

Comprehensive Chemical Profiling in the Ethanol Extract of *Pluchea indica* Aerial Parts by Liquid Chromatography/Mass Spectrometry Analysis of Its Silica Gel Column Chromatography Fractions

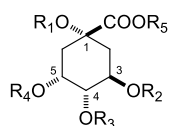
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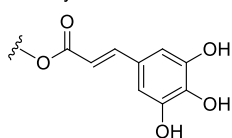
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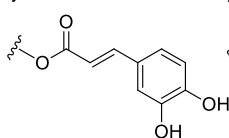


	R ₁	R ₂	R ₃	R ₄	R ₅
4:	H	H	H	Caffeoyl	H
11:	H	Caffeoyl	H	H	H
16:	H	H	Caffeoyl	H	H
29:	H	Caffeoyl	H	H	CH ₃
35:	Caffeoyl	H	Caffeoyl	H	H
37:	Caffeoyl	H	H	Caffeoyl	H
38:	Caffeoyl	Caffeoyl	H	H	H
39:	H	H	Caffeoyl	Caffeoyl	H
40:	H	Caffeoyl	H	Caffeoyl	H
45:	H	Caffeoyl	Caffeoyl	H	H
47:	Caffeoyl	Caffeoyl	H	Caffeoyl	H
51:	H	H	Caffeoyl	Caffeoyl	CH ₃
53:	Caffeoyl	Caffeoyl	Caffeoyl	H	H
55:	H	Caffeoyl	H	Caffeoyl	CH ₃
61:	H	Caffeoyl	Caffeoyl	H	CH ₃
65:	H	Caffeoyl	Caffeoyl	Caffeoyl	H
66:	H	Caffeoyl	H	Caffeoyl	CH ₂ CH ₃
74:	H	Caffeoyl	Caffeoyl	H	CH ₂ CH ₃
76:	Caffeoyl	Caffeoyl	Caffeoyl	Caffeoyl	H
91:	H	Caffeoyl	Caffeoyl	Caffeoyl	CH ₃

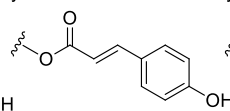
3,4,5-Trihydroxycinnamoyl:



Caffeoyl:



Coumaroyl:



Ferulyl:

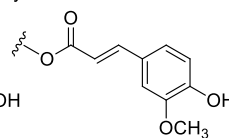


Fig. S1. The structures of 20 quinic acids standard references.

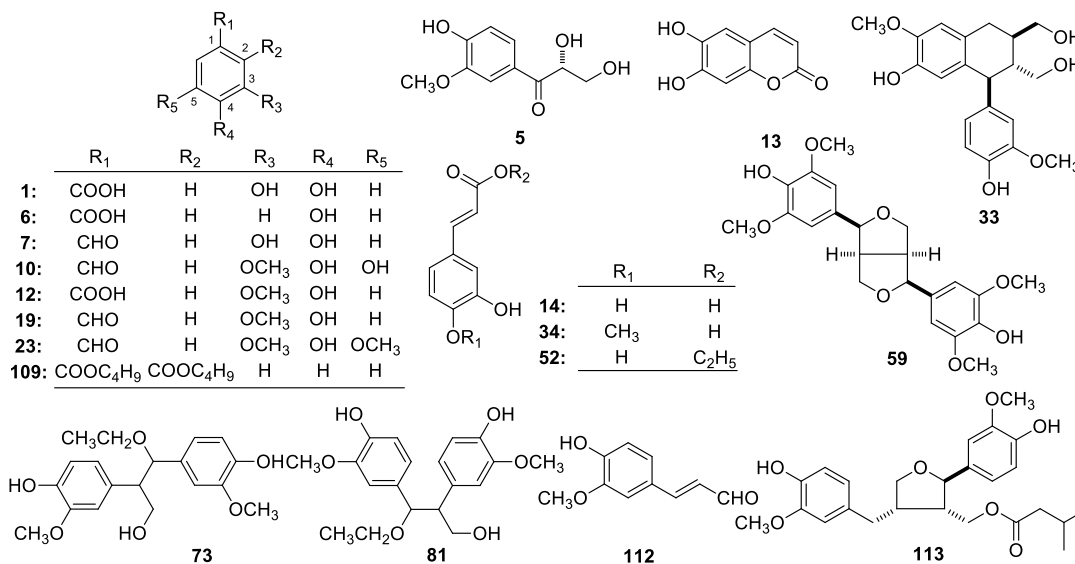
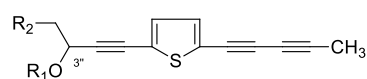
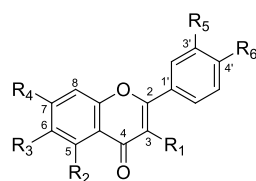


Fig. S2. The structures of 19 phenolic acids standard references.



	R ₁	R ₂	3''
99:	H	OH	R
105:	H	OCCH ₃	R
107:	CH ₂ CH ₃	OH	S
111:	CH ₂ CH ₃	OCCH ₃	S

Fig. S3. The structures of 4 thiophenes standard references.



	R ₁	R ₂	R ₃	R ₄	R ₅	R ₆
31:	OGa	OH	H	OH	OH	OH
32:	OGlc	OH	H	OH	OH	OH
42:	OGlc	OH	H	OH	H	OH
43:	H	OH	H	OGlc	OH	OH
44:	OCH ₃	OH	H	OH	OGlc	OH
54:	OH	OH	H	OH	OH	OH
57:	H	OH	H	OH	OH	OH
68:	OCH ₃	OH	OH	OCH ₃	H	OH
71:	OH	OH	H	OH	H	OH
77:	OH	OH	H	OH	OCH ₃	OH
86:	OCH ₃	OH	OH	OCH ₃	OCH ₃	OH
87:	OCH ₃	OH	OCH ₃	OH	OH	OCH ₃
101:	OCH ₃	OH	OCH ₃	OCH ₃	OH	OCH ₃

Glc: β -D-glucopyranoside; Gal: β -D-galactopyranoside

Fig. S4. The structures of 13 flavonoids standard references.

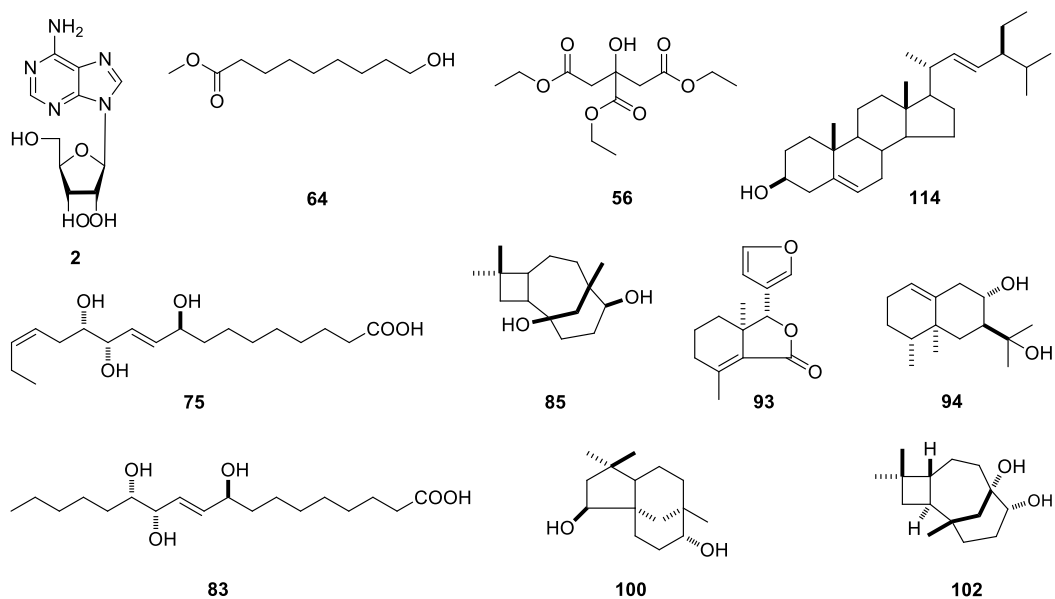


Fig. S5. The structures of 7 other compounds standard references.

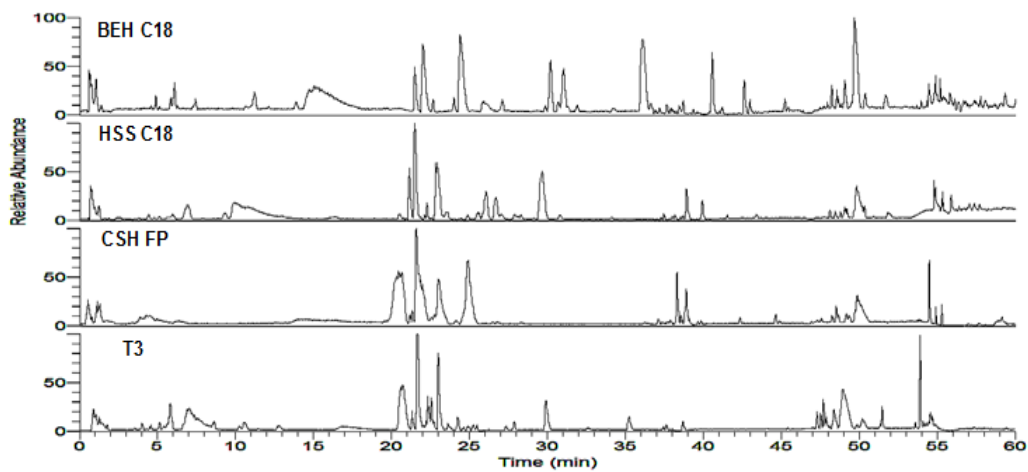


Fig. S6. Base peak chromatograms (BPC) of PI on BEHC18, HSS C18, CSH FP, and T3 columns.

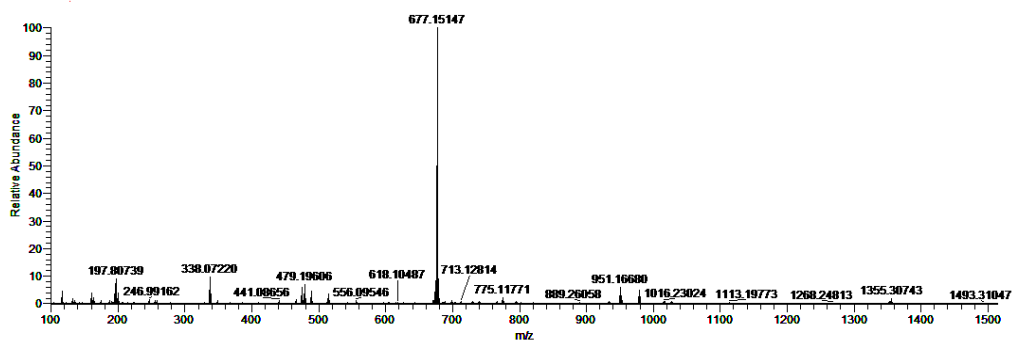


Fig. S7. MS spectrum for peak 40.13 min from TIC of PI.

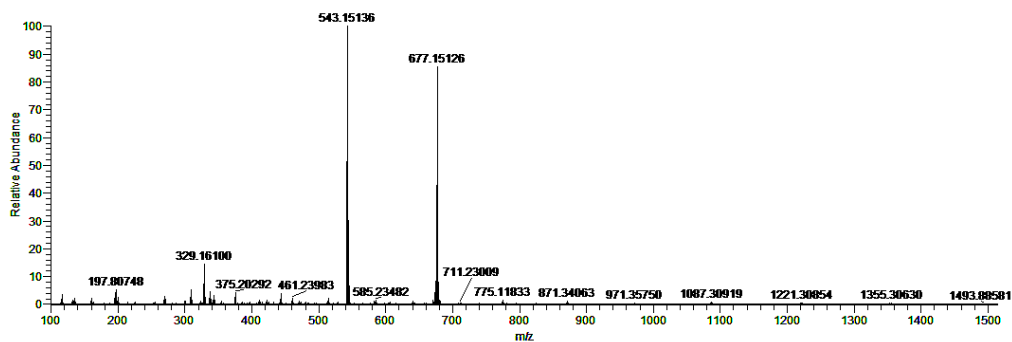


Fig. S8. MS spectrum for peak 40.13 min from TIC of PIE4.

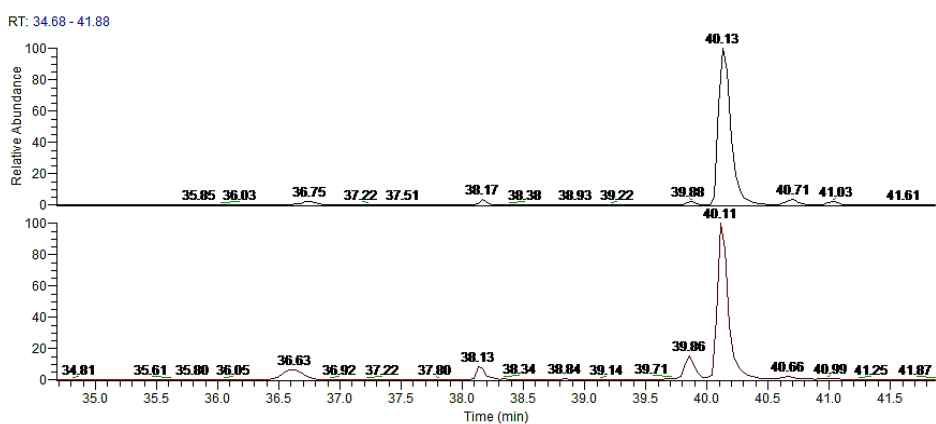


Fig. S9. The EIC of m/z 677.15119. A: EIC from PI; B: EIC from PIE6.

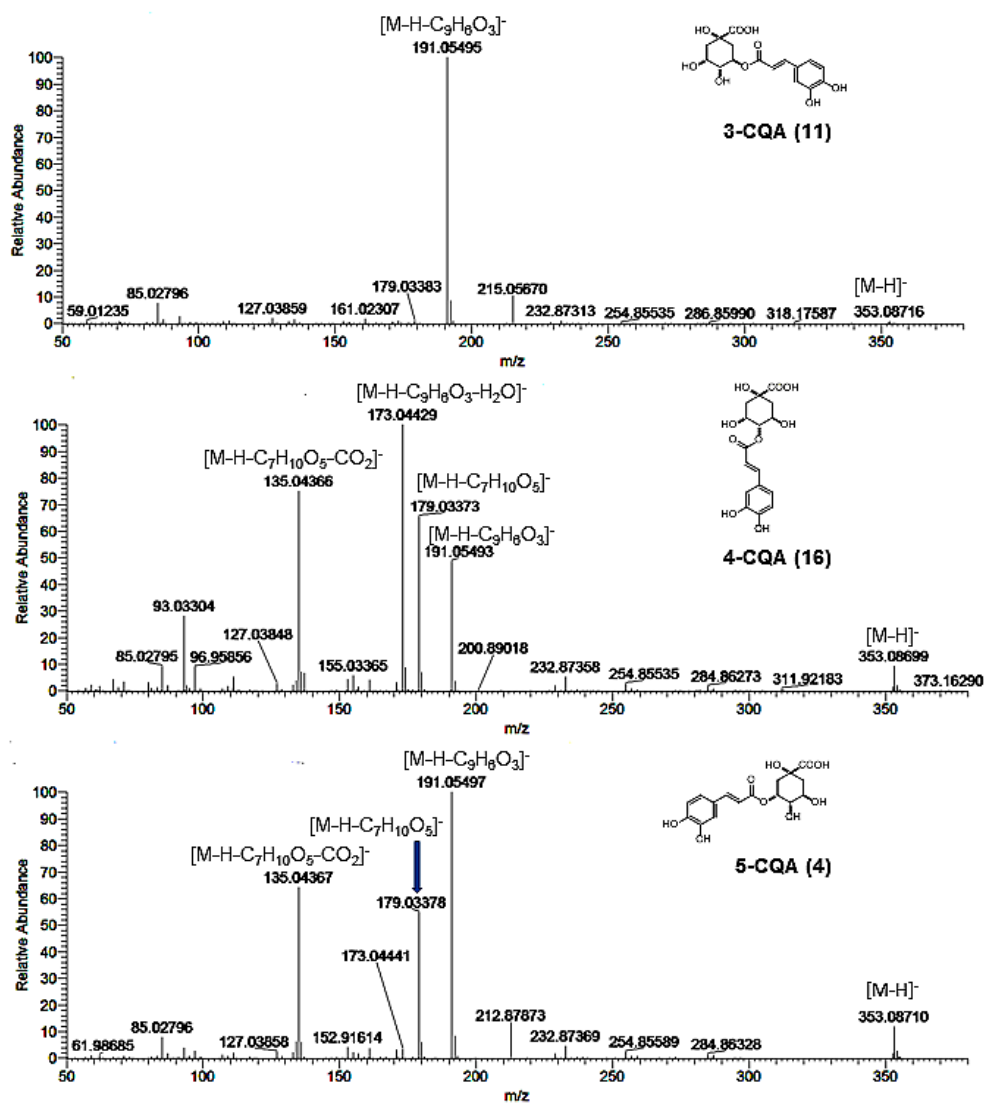


Fig. S10. MS/MS spectrum of the $[M-H]^-$ ions for 11, 16, and 4.

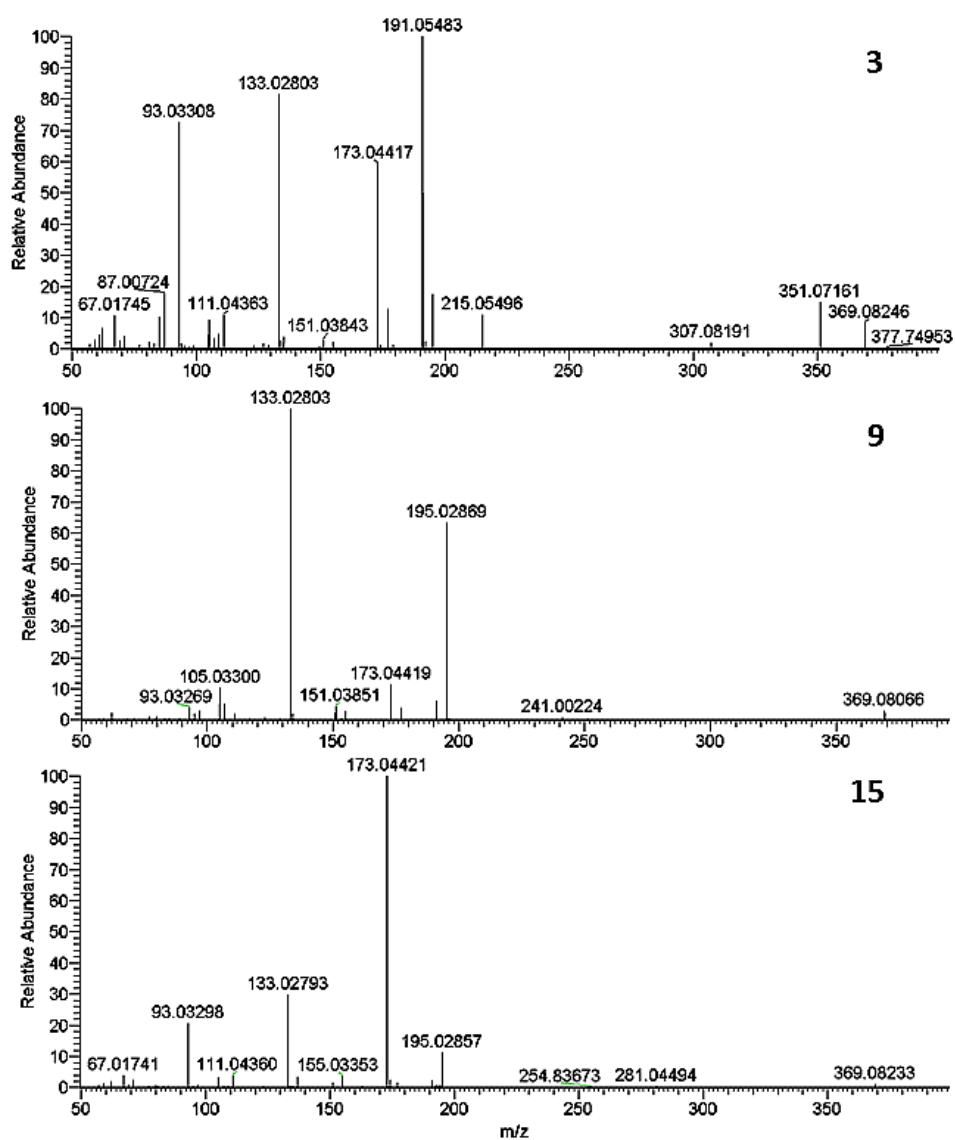


Fig. S11. MS/MS spectrum of the $[M-H]^-$ ions for 3, 5, and 9.

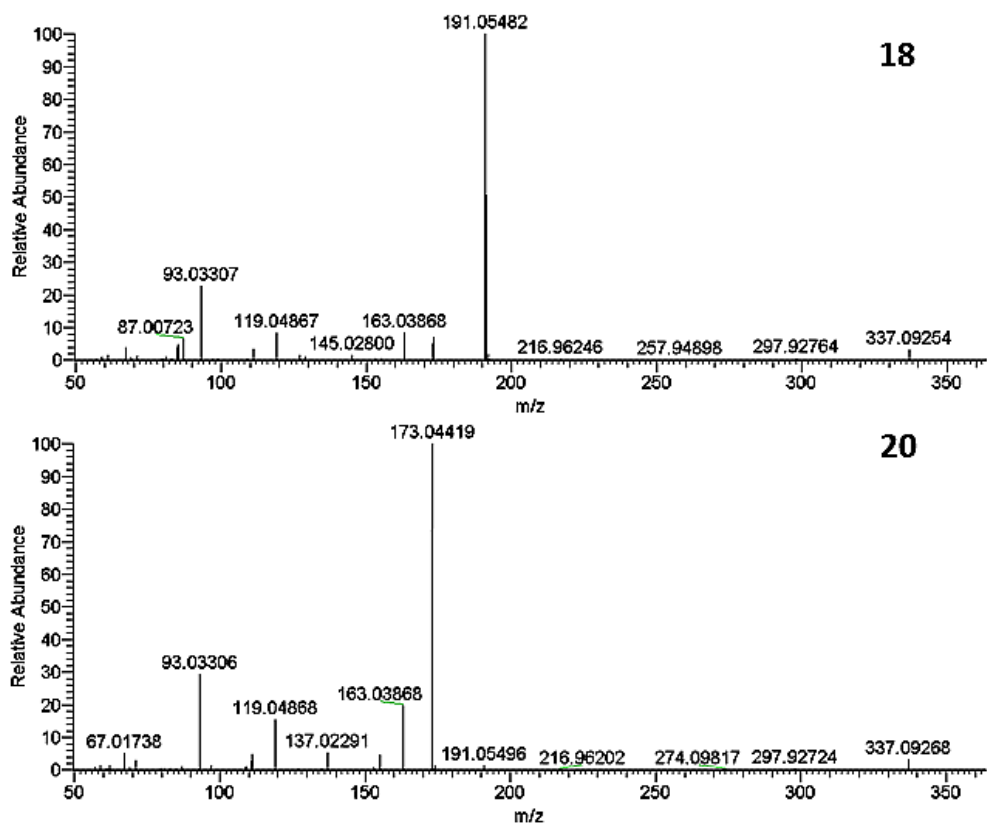


Fig. S12. MS/MS spectrum of the $[M-H]^-$ ions for 18 and 20.

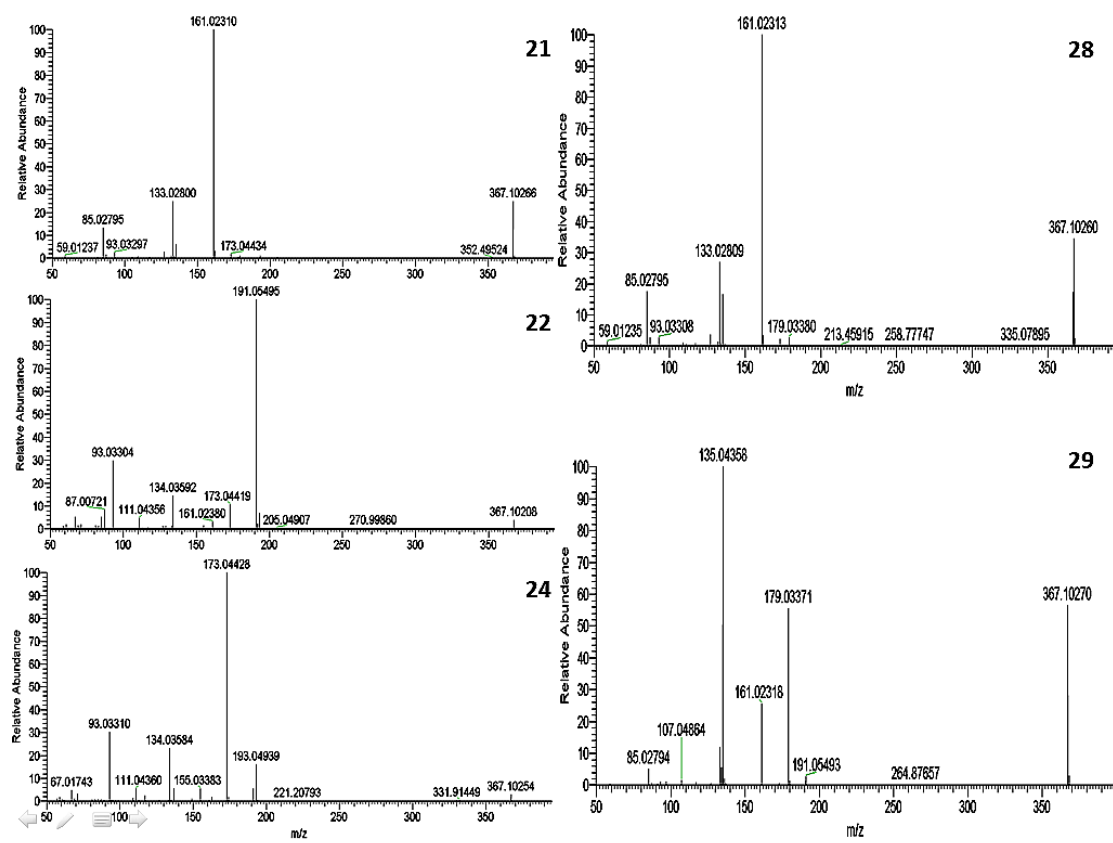


Fig. S13. MS/MS spectrum of the $[M-H]^-$ ions for 21, 22, 24, 28 and 29.

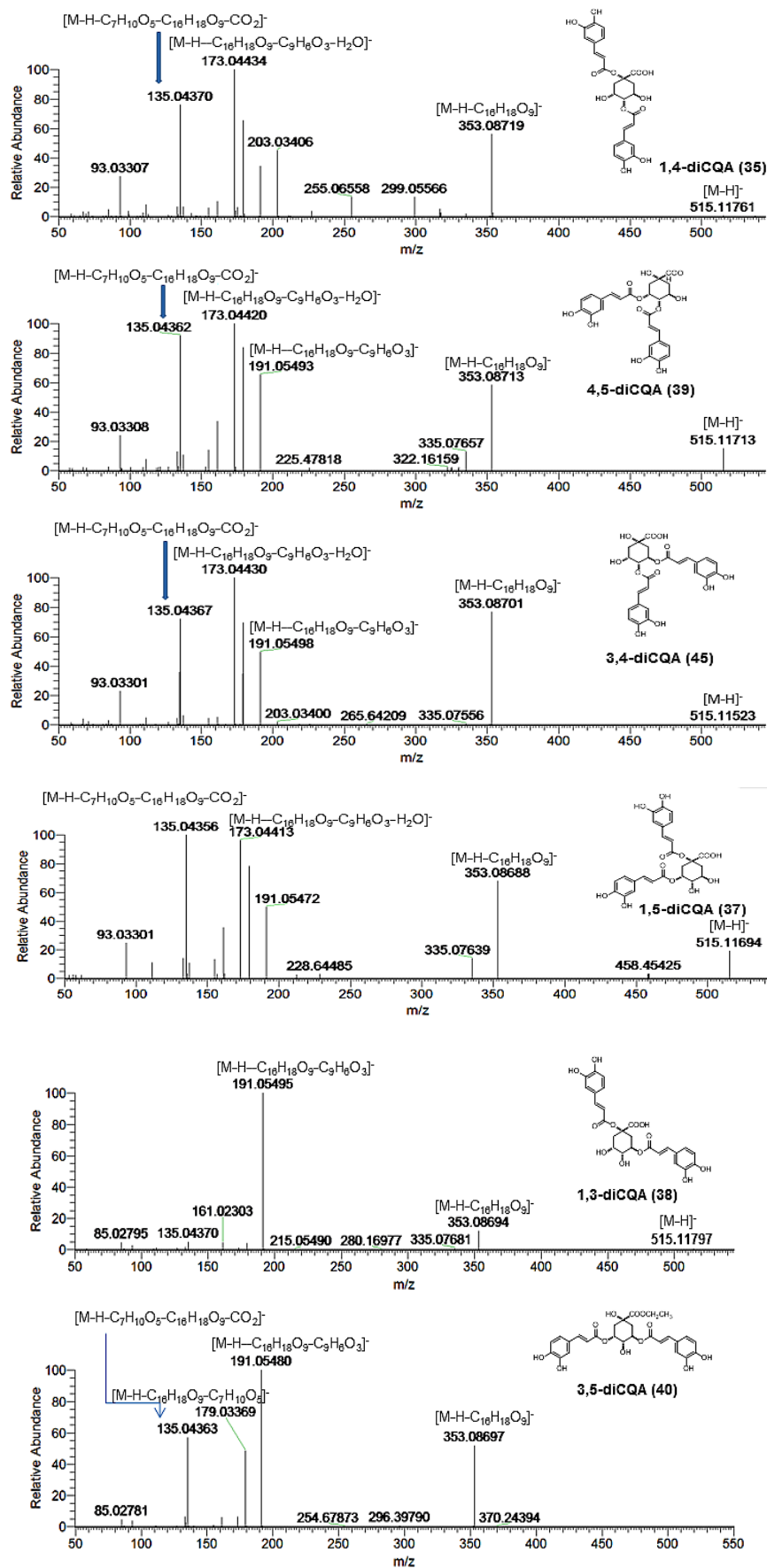


Fig. S14. The MS/MS spectrum of the [M-H]⁻ ions for 35, 37–40, 45.

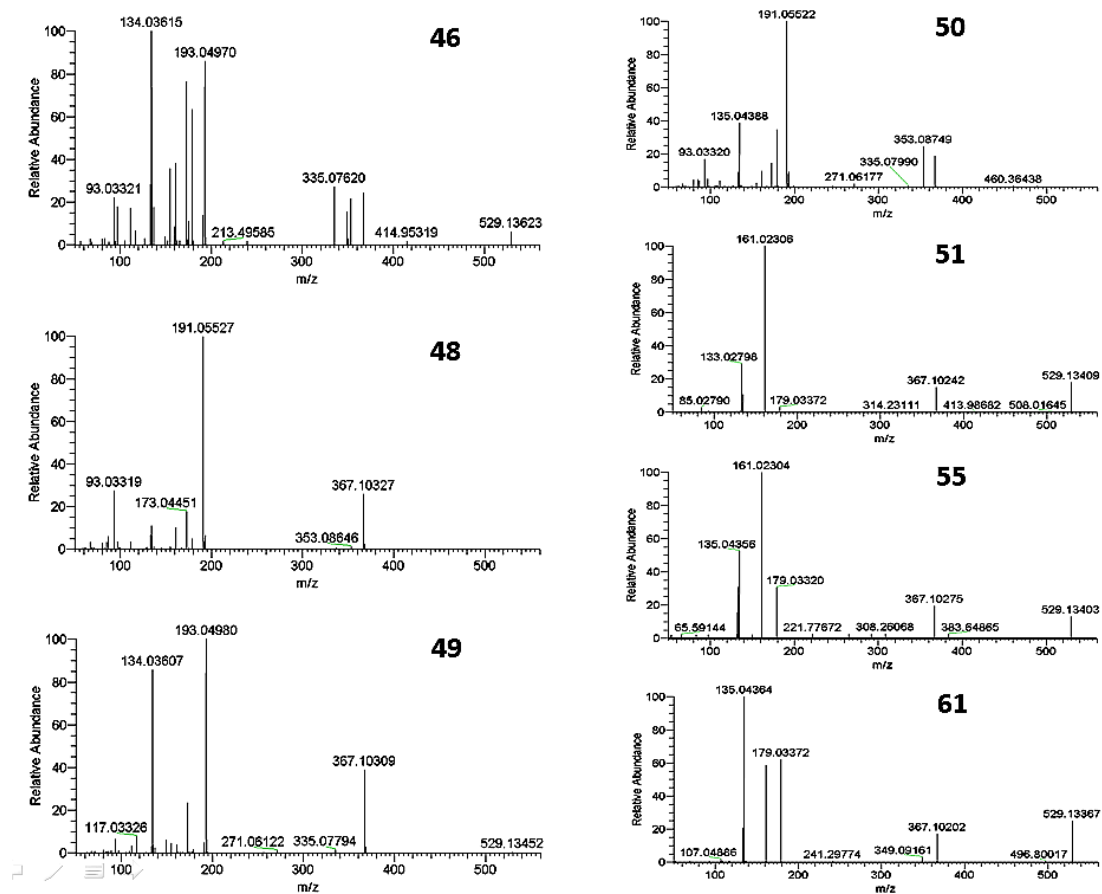


Fig. S15. The MS/MS spectrum of the $[M-H]^-$ ions for peaks 46, 48, 49, 50, 51, 55 and 61.

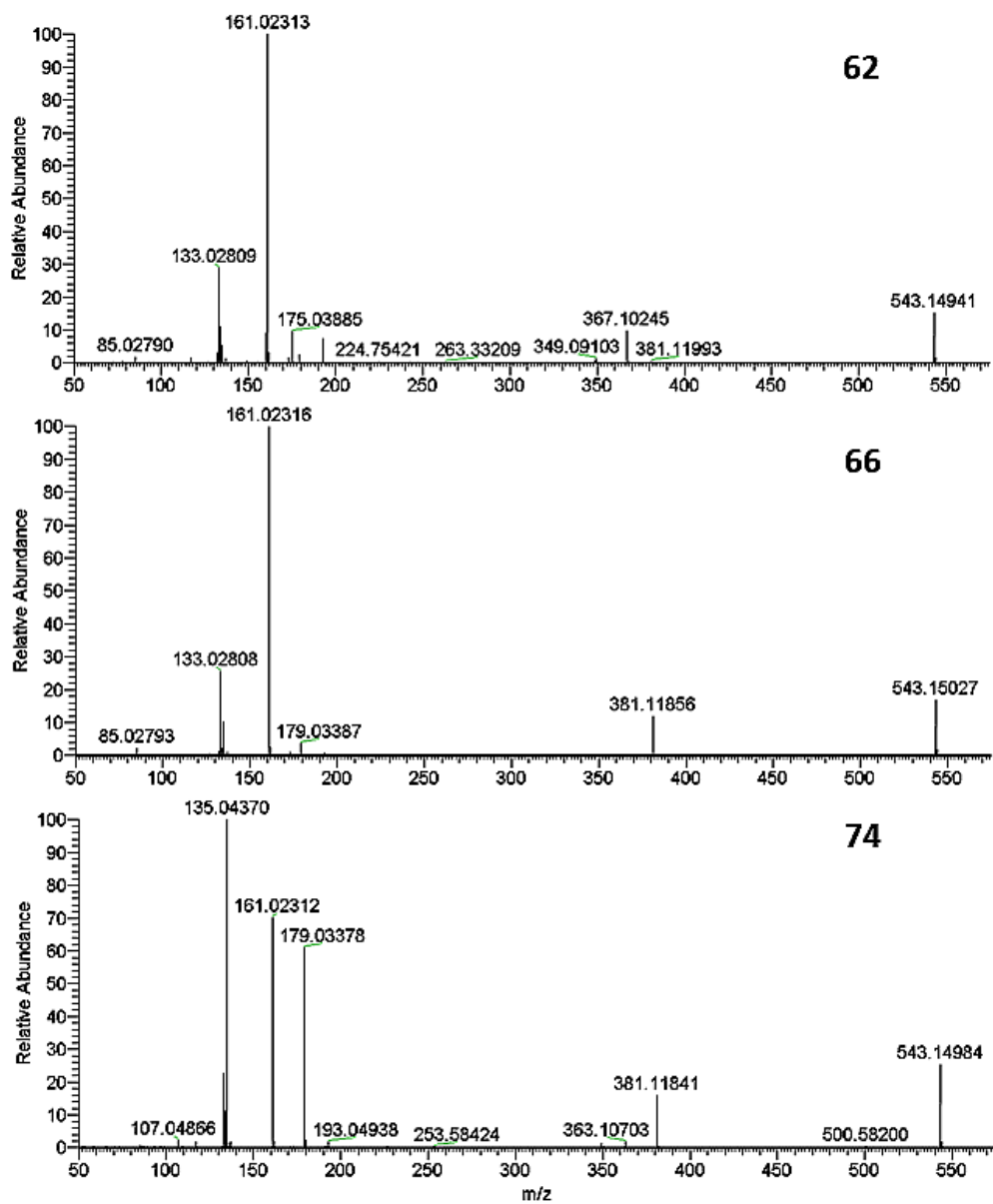


Fig. S16. The MS/MS spectrum of the $[M-H]^-$ ions for peaks 62, 66 and 73.

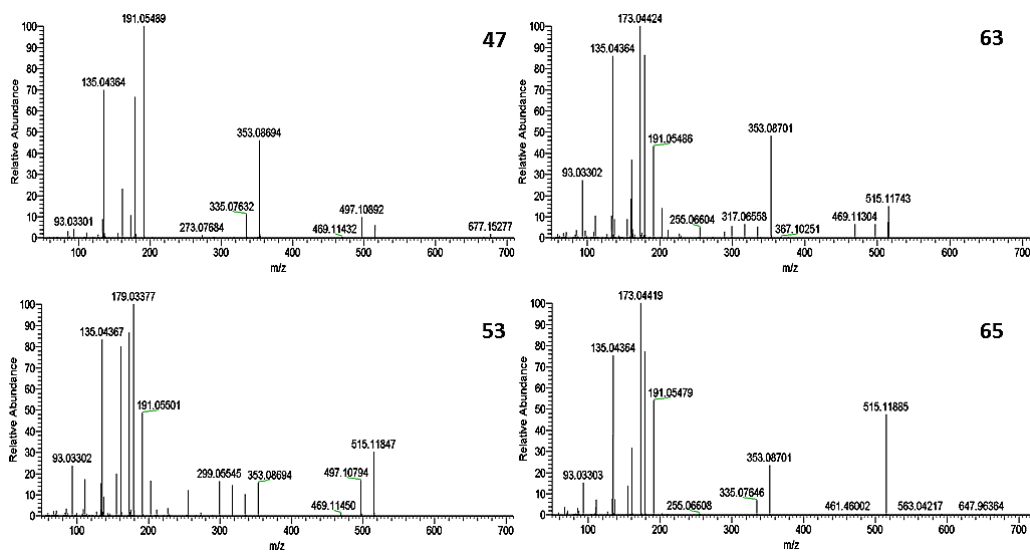


Fig. S17. The MS/MS spectrum of the $[M-H]^-$ ions for peaks 47, 53, 63 and 65.

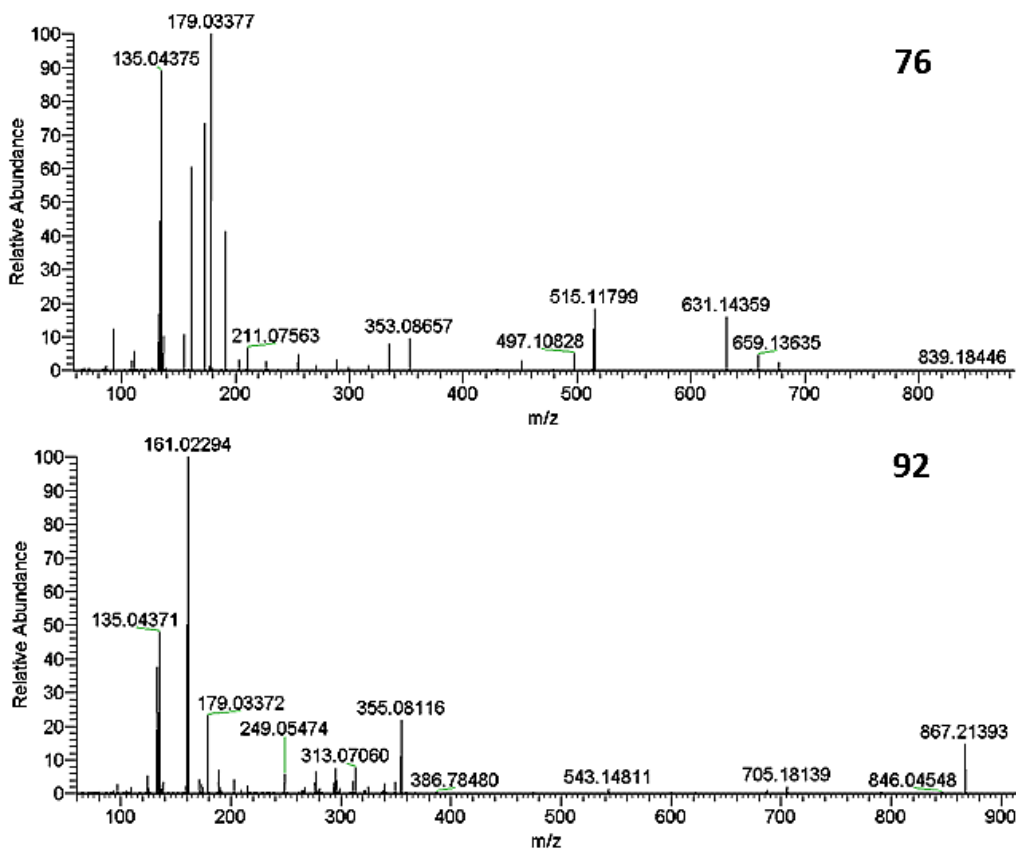


Fig. S18. The MS/MS spectrum of the $[M-H]^-$ ions for peaks 76 and 92.

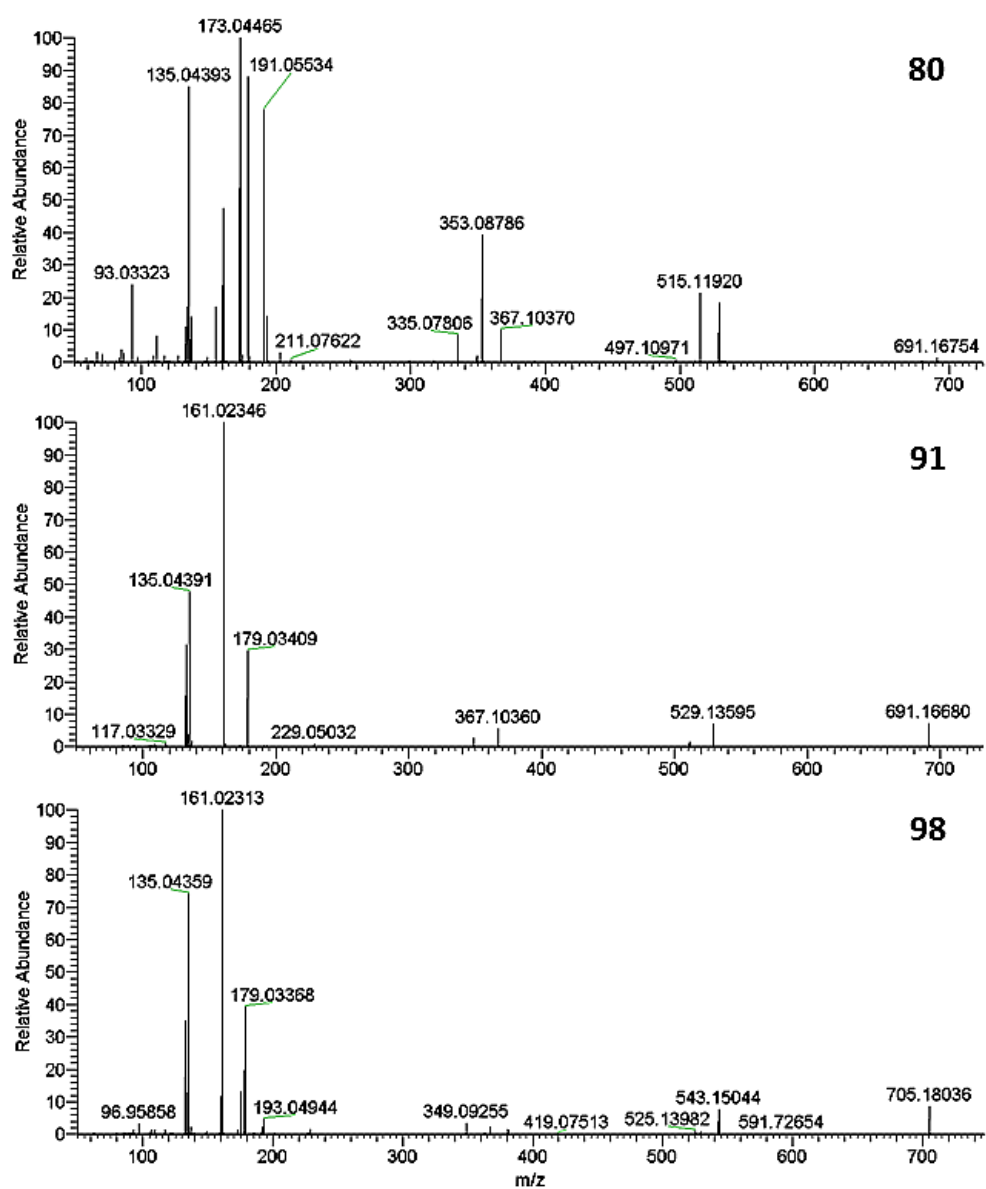


Fig. S19. The MS/MS spectrum of the $[M-H]^-$ ions for peaks 80, 91 and 98.

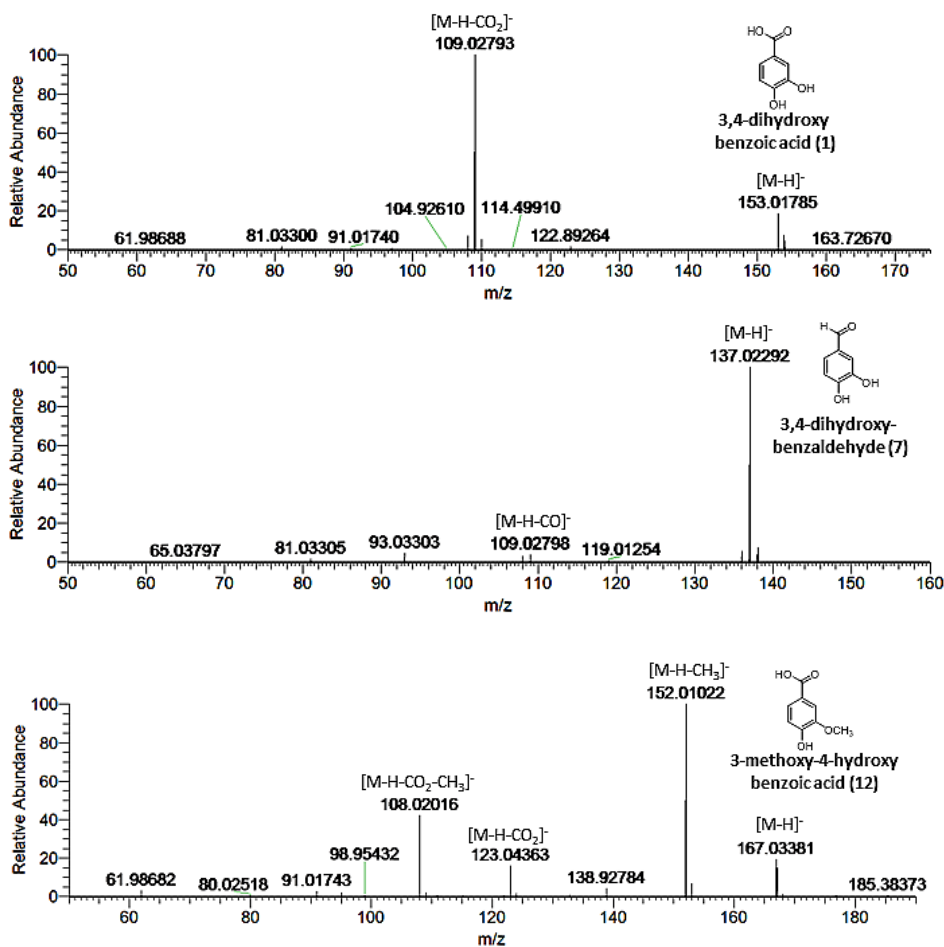


Fig. S20. The MS/MS spectrum of the [M-H]⁻ ions for 1, 7 and 12.

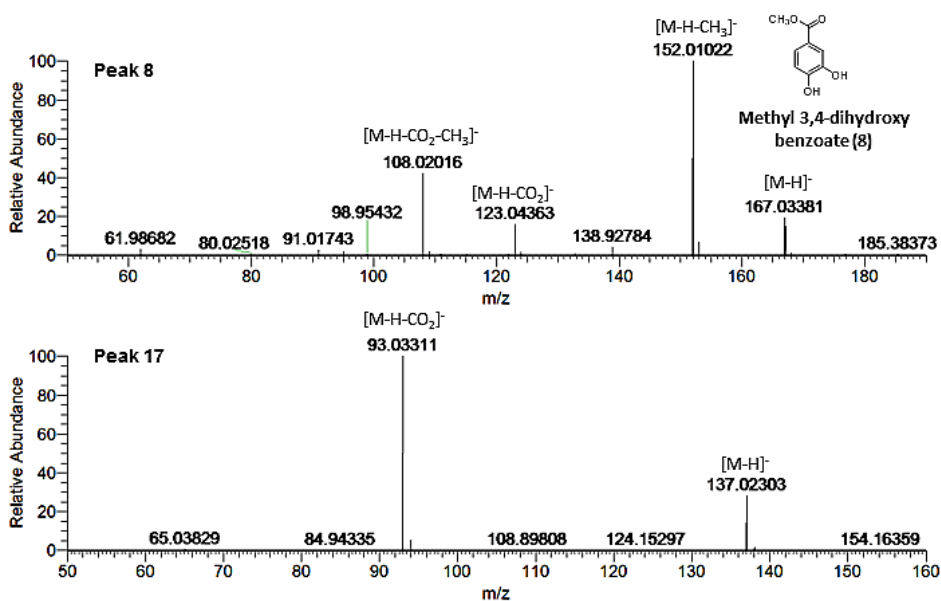
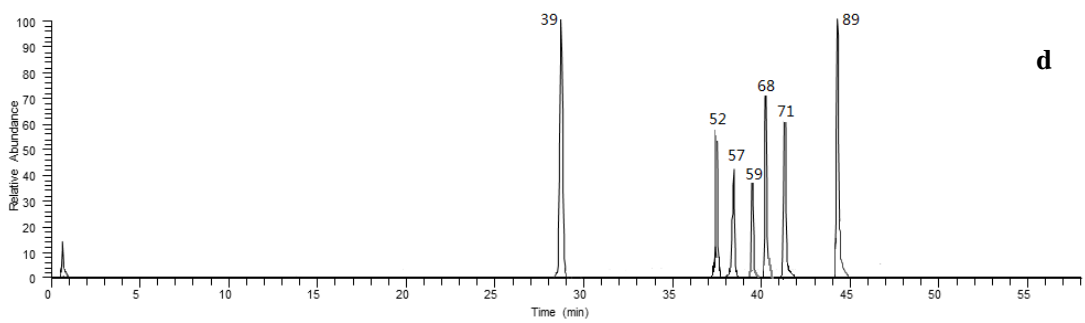
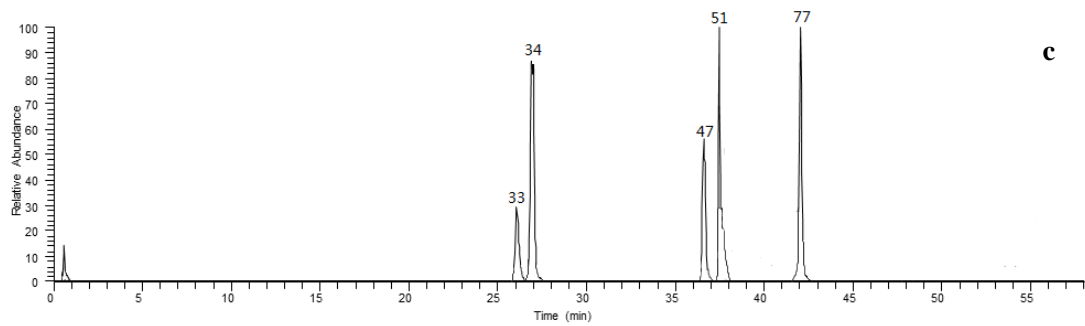
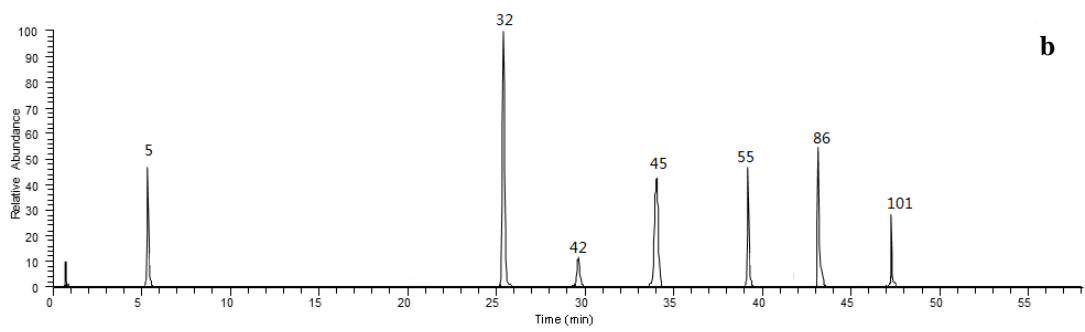
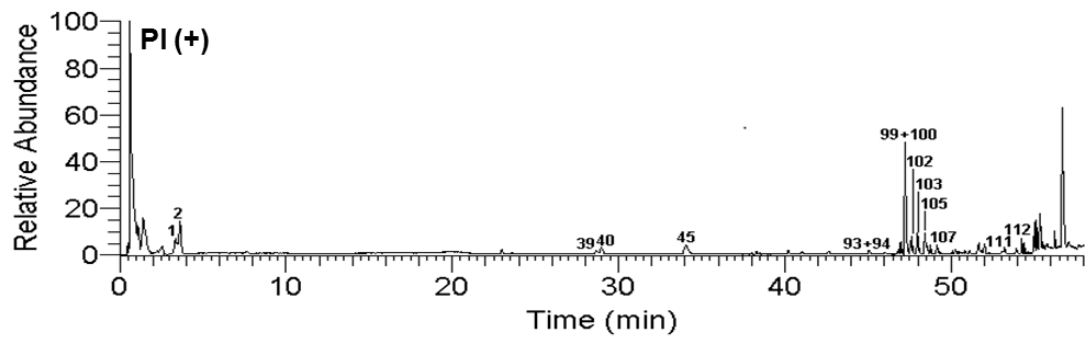
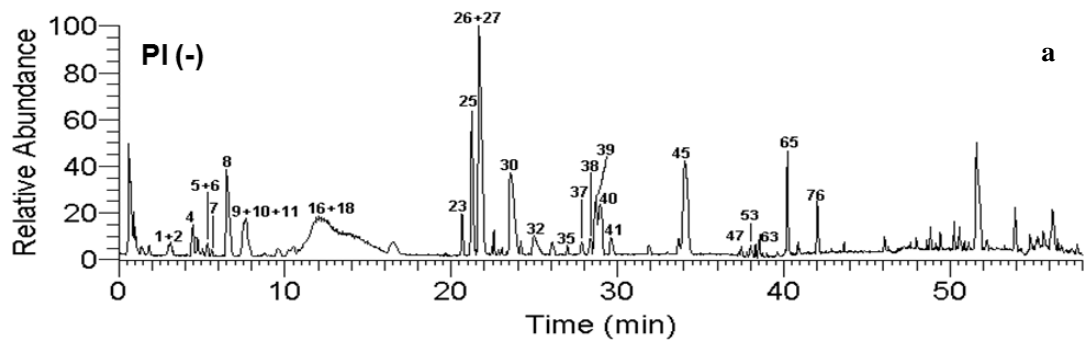
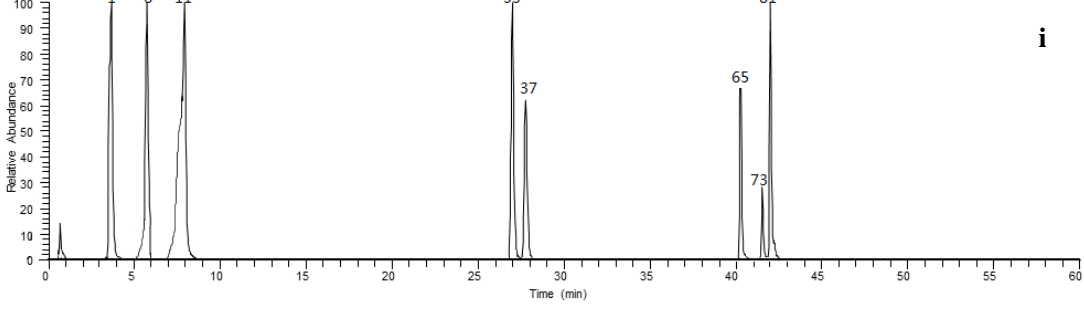
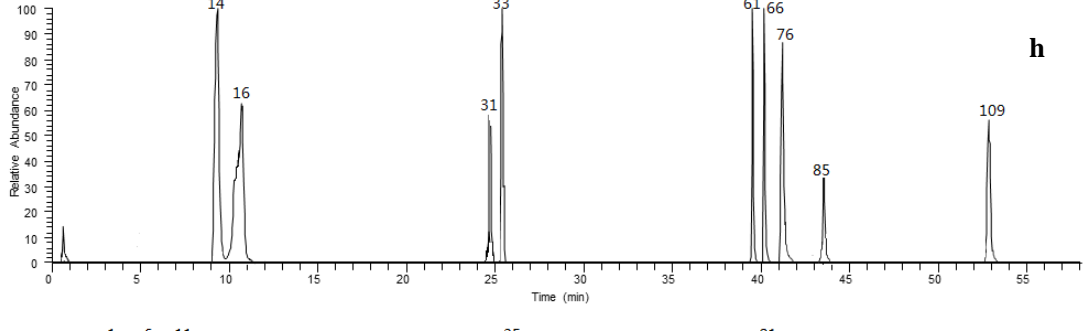
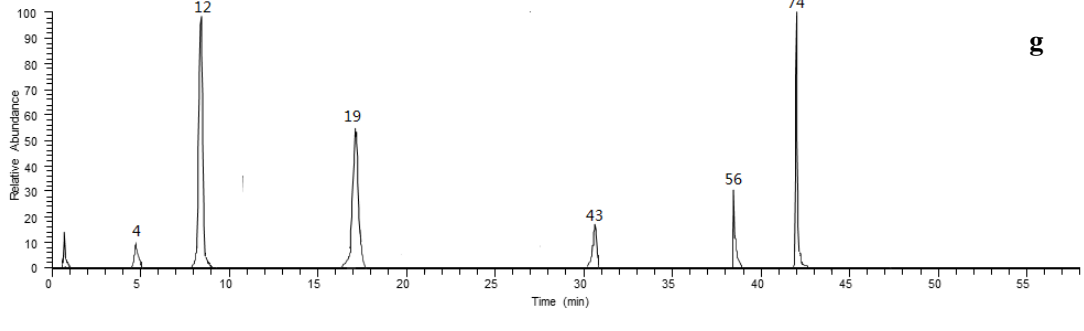
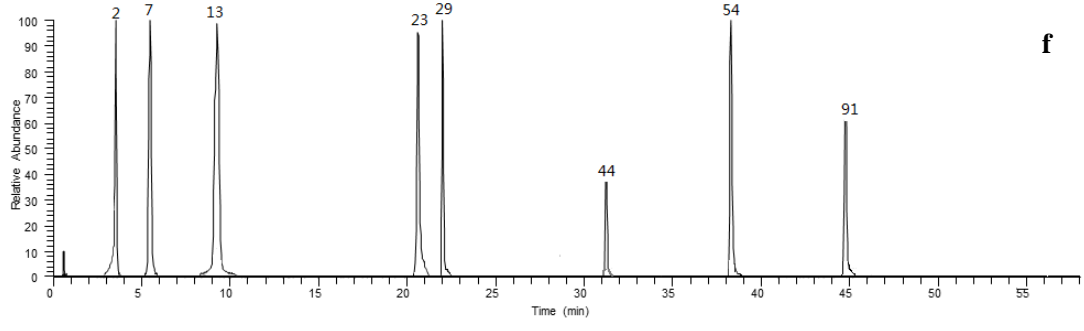
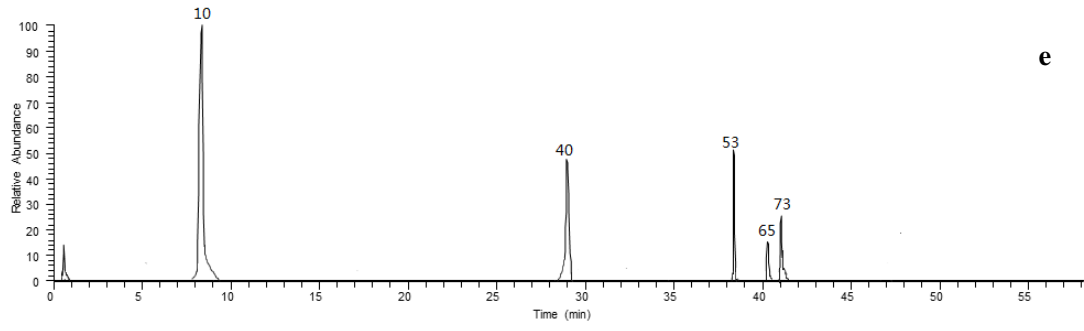


Fig. S21. The MS/MS spectrum of the [M-H]⁻ ions for 8, 17.





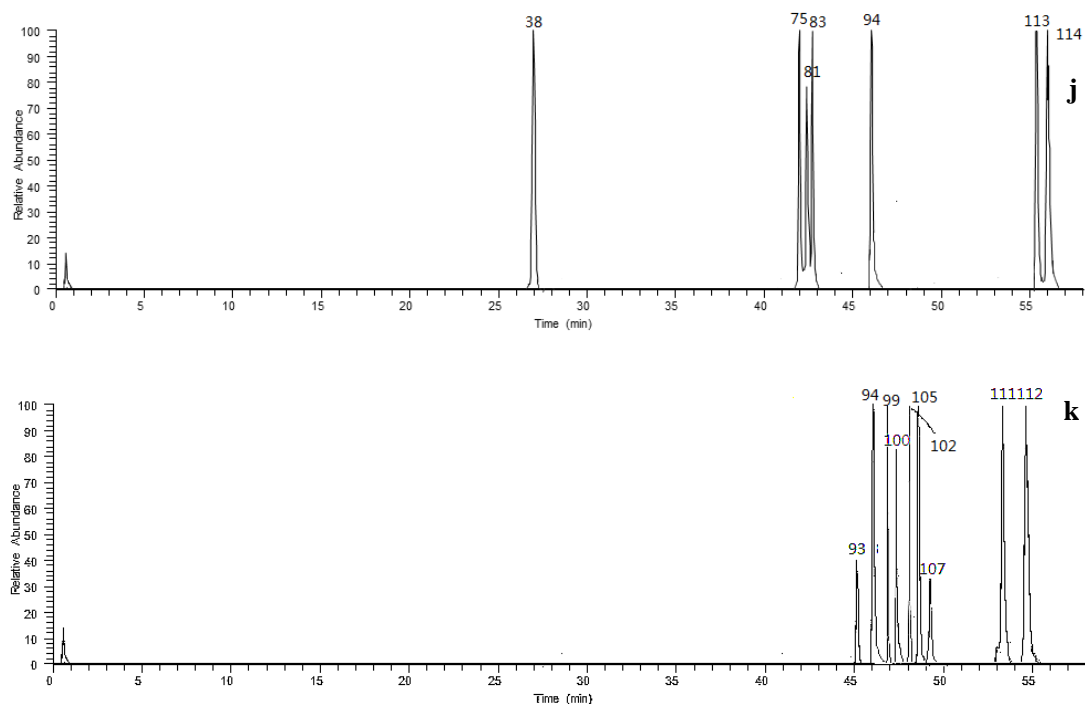


Fig. S22. The UPLC-MS analysis results of 67 standard references in negative and positive mode a: Base peak chromatograms of *P. indica* 70% EtOH extract on BEHC18 column in negative and positive mode; b: Base peak chromatograms of the mixed standard for 5, 32, 42, 45, 55, 86, and 101; c: Base peak chromatograms of the mixed standard for 33, 34, 47, 51, and 77; d: Base peak chromatograms of the mixed standard for 39, 52, 57, 59, 68, 71 and 89; e: Base peak chromatograms of the mixed standard for 10, 40, 53, 65, and 73; f: Base peak chromatograms of the mixed standard for 2, 7, 13, 23, 29, 44, 54, and 91; g: Base peak chromatograms of the mixed standard for 4, 12, 19, 43, 56, 74 and 102; h: Base peak chromatograms of the mixed standard for 14, 16, 31, 33, 61, 66, 76, 85 and 109; i: Base peak chromatograms of the mixed standard for 1, 6, 11, 35, 37, 65, 73 and 81; j: Base peak chromatograms of the mixed standard for 38, 75, 81, 83, 94, 113 and 114; k: Base peak chromatograms of the mixed standard for 93, 94, 99, 100, 102, 105, 107, 111 and 112