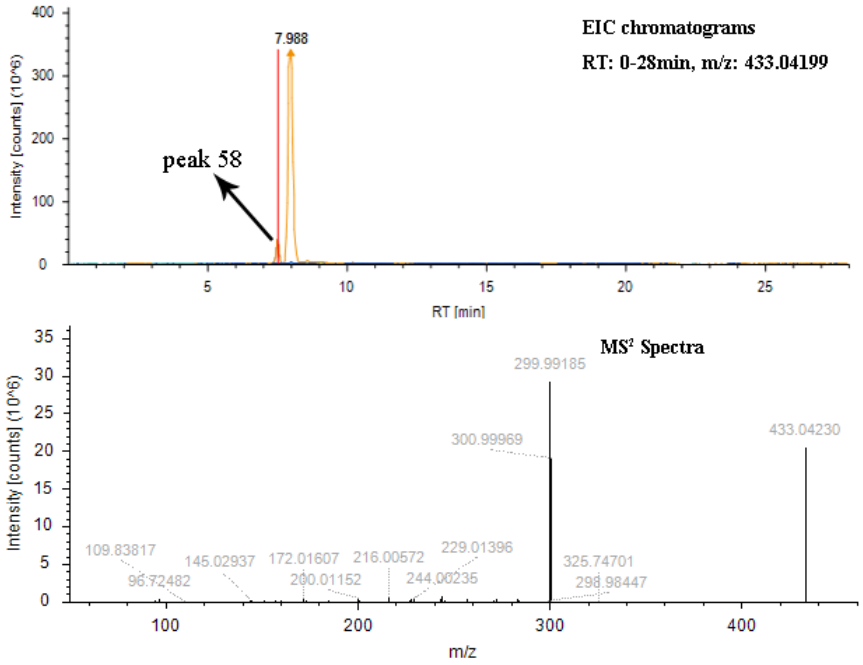


Figure S1. Extracted ion chromatograms (EIC) and tandem mass spectra (MS^2) of ellagitannins identified in the extract of walnut. * The peak numbers are according to Table 1.

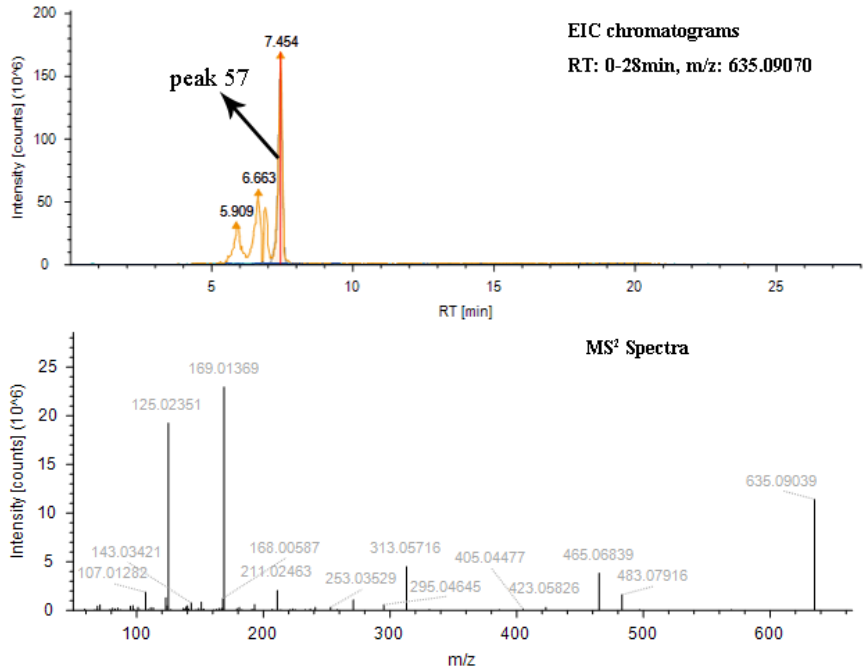


Figure S2. Extracted ion chromatograms (EIC) and tandem mass spectra (MS^2) of gallotannins identified in the extract of walnut.

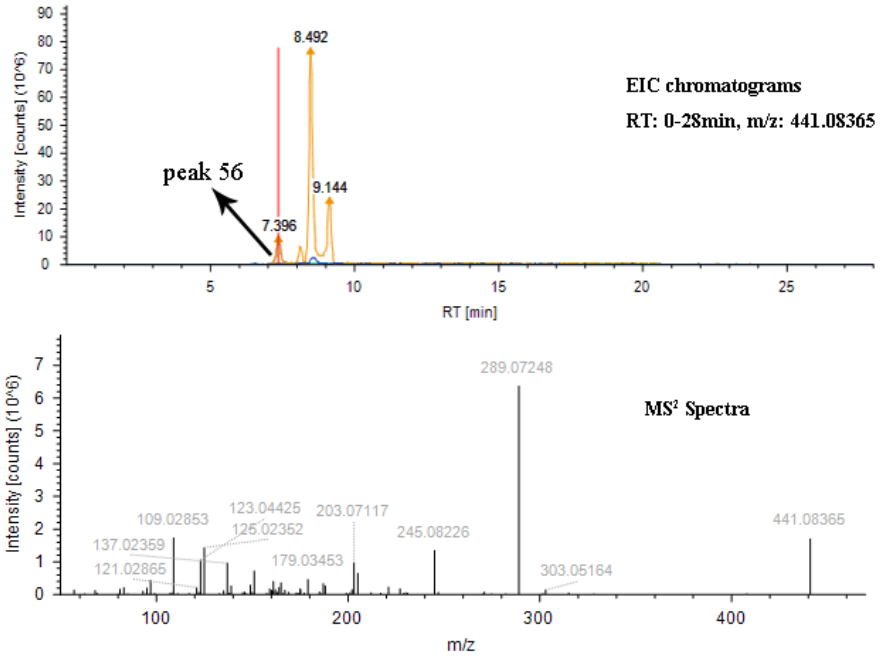


Figure S3. Extracted ion chromatograms (EIC) and tandem mass spectra (MS^2) of flavonoids identified in the extract of walnut.

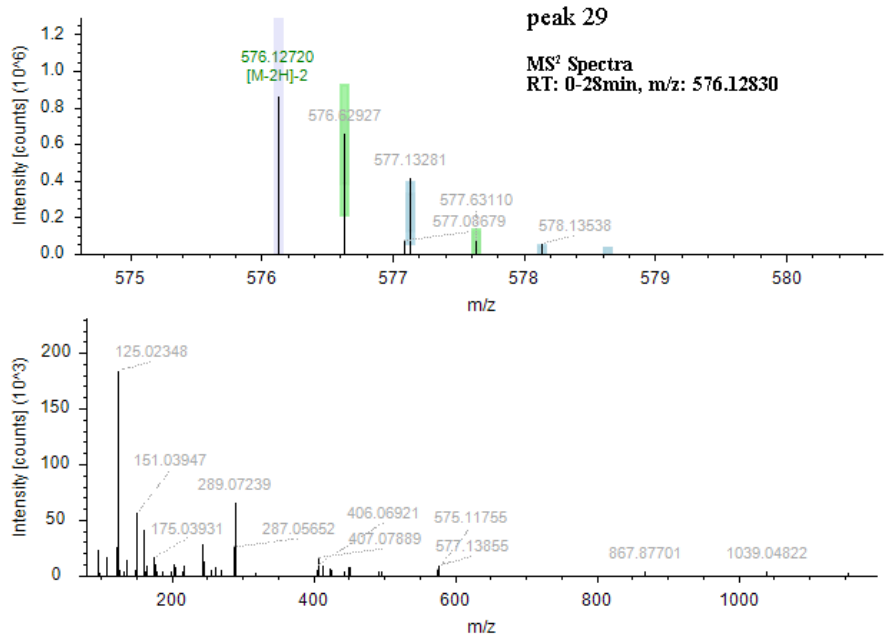


Figure S4. Extracted tandem mass spectra (MS^2) of peak 29 identified in the extract of walnut.

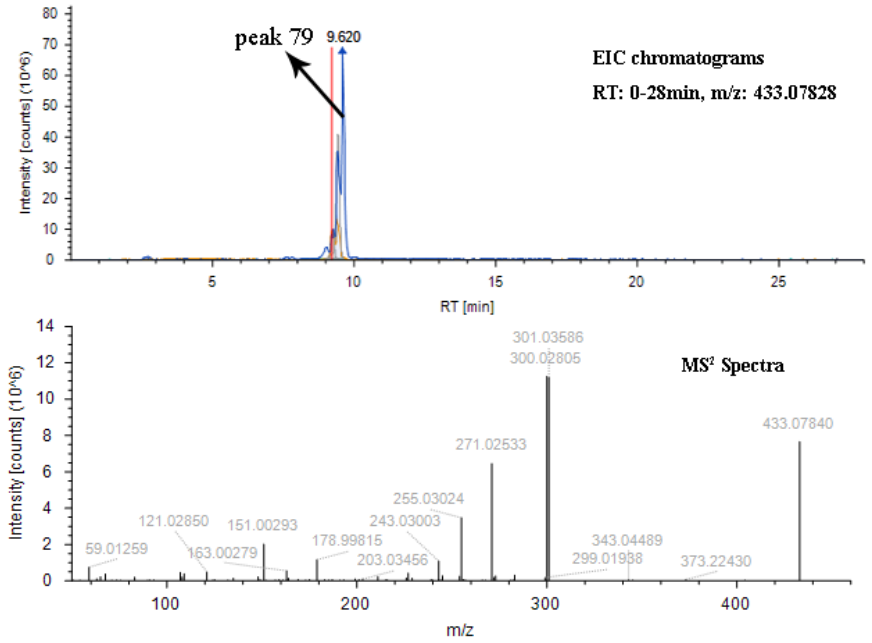


Figure S5. Extracted ion chromatograms (EIC) and tandem mass spectra (MS^2) of flavonol identified in the extract of walnut.

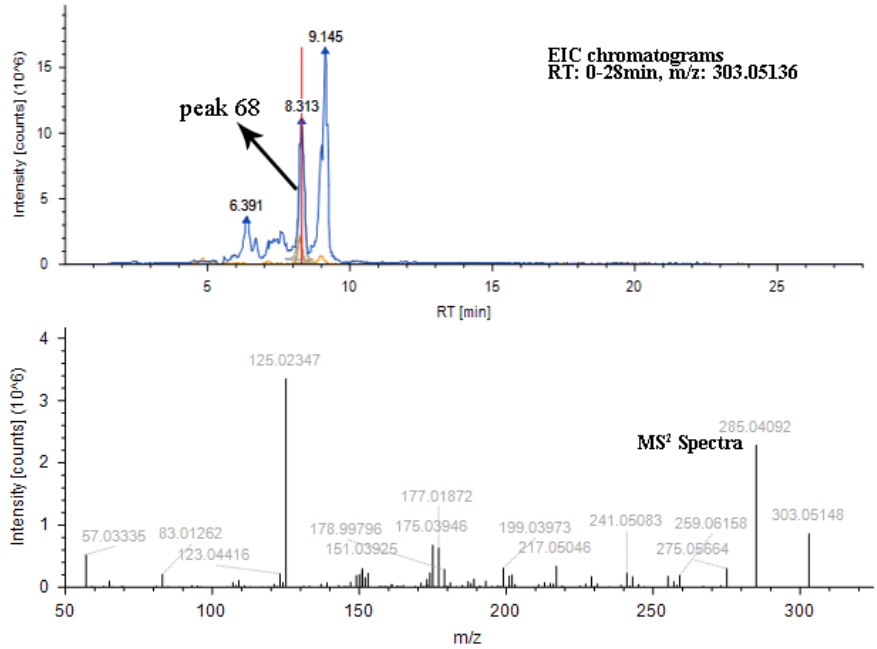


Figure S6. Extracted ion chromatograms (EIC) and tandem mass spectra (MS^2) of flavanol identified in the extract of walnut.

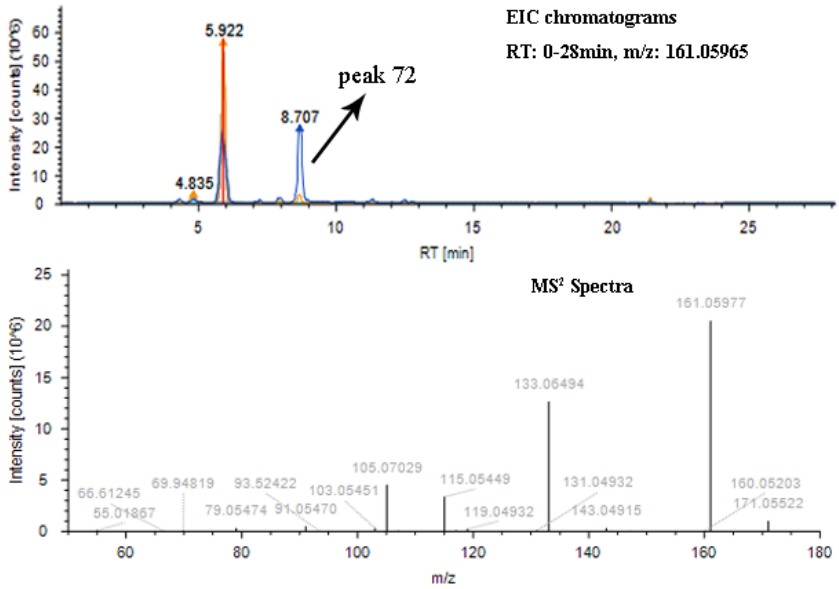
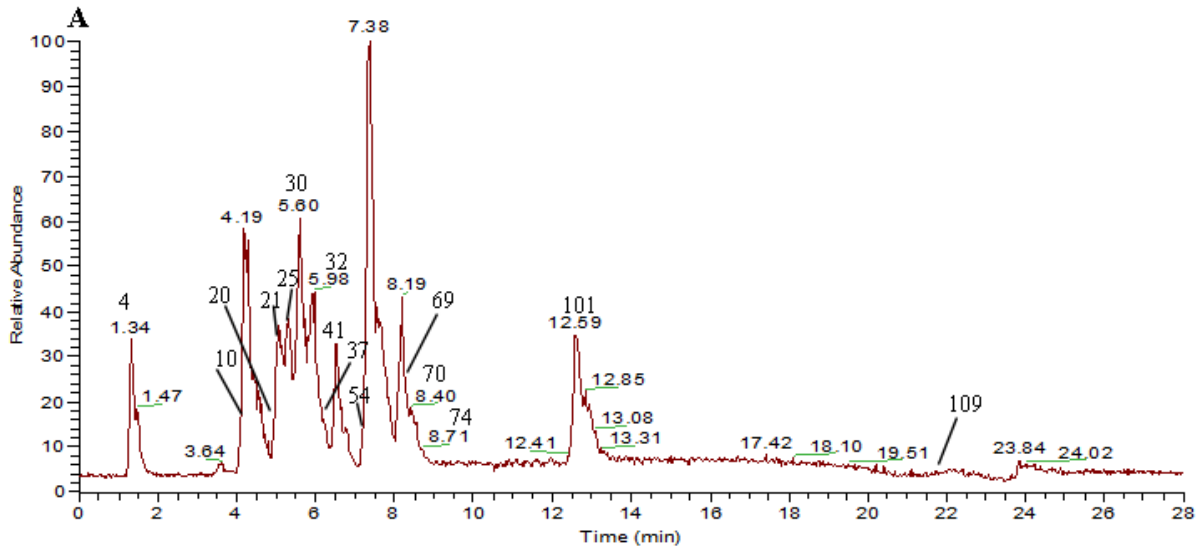
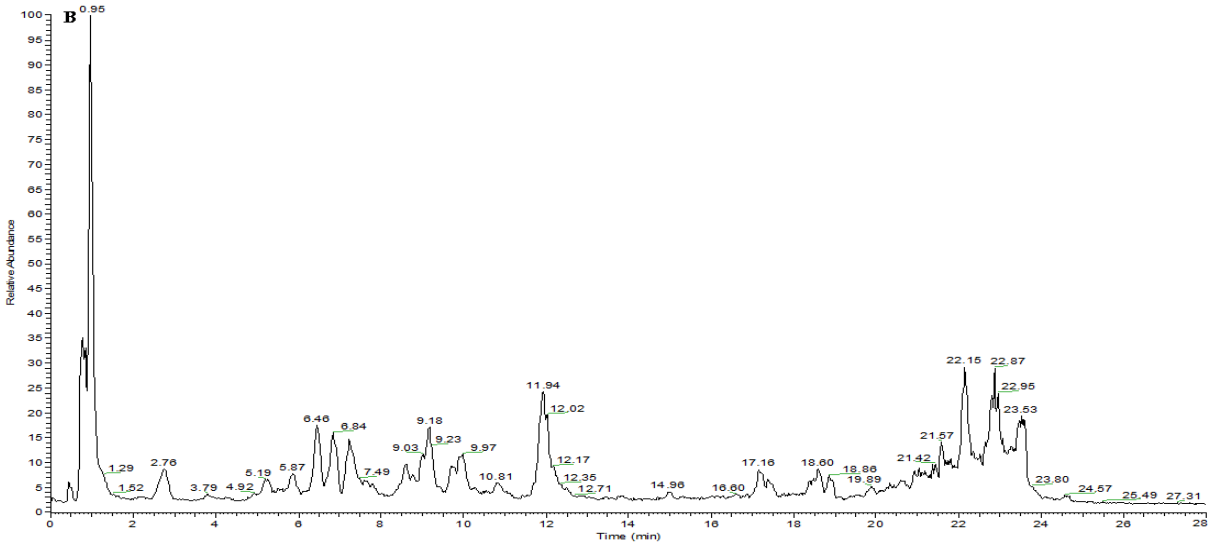


Figure S7. Extracted ion chromatograms (EIC) and tandem mass spectra (MS^2) of quinones identified in the extract of walnut.

Table S1. Calibration curves, Retention time, Linear ranges, LODs and LOQs for 16 analytes

Compound	Calibration curve	R^2	Retention time	UV max (lambda in nm)	Linear ranges (µg/mL)	LOQ (µg/ml)	LOD (µg/ml)
gallic acid	y = 0.0004x - 0.0037	R ²= 0.9992	4.537	280	10.00-625.00	1.20	0.36
neochlorogenic acid	y = 0.0007x - 0.0038	R ²= 0.9993	9.592	280	10.00-625.00	0.52	0.16
chlorogenic acid	y = 0.0016x - 0.0029	R ²= 0.9996	14.470	280	10.00-500.00	0.86	0.26
catechin	y = 0.0008x - 0.0045	R ²= 0.9988	15.428	280	5.00-625.00	0.54	0.16
p-hydroxybenzoic acid	y = 0.0007x - 0.0047	R ²= 0.9986	16.959	280	10.00-625.00	0.83	0.25
vanillic acid	y = 0.0007x - 0.0042	R ²= 0.999	19.426	280	10.00-625.00	1.00	0.30
caffeic acid	y = 0.0003x - 0.0006	R ²= 0.9997	19.904	280	5.00-500.00	0.40	0.12
epicatechin	y = 0.0016x + 0.0014	R ²= 0.9988	22.004	280	10.00-500.00	0.83	0.25
syringic acid	y = 0.0004x - 0.0010	R ²= 0.9998	22.454	280	5.00-500.00	0.38	0.11
p-coumaric acid	y = 0.0002x - 0.0005	R ²= 0.9998	28.144	280	5.00-500.00	0.23	0.07
ferulic acid	y = 0.0004x - 0.0011	R ²= 0.9997	31.285	280	5.00-500.00	0.43	0.13
o-coumaric acid	y = 0.0002x - 0.0030	R ²= 0.9994	35.168	280	10.00-625.00	0.31	0.09
rutin	y = 0.0013x - 0.0336	R ²= 0.9971	10.410	251	50.00-5000.00	1.88	0.56
myricetin	y = 0.0123x - 0.1200	R ²= 0.9947	11.741	251	50.00-5000.00	11.21	3.36
quercetin	y = 0.0062x + 0.0025	R ²= 0.9981	14.710	251	50.00-500.00	11.23	3.37
juglone	y = 0.0007x + 0.0004	R ²= 0.9985	16.448	251	10.00-500.00	1.10	0.33


A
Relative Abundance
Time (min)
7.38
4.19
30
5.60
32
5.98
25
20
21
41
37
10
54
4
1.34
1.47
3.64
8.19
69
70
8.40
74
8.71
101
12.59
12.85
13.08
13.31
12.41
17.42
18.10
19.51
109
23.84
24.02


B
0.95
Relative Abundance
Time (min)
11.94
12.02
22.15
22.87
22.95
23.53
6.46
6.84
9.18
9.23
9.03
9.97
21.57
21.42
12.17
12.35
12.71
10.81
7.49
5.87
5.19
4.92
3.79
2.76
1.29
1.52
14.96
16.60
17.16
18.60
18.86
19.89
23.80
24.57
25.49
27.31

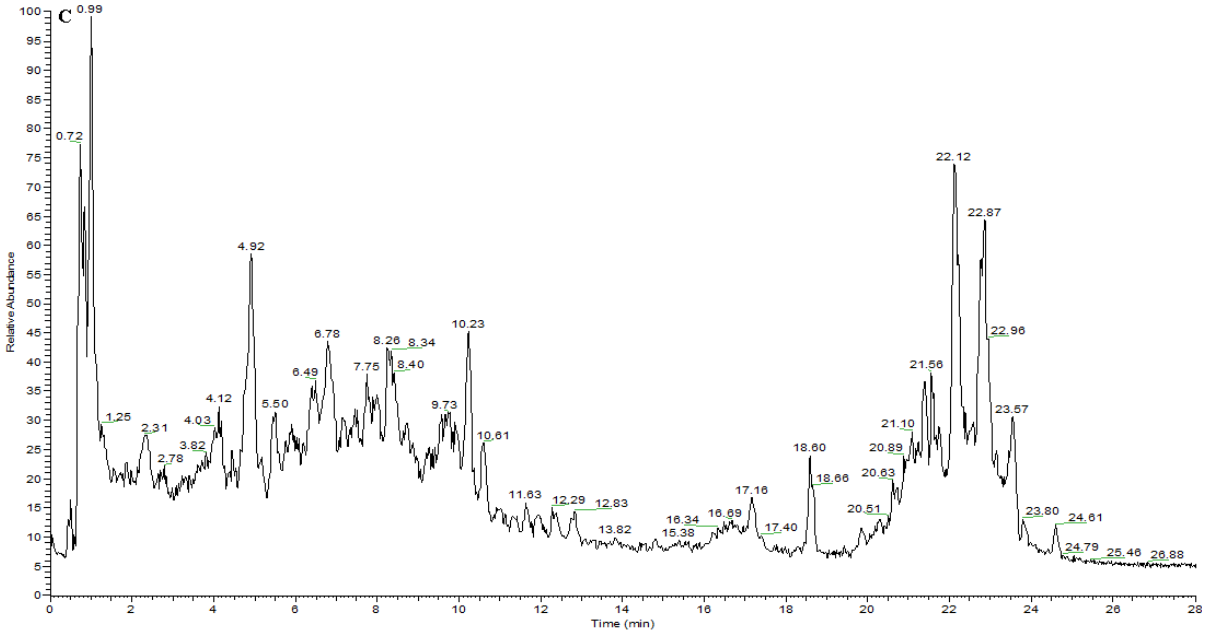

C
0.99
0.72
Relative Abundance
Time (min)
22.12
22.87
22.96
4.92
10.23
6.78
8.26
8.34
8.40
6.49
7.75
21.56
23.57
4.12
5.50
9.73
10.61
4.03
3.82
2.78
2.31
1.25
18.60
18.66
20.89
20.63
21.10
20.51
17.16
17.40
16.34
16.69
15.38
13.82
11.63
12.29
12.83
23.80
24.61
24.79
25.46
26.88

Figure S8. Total-ion chromatograms in negative mode of walnut husk and pellicle extracts. (A: Chromatogram of quantitative standards; B: Chromatogram of walnut husk; C: Chromatogram of walnut pellicle)

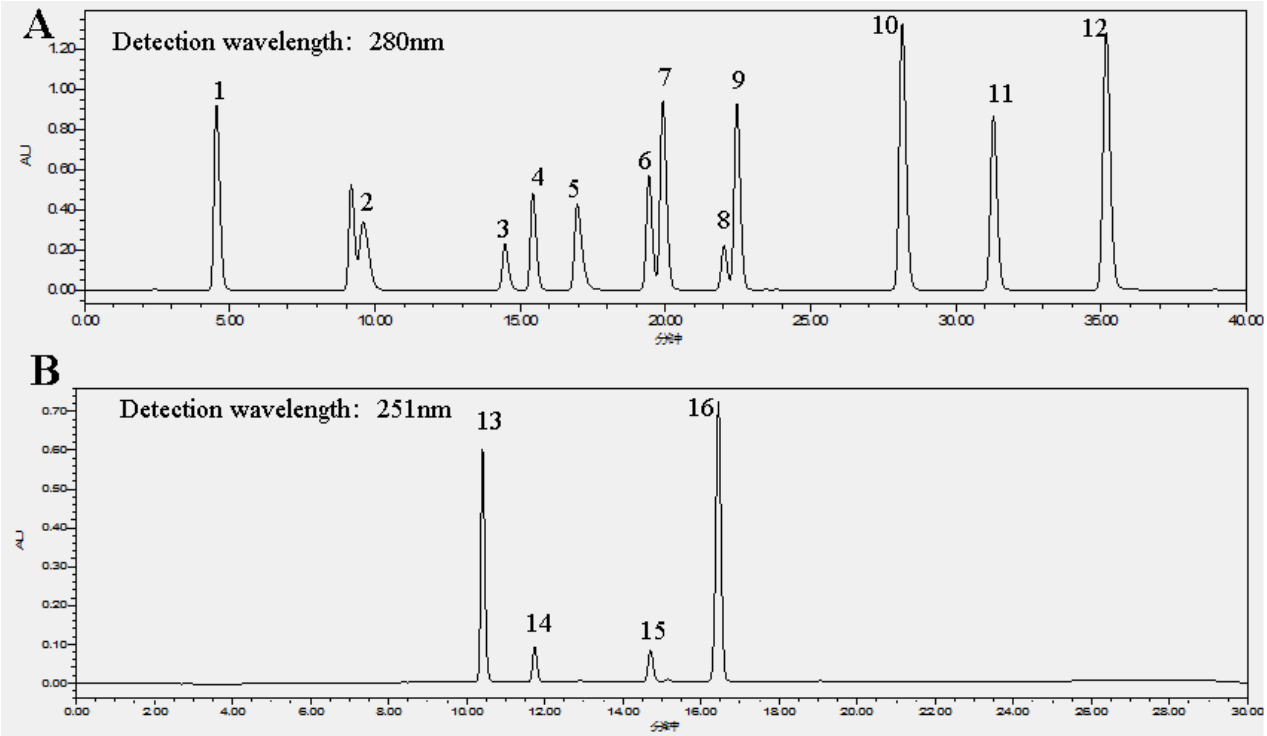


Figure S9. HPLC chromatogram of the standard optimized system (Note: 1. gallic acid; 2. neochlorogenic acid; 3. catechin; 4. *p*-hydroxybenzoic acid; 5. chlorogenic acid ; 6. vanillic acid; 7. caffeic acid; 8. epicatechin; 9. syringic acid; 10. *p*-coumaric acid; 11. ferulic acid; 12. *o*-coumaric acid; 13. rutin; 14. myricetin; 15. quercetin; 16. juglone)