °C

Time (min)	Flow (mL/min)	% MeCN w/ 0.05% FA	% Water w/ 0.05% FA
0.00	0.30	10.0	90.0
22.00	0.30	10.0	90.0
30.00	0.30	25.0	75.0
32.00	0.30	100.0	0.0



f) Column: Cortecs UPLC C18, 1.6 um, 2.1 x 100 mm at 30 °C

Time (min)	Flow (mL/min)	% MeCN w/ 0.05% FA	% Water w/ 0.05% FA
0.00	0.25	10.0	90.0
22.00	0.25	10.0	90.0
30.00	0.25	25.0	75.0
32.00	0.25	100.0	0.0

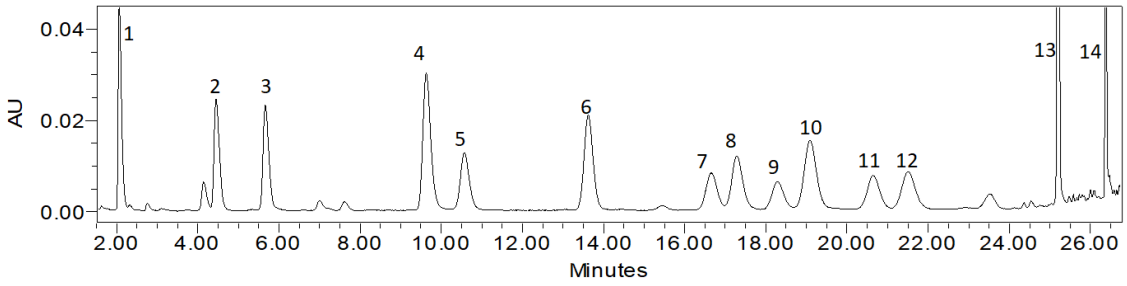


Figure S5. Different chromatograms for different columns and flow rates tried in the method development and optimization at 280 nm.

Table S1. Inter-day and Intra-day precision (% RSD) and recovery analysis for *A. linearis* #16850 samples.

Compound No.	Analytes	Intra-Day (n=3)			Inter-day (n=9)	Amount added (µg)	Amount Found (µg)	Recovery Rate (%)	LOD (mg/100 mg)	LOD (µg/mL)	LOQ (mg/100 mg)	LOQ (µg/mL)
		Day 1	Day 2	Day 3								
1	Syringin	1.54	1.07	0.60	2.5	6.87	6.48	94.21	0.003	0.5	0.012	2
2	Eriodictyol 1	1.73	2.25	1.55	5.1	6.69	6.77	101.27	0.006	1	0.031	5
3	Eriodictyol 2	2.21	2.06	1.09	5.9	8.10	8.06	99.46	0.006	1	0.031	5
4	Isoorientin	1.57	1.04	1.52	1.5	13.31	13.08	98.25	0.004	0.5	0.018	2
5	Orientin	0.78	1.12	1.21	1.2	13.92	12.46	89.50	0.010	1	0.050	5
6	Aspalathin	1.41	1.29	1.06	1.3	15.89	17.13	107.82	0.002	0.5	0.007	2
7	Vitexin	1.32	3.80	4.26	3.9	5.66	6.19	109.36	0.010	1	0.050	5
8	Bioquercetin	1.36	4.12	1.30	3.1	4.67	4.25	91.04	0.004	1	0.020	5
9	Hyperoside	1.38	3.63	2.79	2.7	8.20	8.95	109.09	0.004	1	0.019	5
10	Isovitexin	1.34	1.33	1.74	1.5	6.08	6.05	99.50	0.006	0.5	0.025	2
11	Rutin	0.74	3.25	3.71	2.5	6.78	6.42	94.60	0.007	1	0.030	5
12	Isoquercitrin	1.75	1.73	2.67	2.3	6.61	7.18	108.64	0.004	1	0.019	5
13	Nothofagin	1.13	1.69	0.15	2.3	5.29	5.21	98.47	0.001	0.2	0.005	1
14	Thermopsoside	1.08	0.54	0.73	2.2	6.49	6.05	93.16	0.005	0.5	0.020	2