

Supplementary Material

for

Identification of the chemical compositions of Ponkan peel by ultra performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry

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Additional figures

Fig. S1 UPLC chromatogram of 8 standards. a: Eriocitrin; b: Narirutin; c: Hesperidin; d Rhoifolin; e: Isosakuranetin-7-O-rutinoside; f: Tangeretin; g: Nobiletin; h: Sinensetin.

Fig. S2 The negative MS (a1, b1, c1, d1, e1) and MS² (a2, b2, c2, d2, e2) spectra of five flavonoids. a: Eriocitrin; b: Narirutin; c: Hesperidin; d Rhoifolin; e: Isosakuranetin-7-O-rutinoside.

Fig. S3 The positive MS (f1, g1, h1) and MS² (f2, g2, h2) spectra of three polymethoxyflavones. f: Tangeretin; g: Nobiletin; h: Sinensetin.

Fig. S4 The enlarged BPI chromatogram (2.20 min - 2.83min) in the negative ion mode.

Fig. S5 The negative MS spectrum of compound 6.

Fig. S6 The enlarged BPI chromatogram (3.74min - 4.16min) in the negative ion mode.

Fig. S7 The negative MS spectrum of compound 17.

Fig. S8 The enlarged BPI chromatogram (4.4min - 5.08min) in the negative ion mode.

Fig. S9 The negative MS spectrum of compound 21.

Fig. S10 The negative MS² spectrum of compound 24.

Fig. S11 The negative MS² spectrum of compound 26.

Fig. S12 The negative MS² spectrum of compound 27.

Channel name: PDA 283@1.2

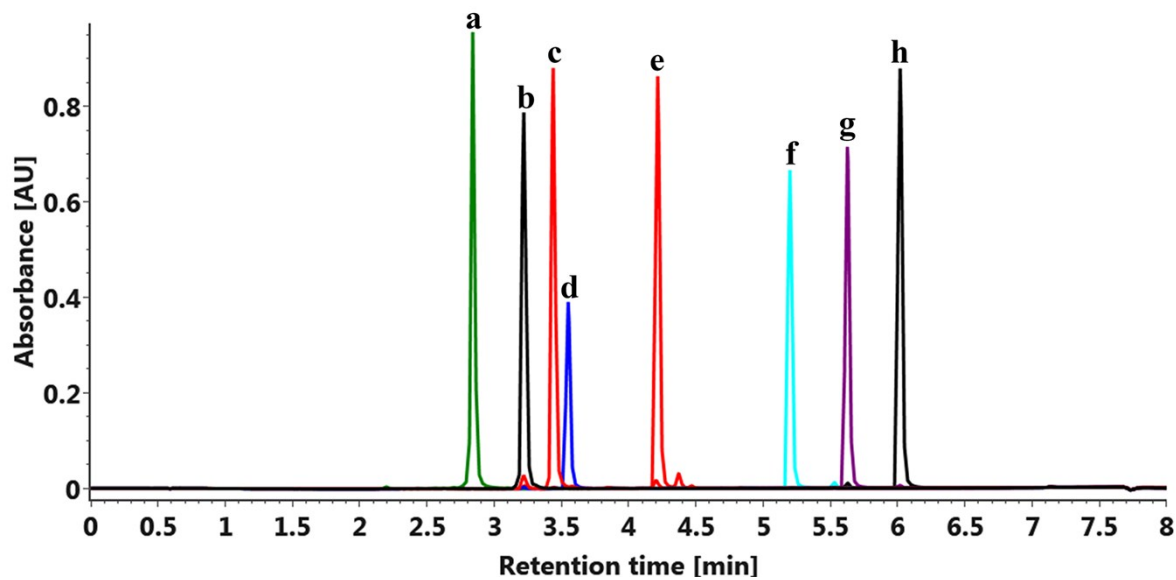


Fig. S1 UPLC chromatogram of 8 standards. a: Eriocitrin; b: Narirutin; c: Hesperidin; d: Rhoifolin; e: Isosakuranetin-7-O-rutinoside; f: Tangeretin; g: Nobiletin; h: Sinensetin.

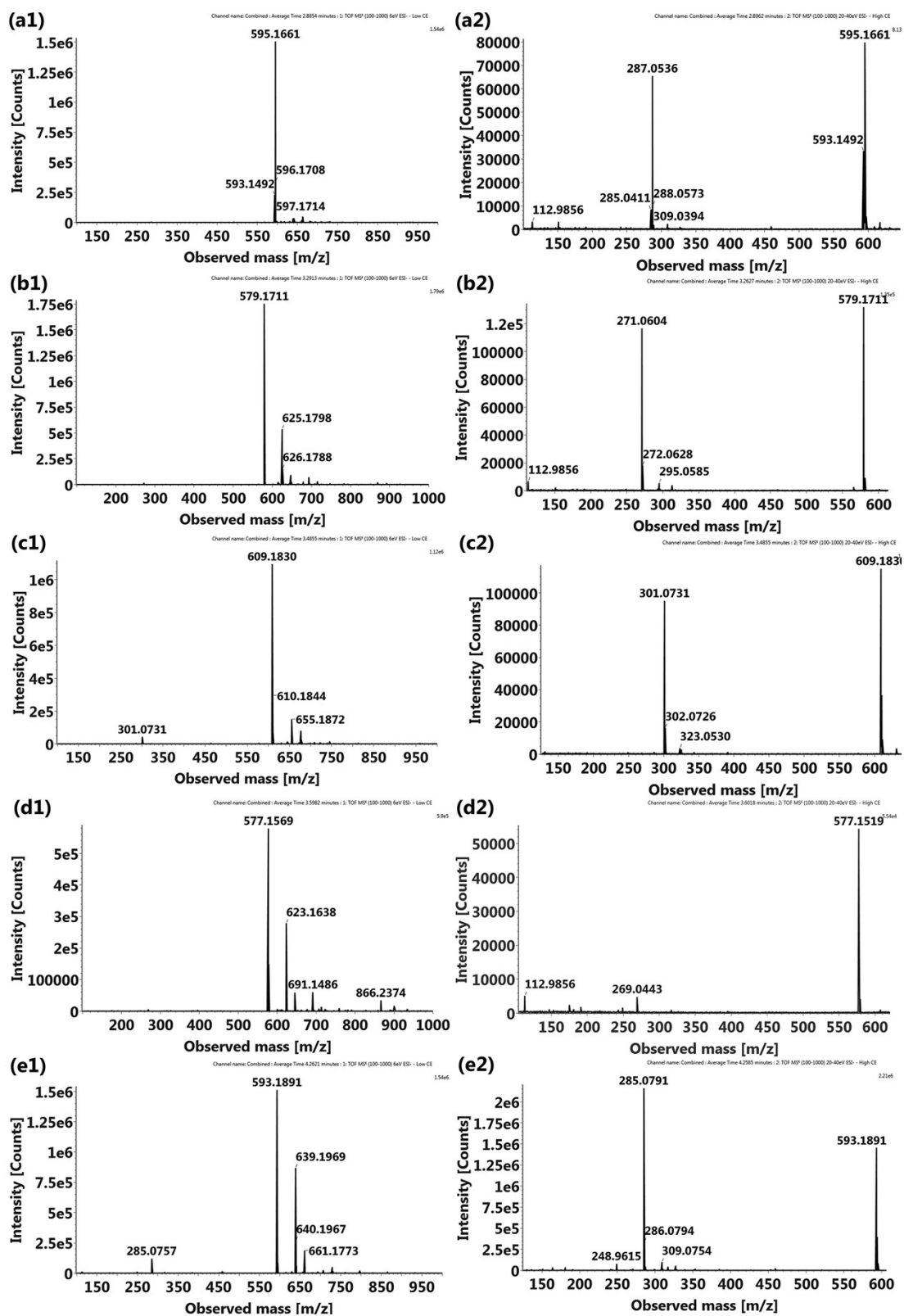


Fig. S2 The negative MS (a1, b1, c1, d1, e1) and MS² (a2, b2, c2, d2, e2) spectra of five flavonoids. a: Eriocitrin; b: Narirutin; c: Hesperidin; d: Rhoifolin; e: Isosakuranetin-7-O-rutinoside.

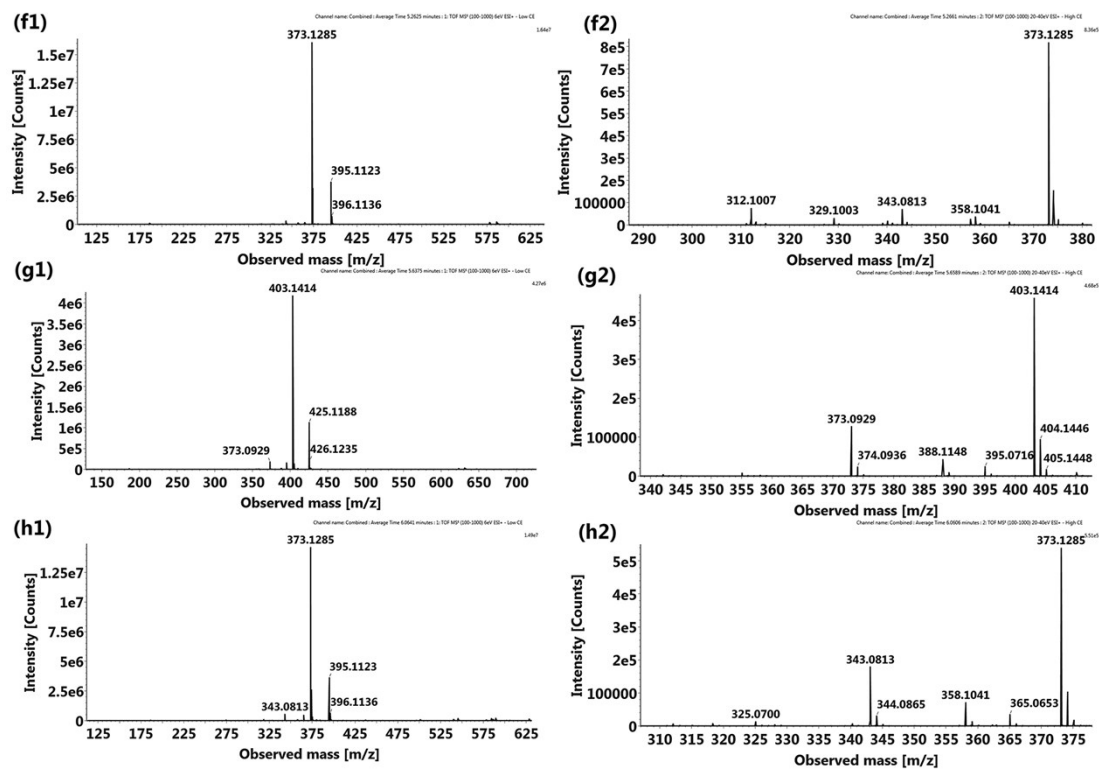


Fig. S3 The positive MS (f1, g1, h1) and MS² (f2, g2, h2) spectra of three polymethoxyflavones. f: Tangeretin; g: Nobiletin; h: Sinensetin.

Item name: Ponkan peel
 Channel name: 1: TOF MS^E (100-1000) 6eV ESI⁻ - Low CE (BPI)

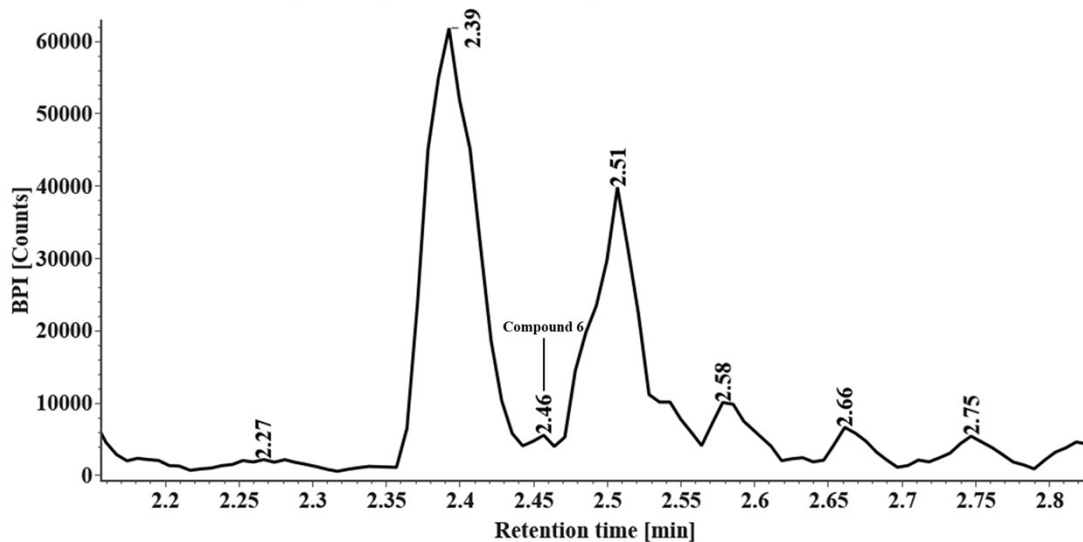


Fig. S4 The enlarged BPI chromatogram (2.20 min - 2.83min) in the negative ion mode.

Channel name: Combined : Average Time 2.4603 minutes : 1: TOF MS^E (100-10...

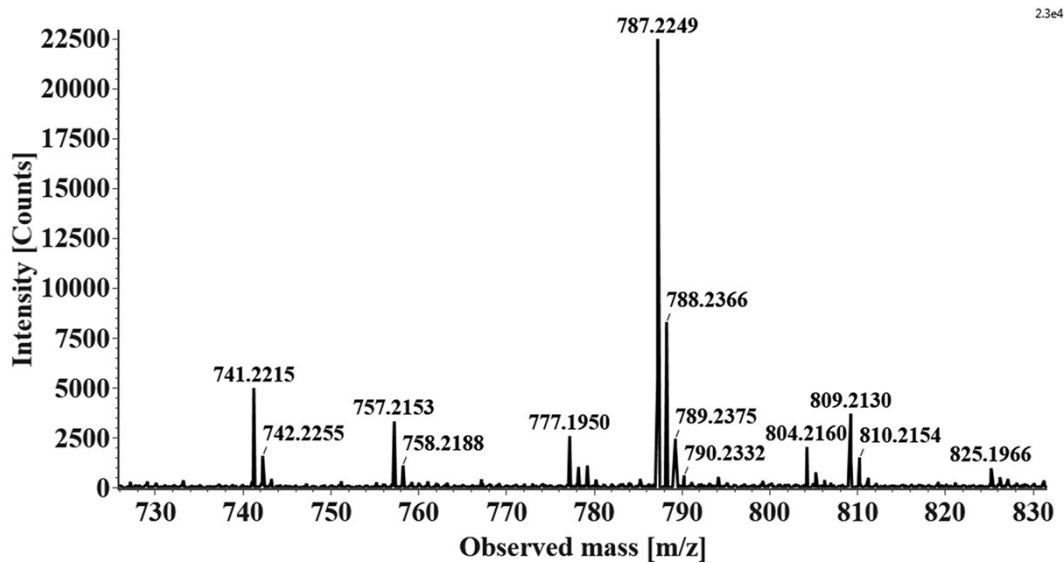


Fig. S5 The negative MS spectrum of compound 6.

Item name: Ponkan peel

Channel name: 1: TOF MS^E (100-1000) 6eV ESI- - Low CE (BPI)

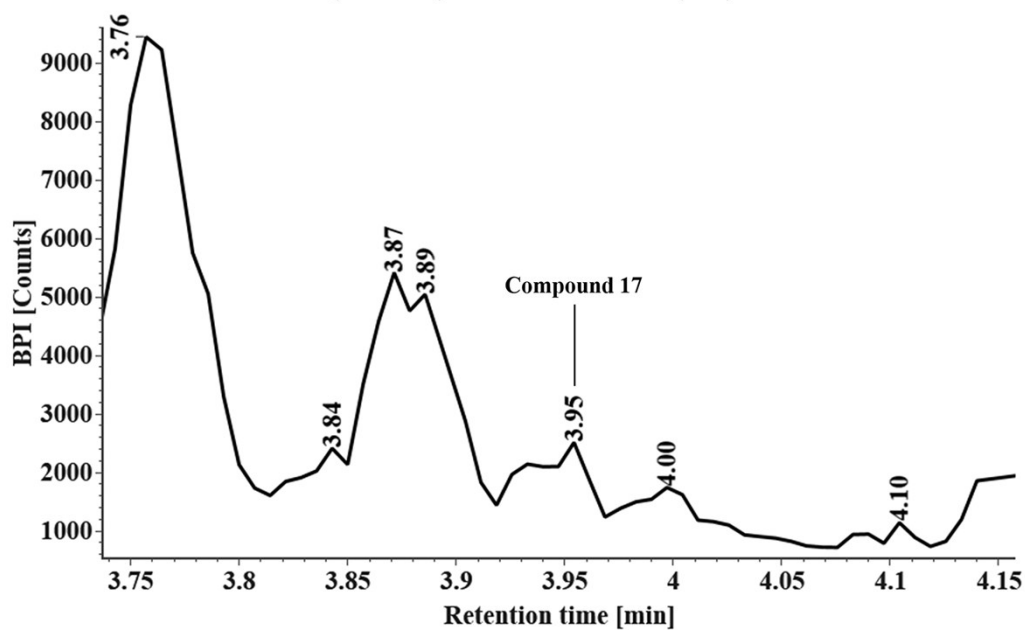


Fig. S6 The enlarged BPI chromatogram (3.74min - 4.16min) in the negative ion mode.

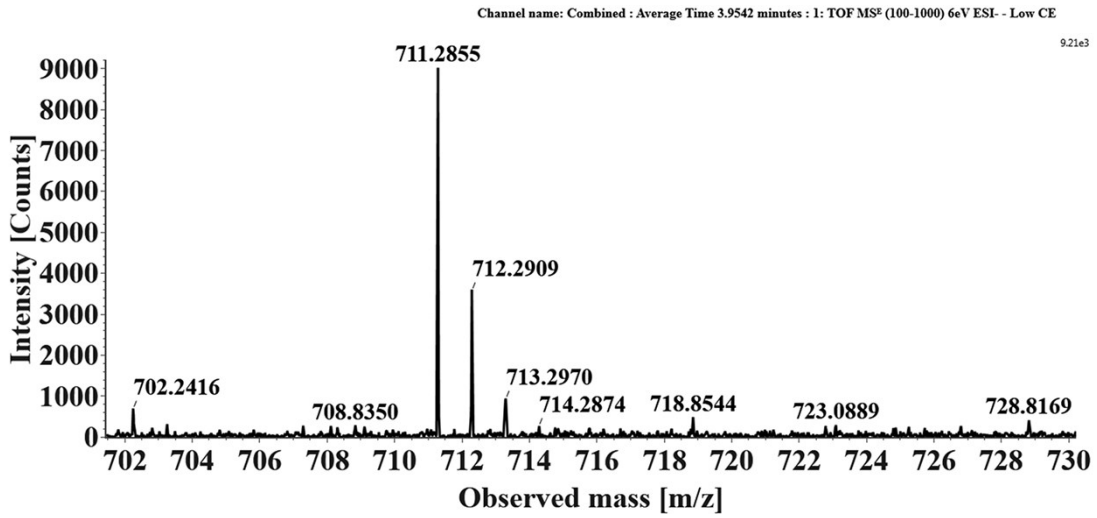


Fig. S7 The negative MS spectrum of compound 17.

Item name: Ponkan peel

Channel name: 1: TOF MS^E (100-1000) 6eV ESI- - Low CE (BPI)

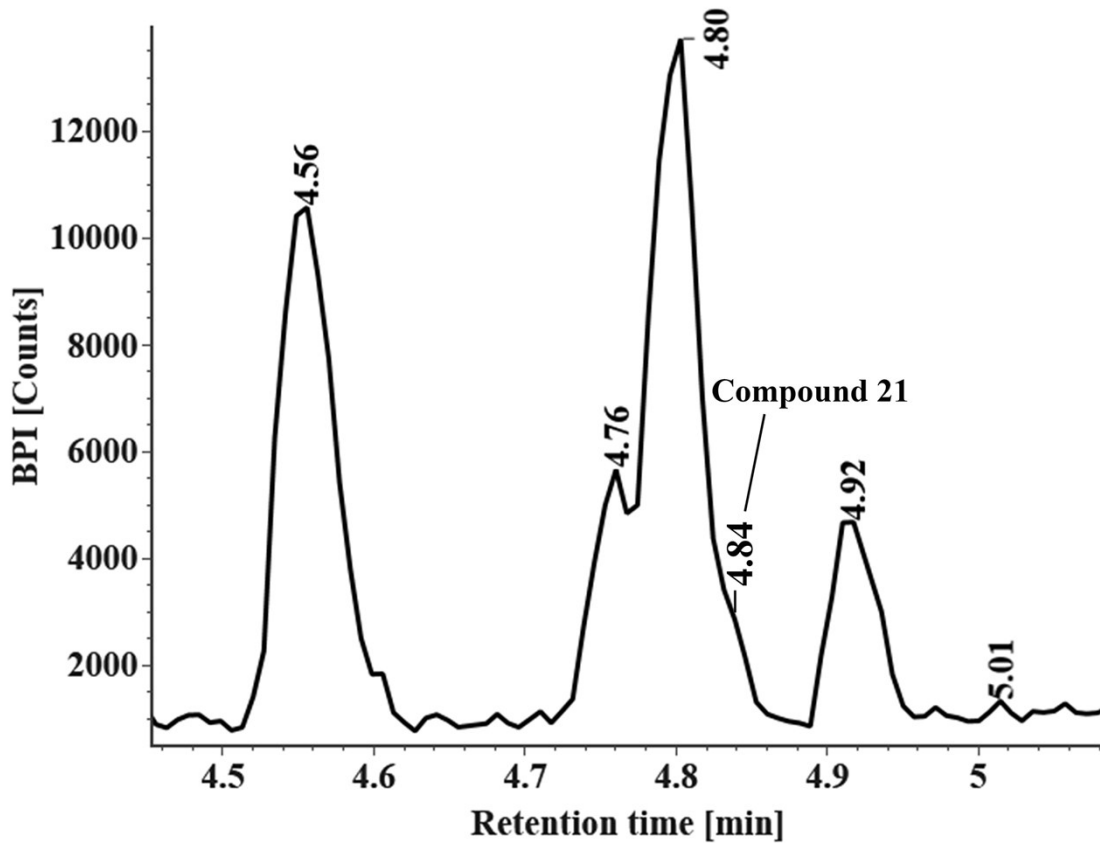


Fig. S8 The enlarged BPI chromatogram (4.4min - 5.08min) in the negative ion mode.

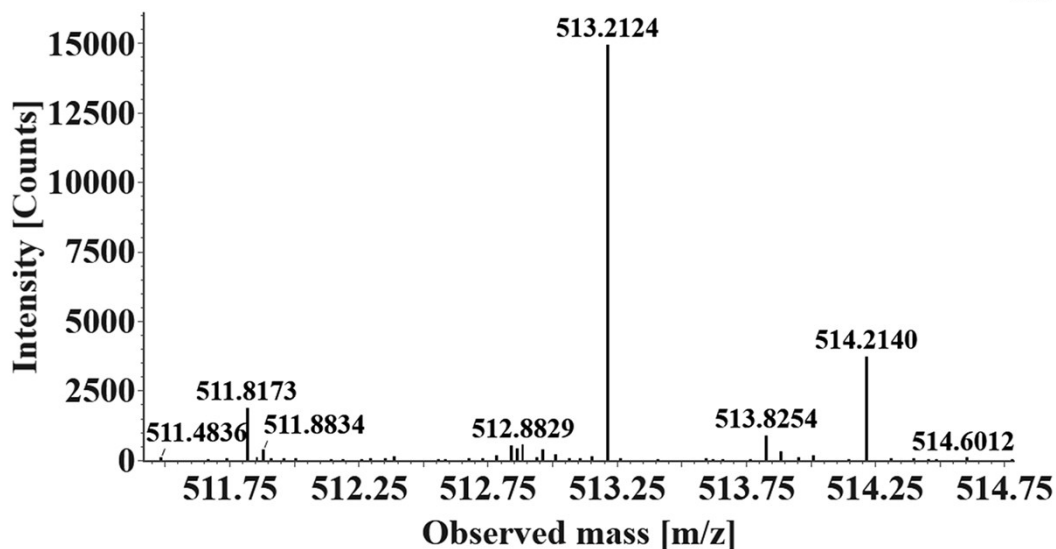


Fig. S9 The negative MS spectrum of compound 21.

Item name: Ponkan peel
Description:

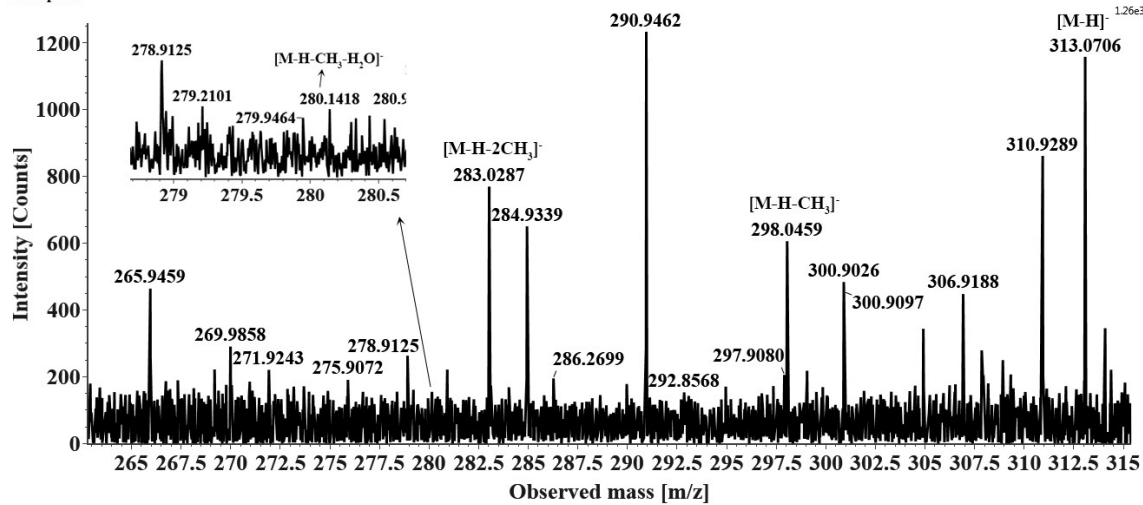


Fig. S10 The negative MS² spectrum of compound 24.

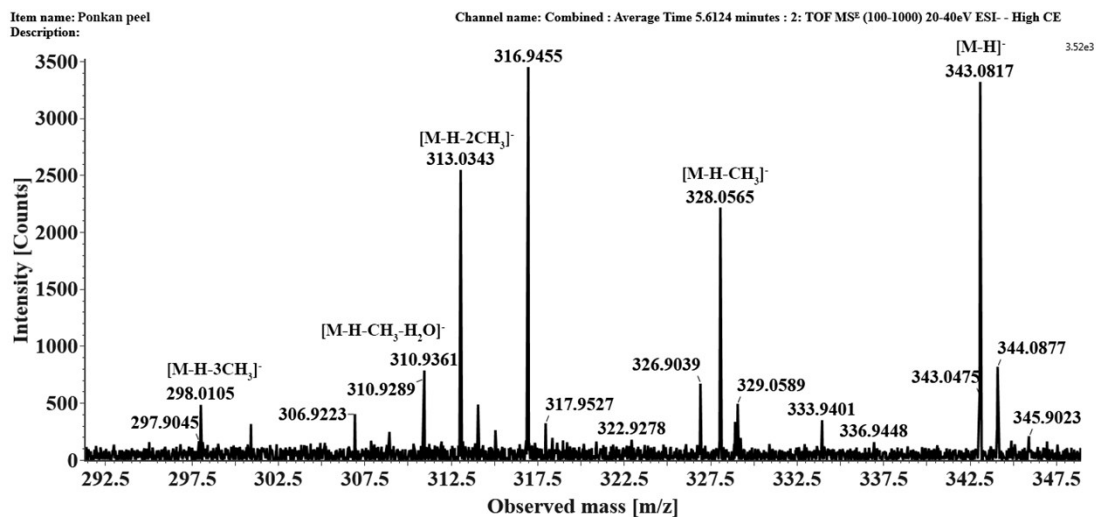


Fig. S11 The negative MS² spectrum of compound 26.

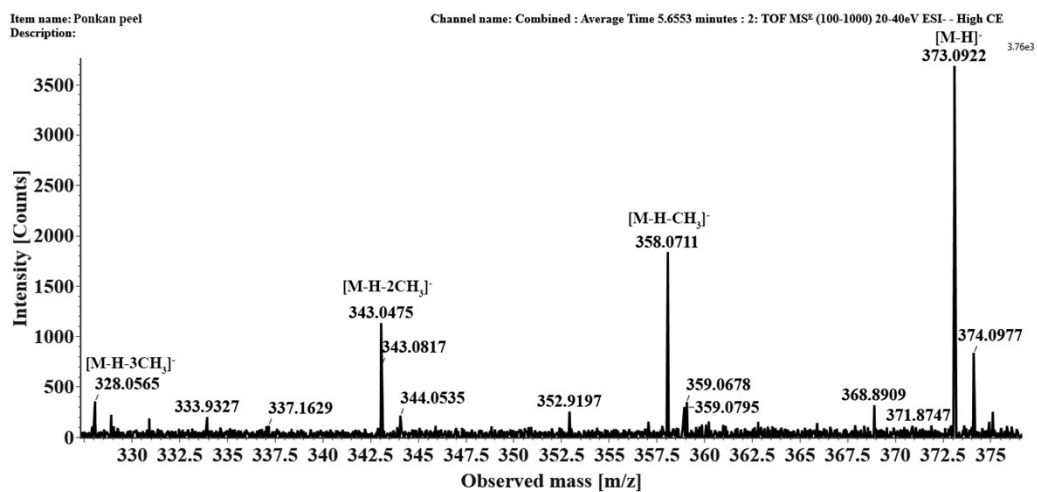


Fig. S12 The negative MS² spectrum of compound 27.