Exploring the efficacious subfractions and underlying mechanisms of Herba Siegesbeckiae against myocardial ischemia/reperfusion injury via UCHL5/NLRP3 pathway

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Supplementary Materials

Contents

All sample data collected by UPLC-HRMS were processed using Compound Discoverer software. Each compound was initially identified by comparing the data with the published literature, the online database mzCloud, and the multistage fragment mass spectra containing the compounds in PubChem. Among them, compounds 1-5 and 7 were preliminarily demonstrated in the published literature[1-5], compounds 6-10 were preliminarily proved by comparing the secondary mass spectrum information in mzCloud database[6,7], and compound 11 was preliminarily determined by comparing the secondary mass spectrum information with the PubChem database[8].

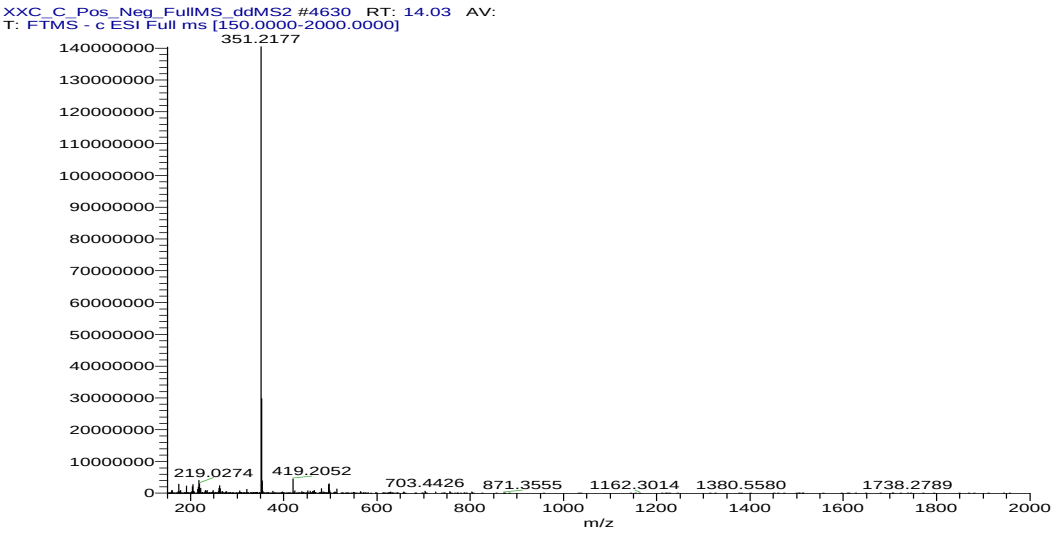

Fig.S1. Primary mass spectrometry of ent-2*β*,15,16-trihydroxypimar-8(14)-en-18-oic acid (Compound 1).

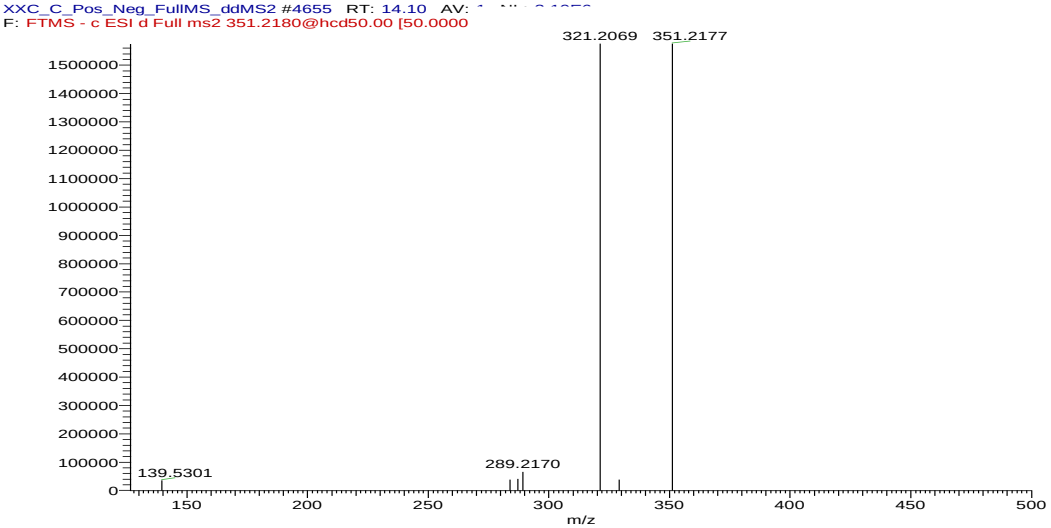

Fig.S2. Secondary mass spectrometry of ent-2*β*,15,16-trihydroxypimar-8(14)-en-18-oic acid (Compound 1).

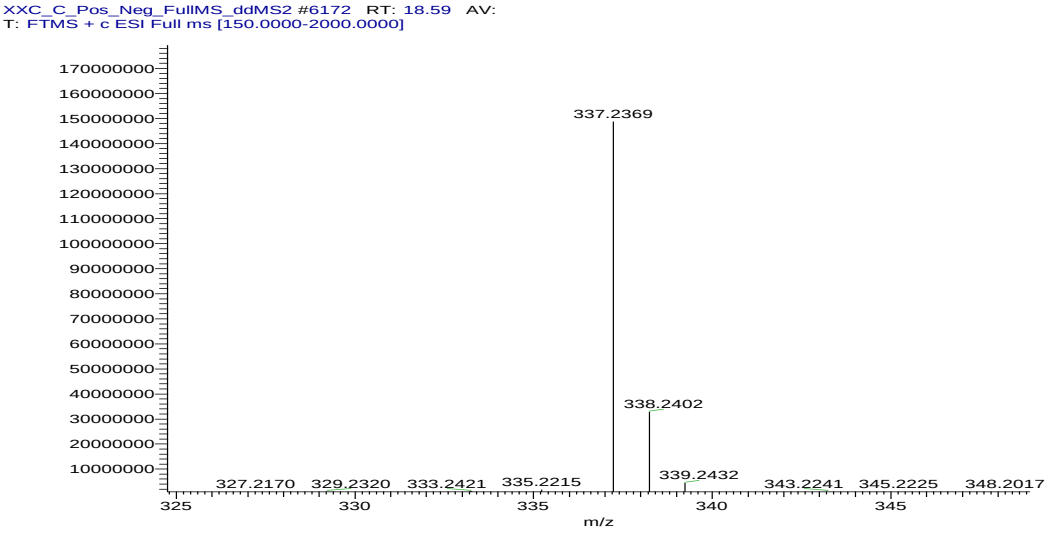

Fig.S3. Primary mass spectrometry of ent-15-oxo-2β,16,19-trihydroxypimar-8(14)-ene (Compound 2).

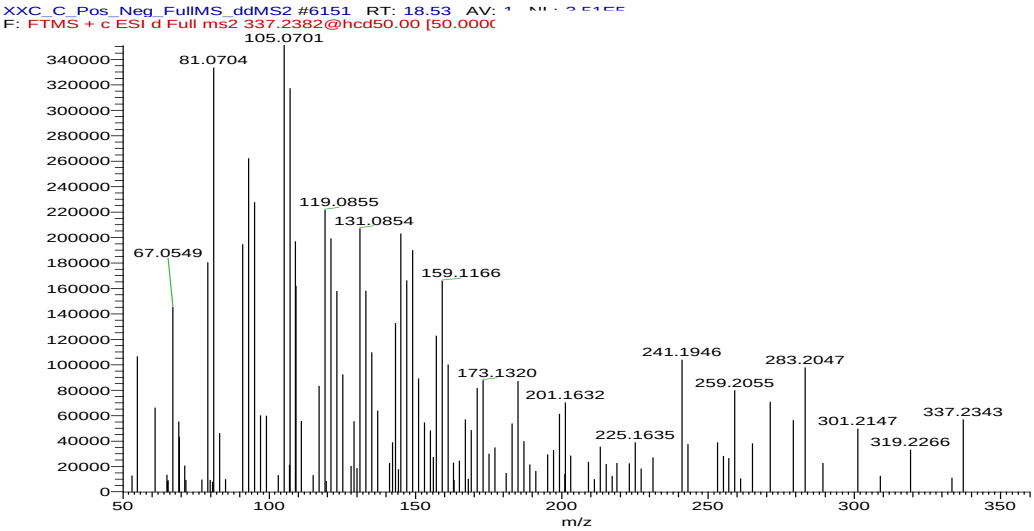

Fig.S4. Secondary mass spectrometry of ent-15-oxo-2β,16,19-trihydroxypimar-8(14)-ene (Compound 2).

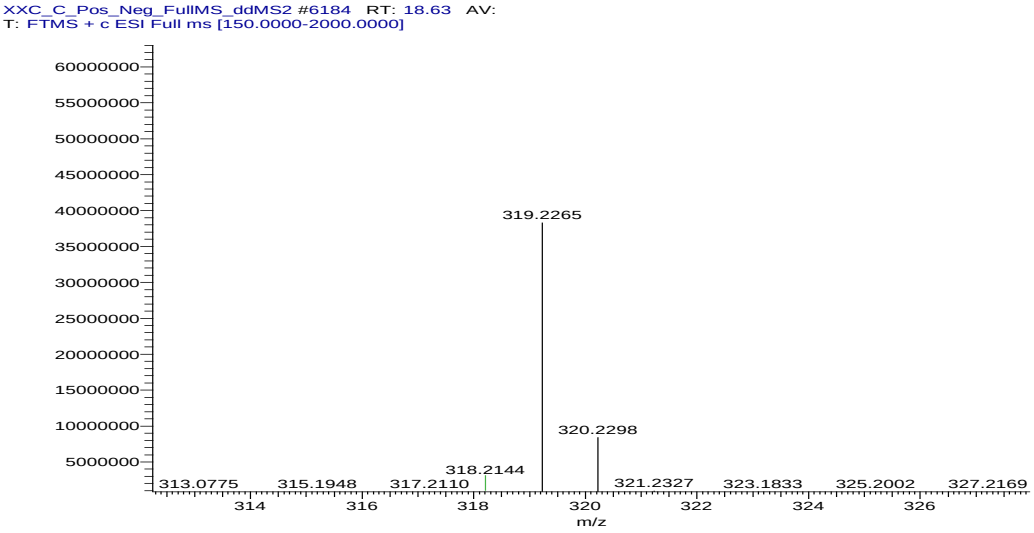

Fig.S5. Primary mass spectrometry of ent-15,16-dihydroxypimar-1,8(14)-dien-3-one (Compound 3).

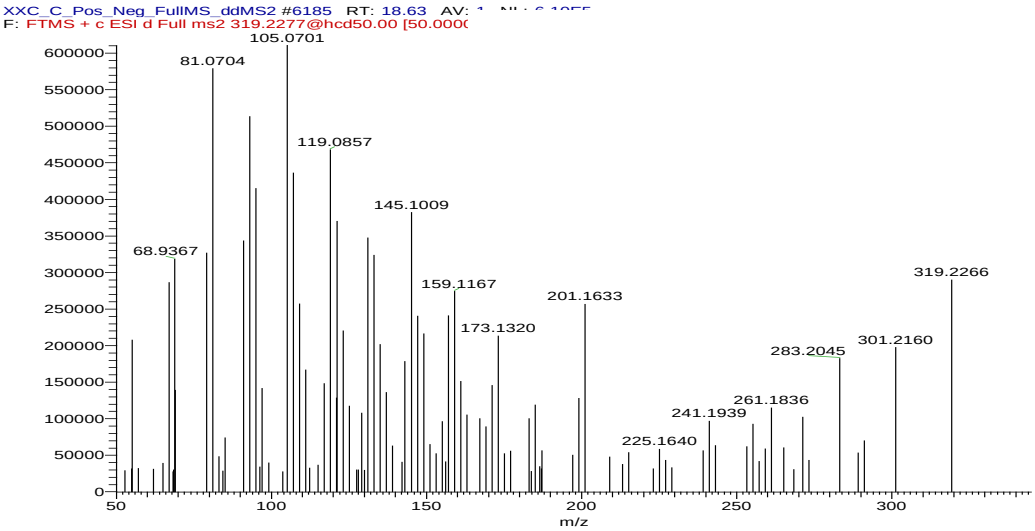

Fig.S6. Secondary mass spectrometry of ent-15,16-dihydroxypimar-1,8(14)-dien-3-one (Compound 3).

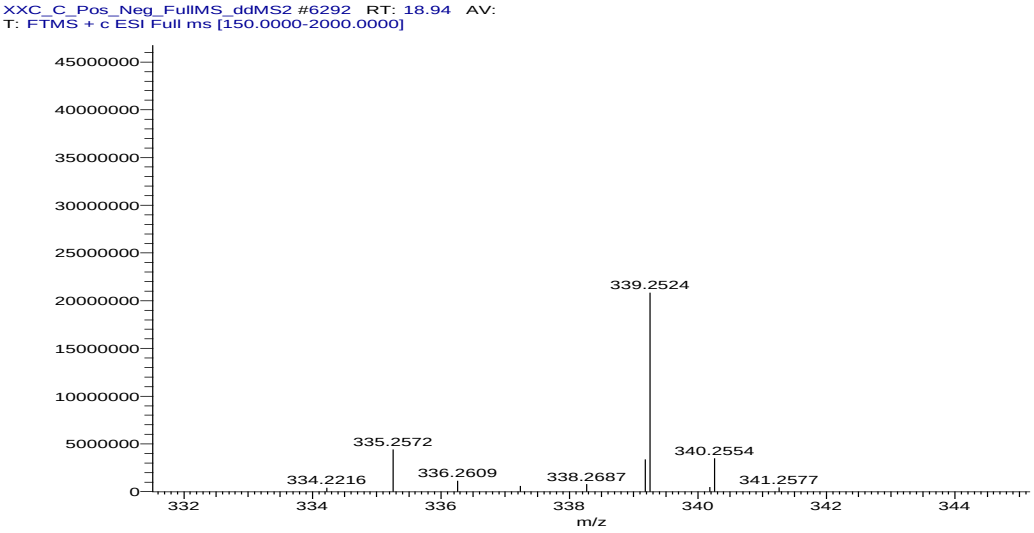

Fig.S7. Primary mass spectrometry of kirenol (Compound 4).

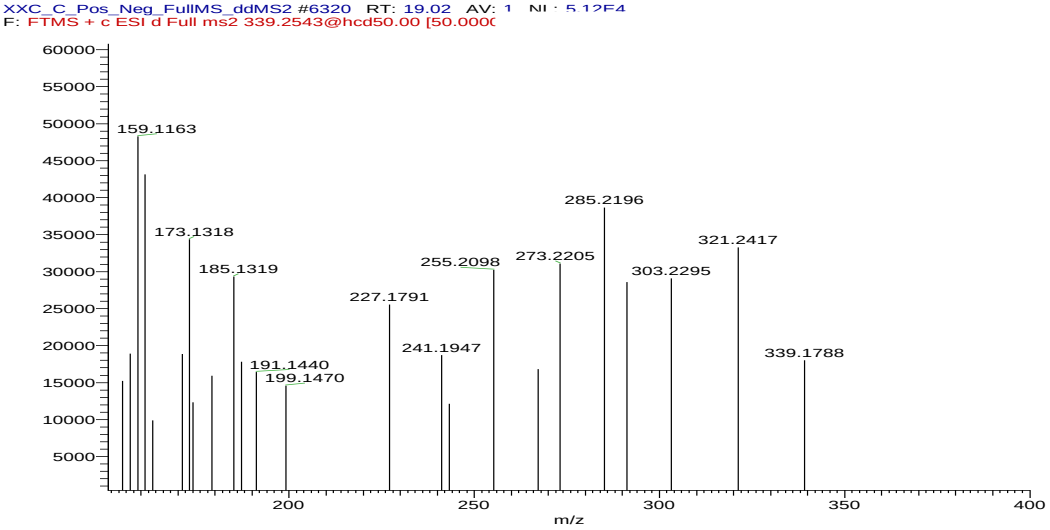

Fig.S8. Secondary mass spectrometry of kirenol (Compound 4).

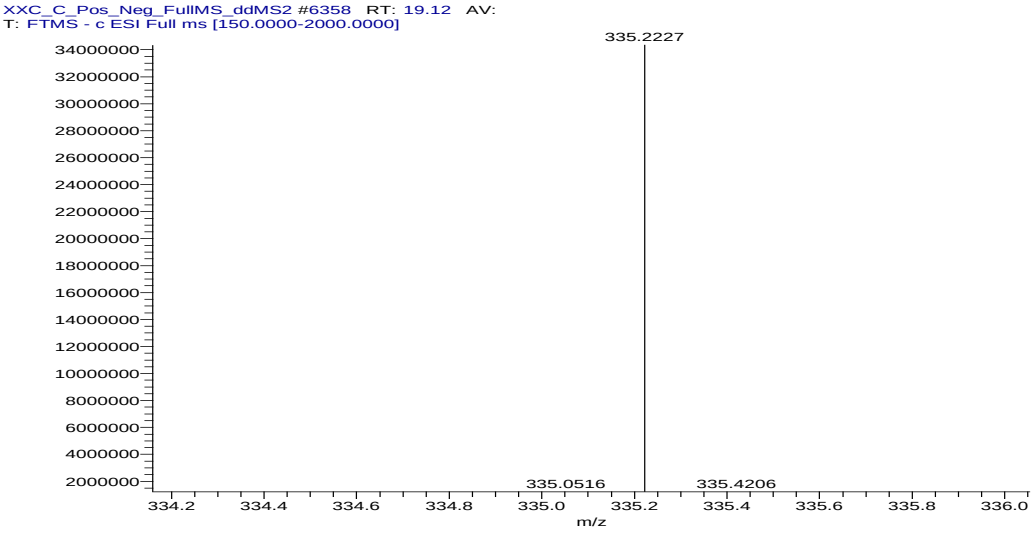

Fig.S9. Primary mass spectrometry of siegesbeckic acid (Compound 5).

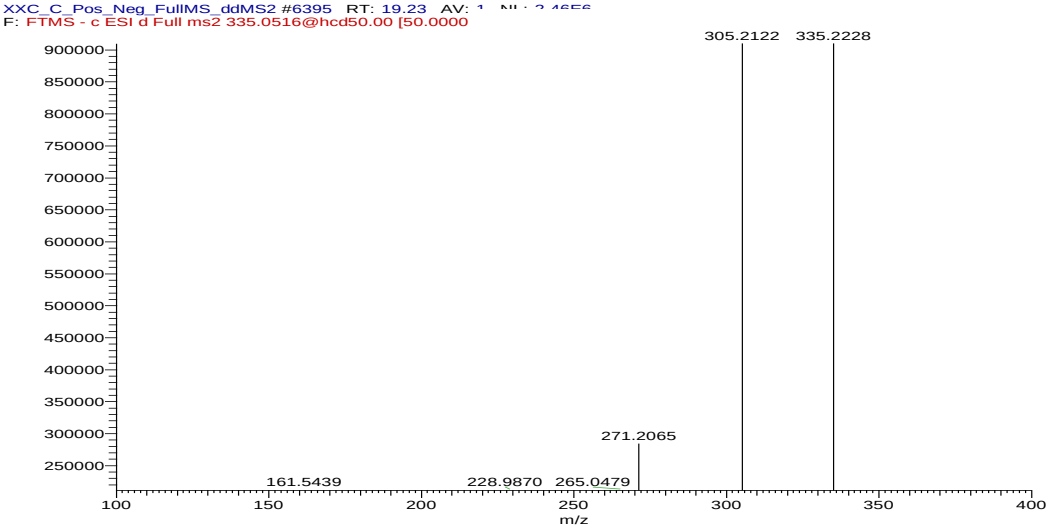

Fig.S10. Secondary mass spectrometry of siegesbeckic acid (Compound 5).

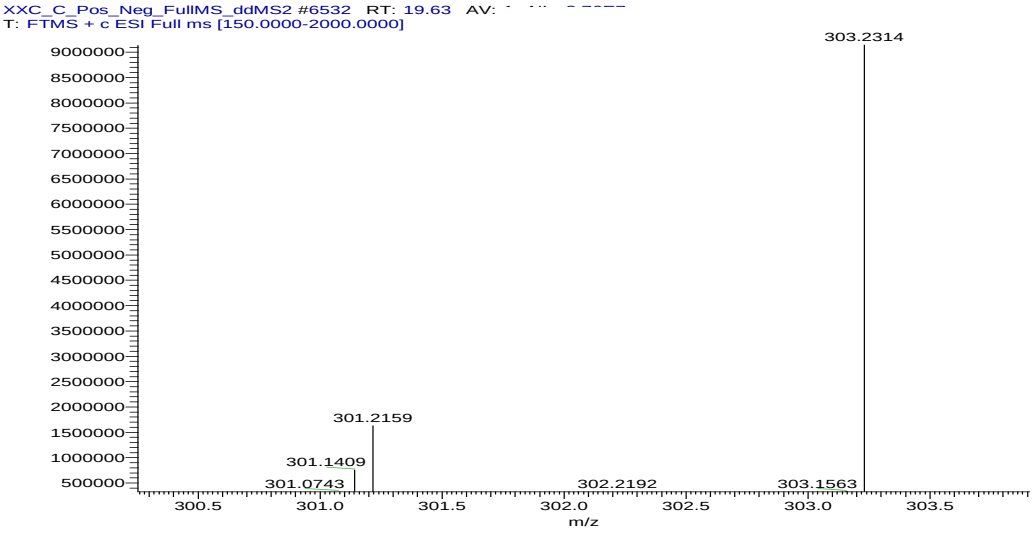

Fig.S11. Primary mass spectrometry of eicosapentaenoic acid (Compound 6).

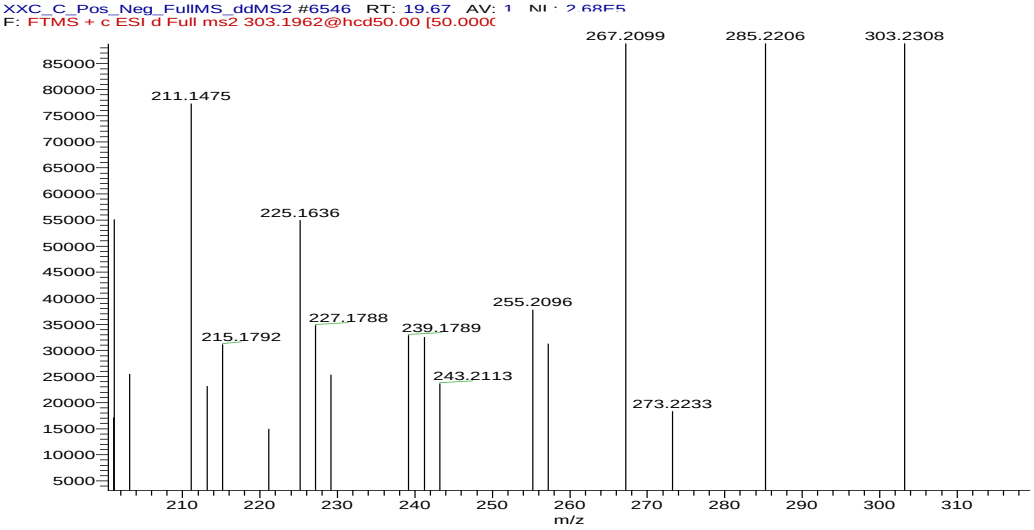

Fig.S12. Secondary mass spectrometry of eicosapentaenoic acid (Compound 6).

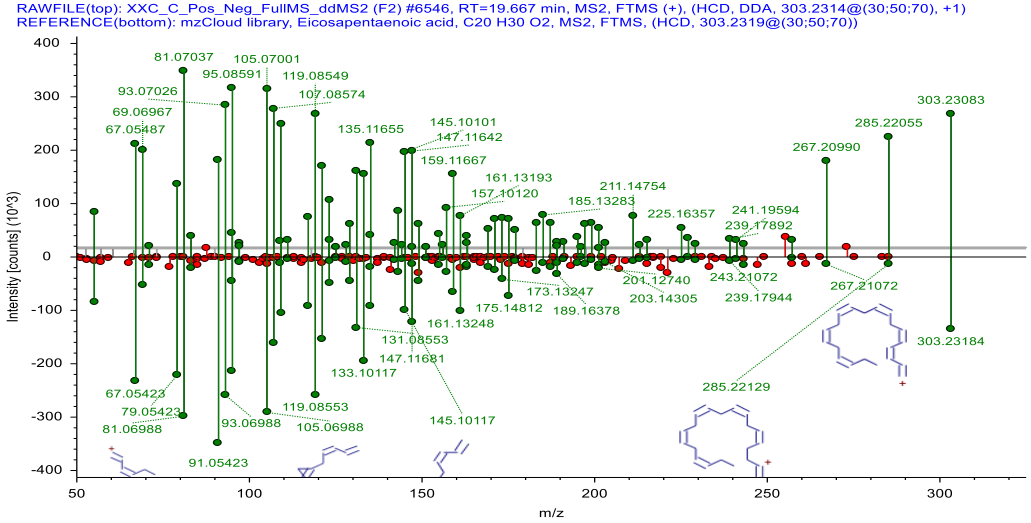

Fig.S13. Comparison of secondary mass spectra of eicosapentaenoic acid (compound 6) standards retrieved by UPLC-HRMS and mzCloud.

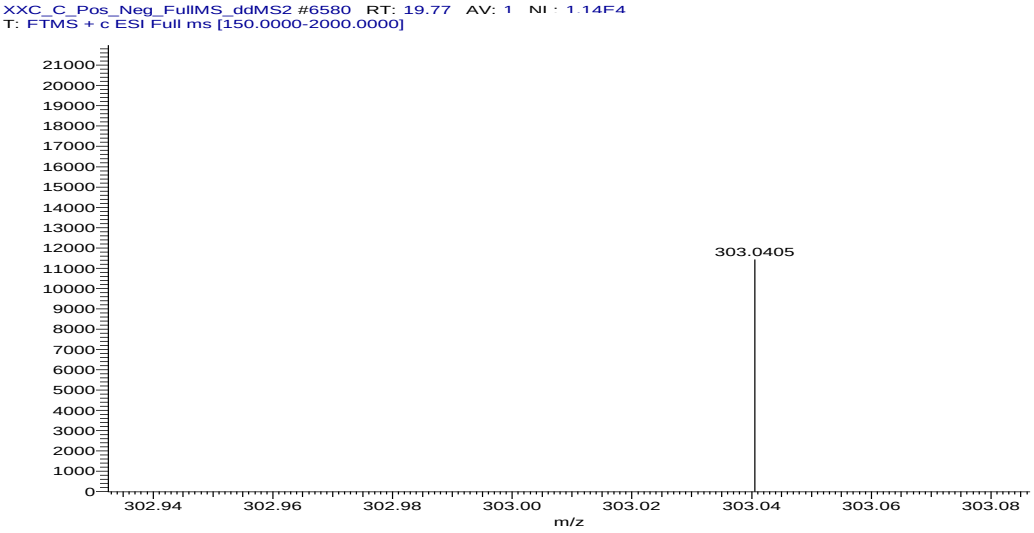

Fig.S14. Primary mass spectrometry of quercetin (Compound 7).

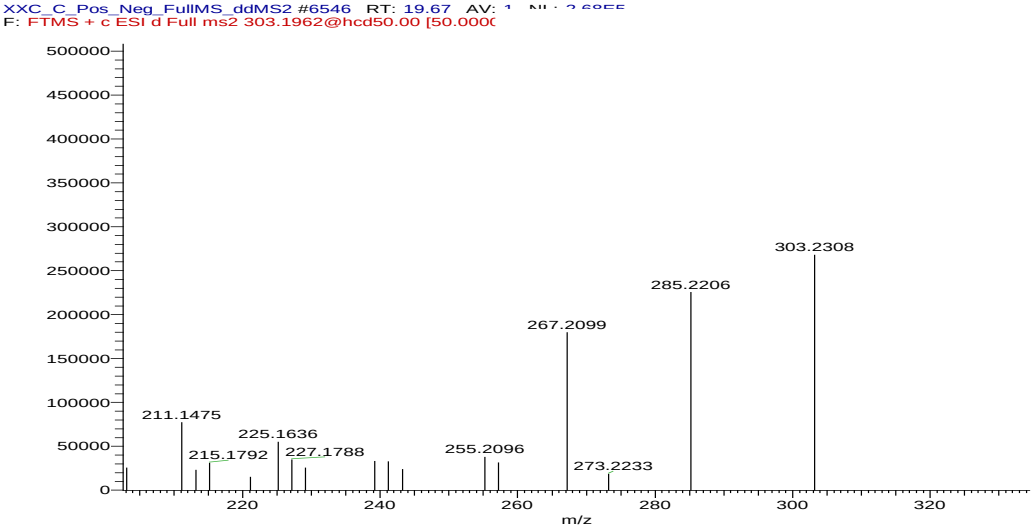

Fig.S15. Secondary mass spectrometry of quercetin (Compound 7).

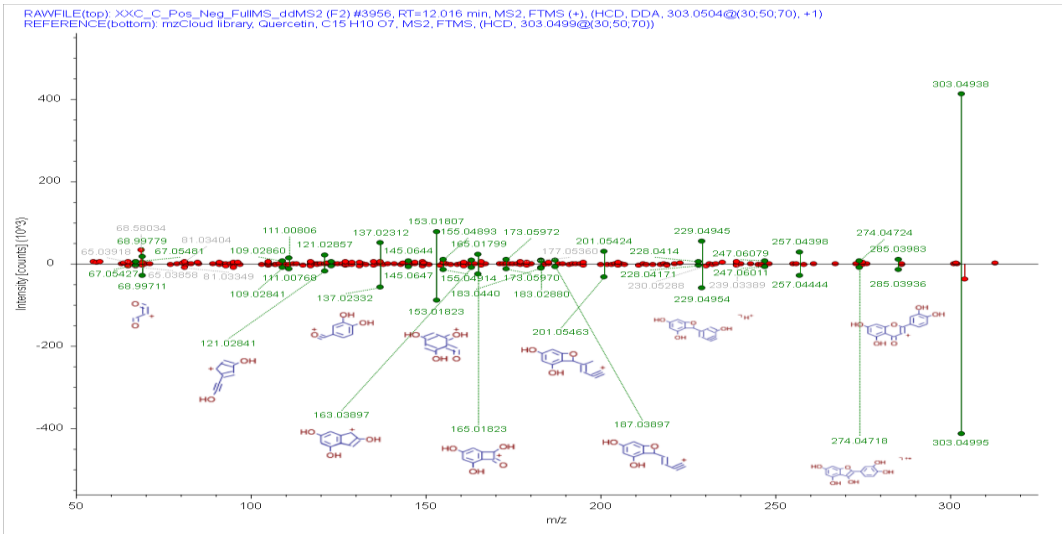

Fig.S16. Comparison of secondary mass spectra of quercetin (compound 7) standards retrieved by UPLC-HRMS and mzCloud.

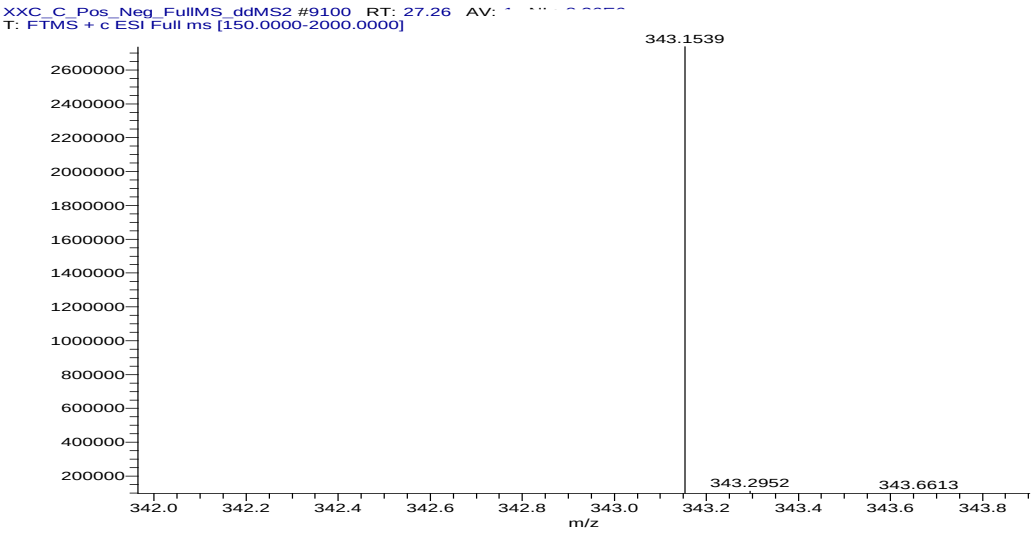

Fig.S17. Primary mass spectrometry of oxydipropyl dibenzoate (Compound 8).

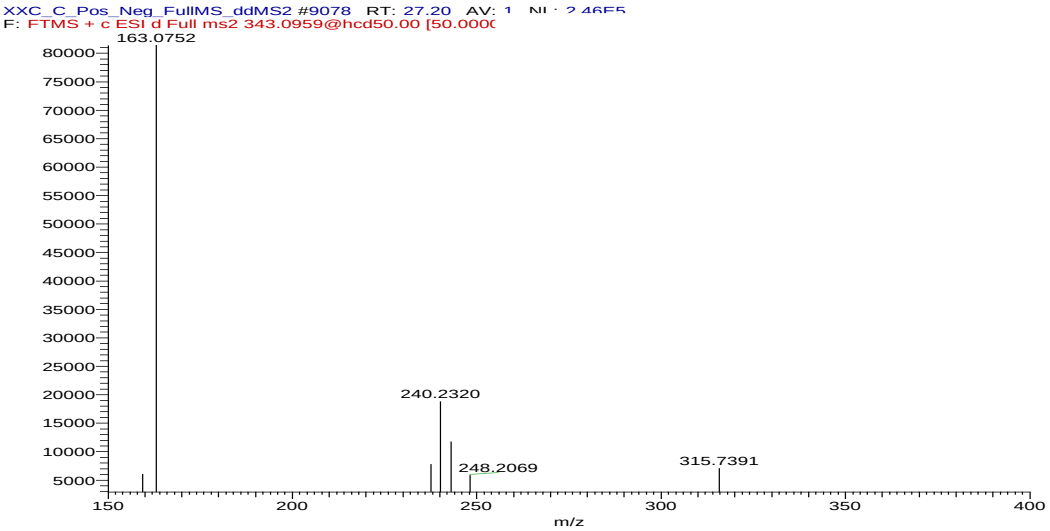

Fig.S18. Secondary mass spectrometry of oxydipropyl dibenzoate (Compound 8).

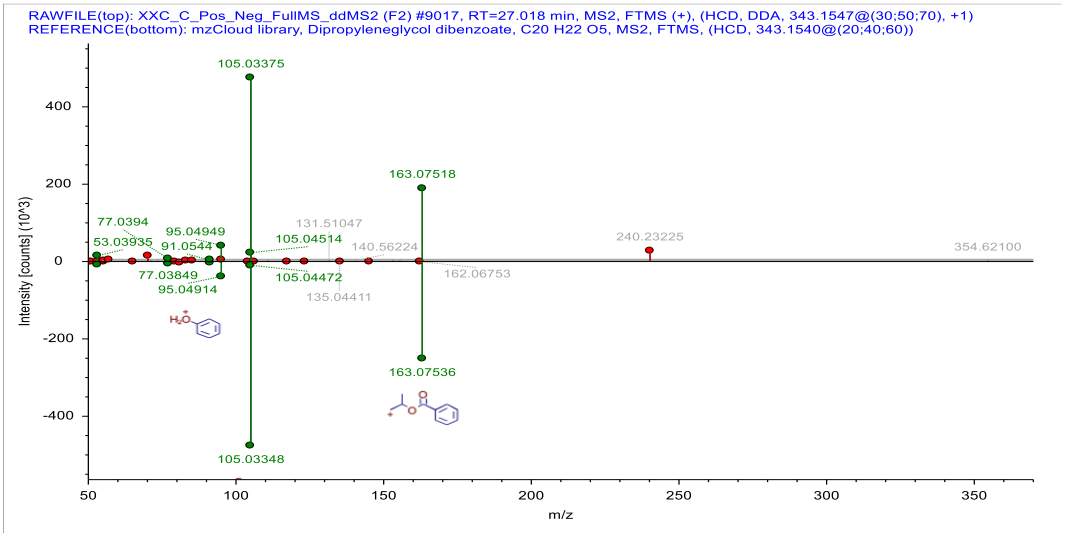

Fig.S19. Comparison of secondary mass spectra of oxydipropyl dibenzoate (Compound 8) standards retrieved by UPLC-HRMS and mzCloud.

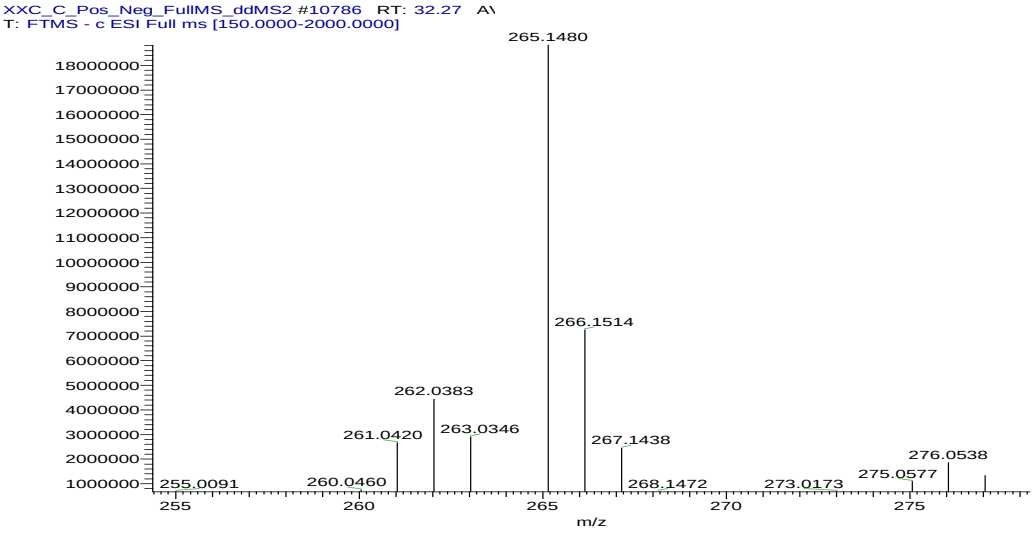

Fig.S20. Primary mass spectrometry of dodecyl hydrogen sulphate (Compound 9).

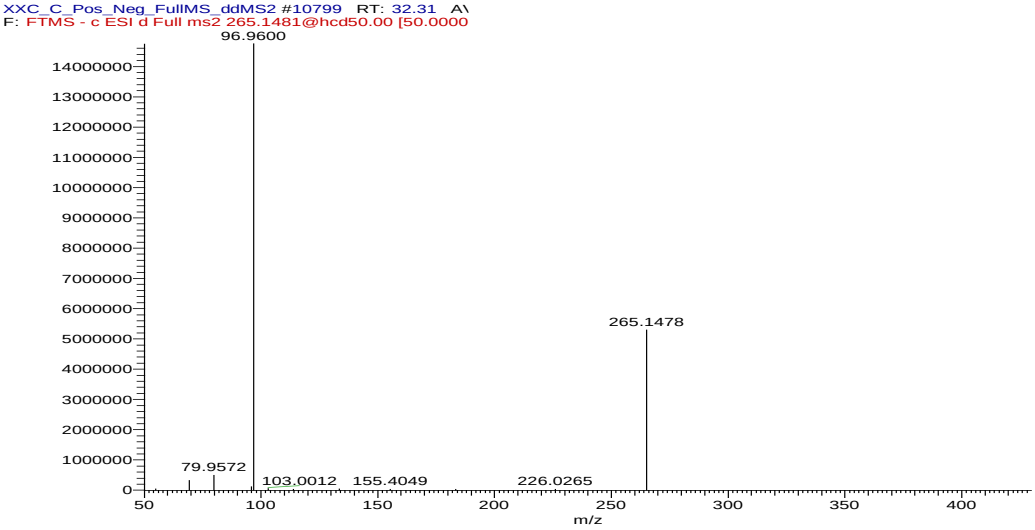

Fig.S21. Secondary mass spectrometry of dodecyl hydrogen sulphate (Compound 9).

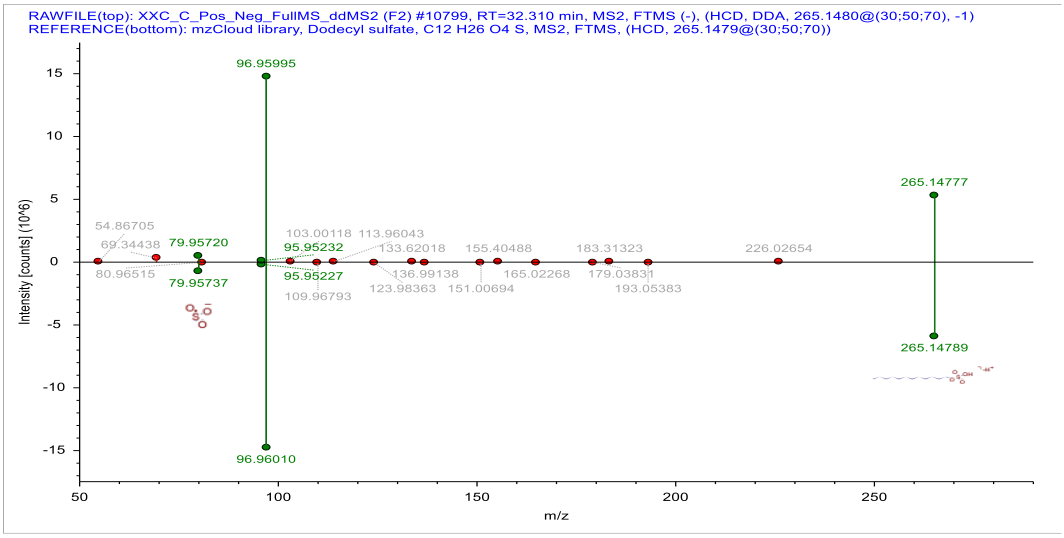

Fig.S22. Comparison of secondary mass spectra of dodecyl hydrogen sulphate (Compound 9) standards retrieved by UPLC-HRMS and mzCloud.

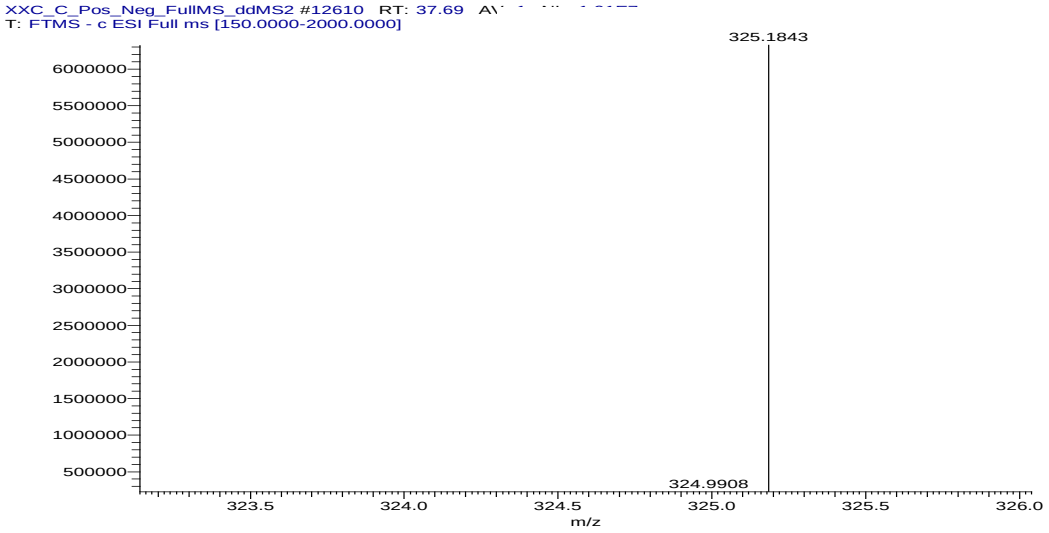

Fig.S23. Primary mass spectrometry of 4-dodecylbenzenesulfonic acid (Compound 10).

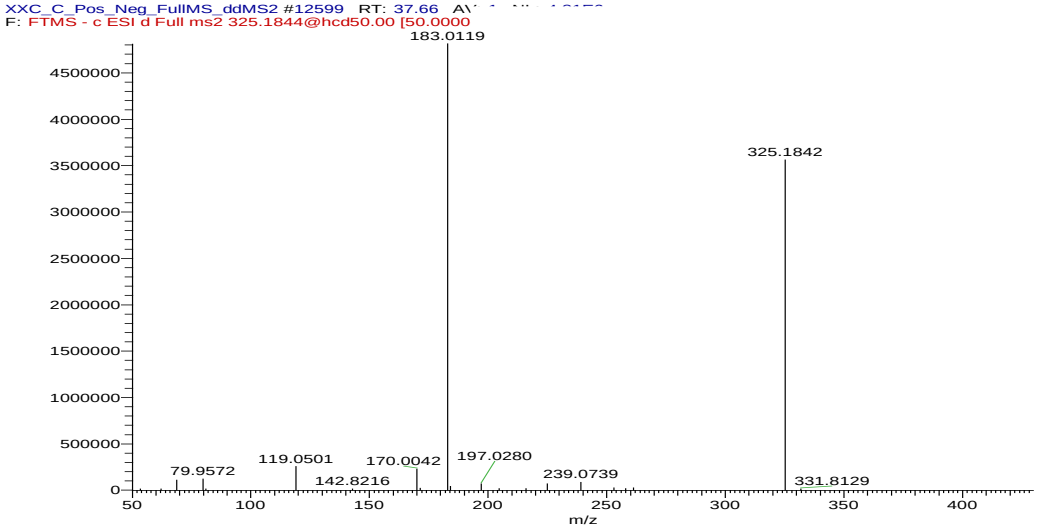

Fig.S24. Secondary mass spectrometry of 4-dodecylbenzenesulfonic acid (Compound 10).

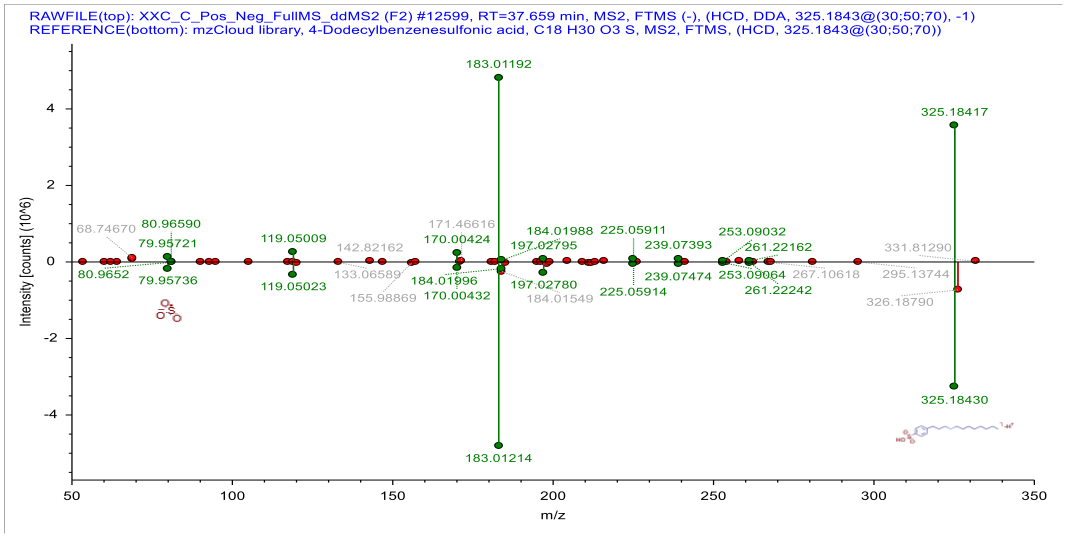

Fig.S25. Comparison of secondary mass spectra of 4-dodecylbenzenesulfonic acid (Compound 10) standards retrieved by UPLC-HRMS and mzCloud.

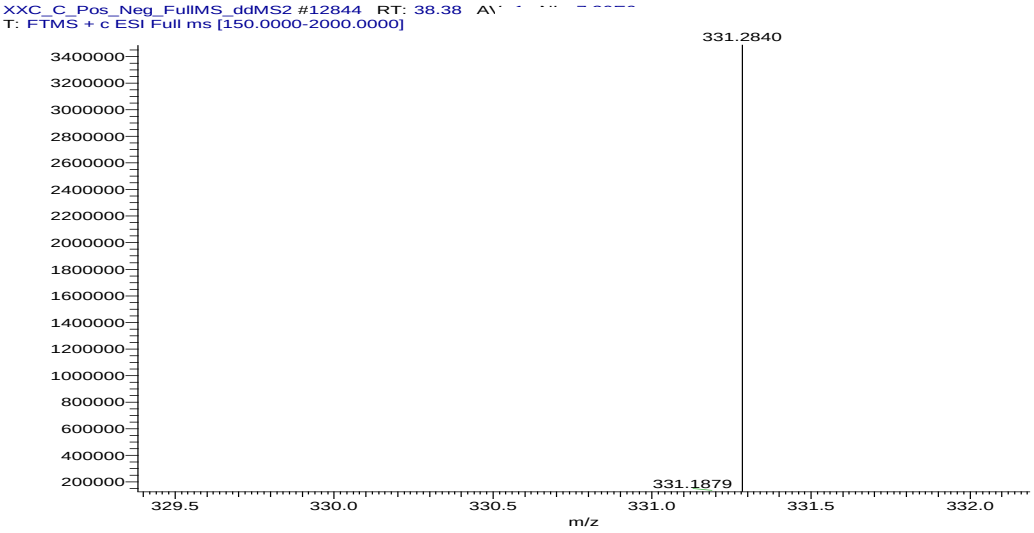

Fig.S26. Primary mass spectrometry of monopalmitin (Compound 11).

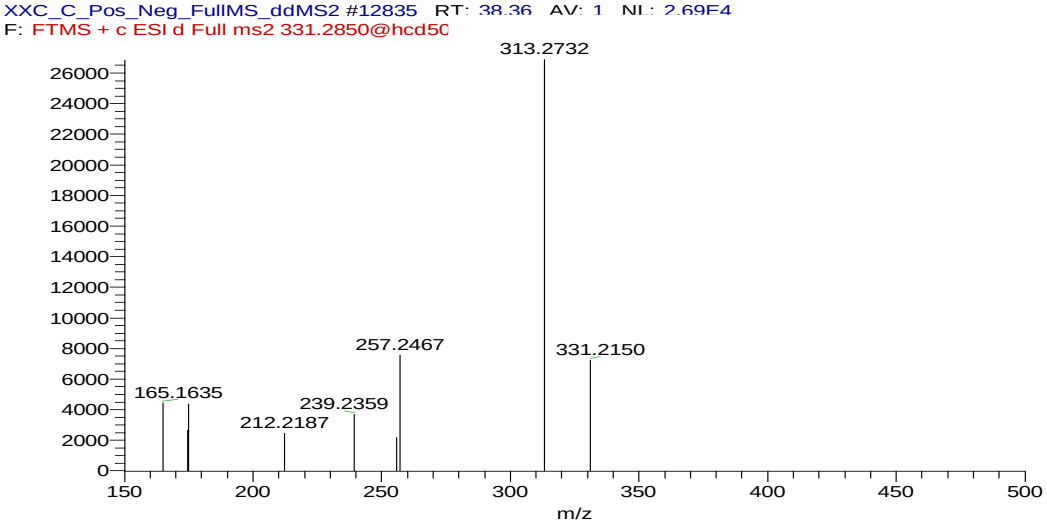

Fig.S27. Secondary mass spectrometry of monopalmitin (Compound 11).

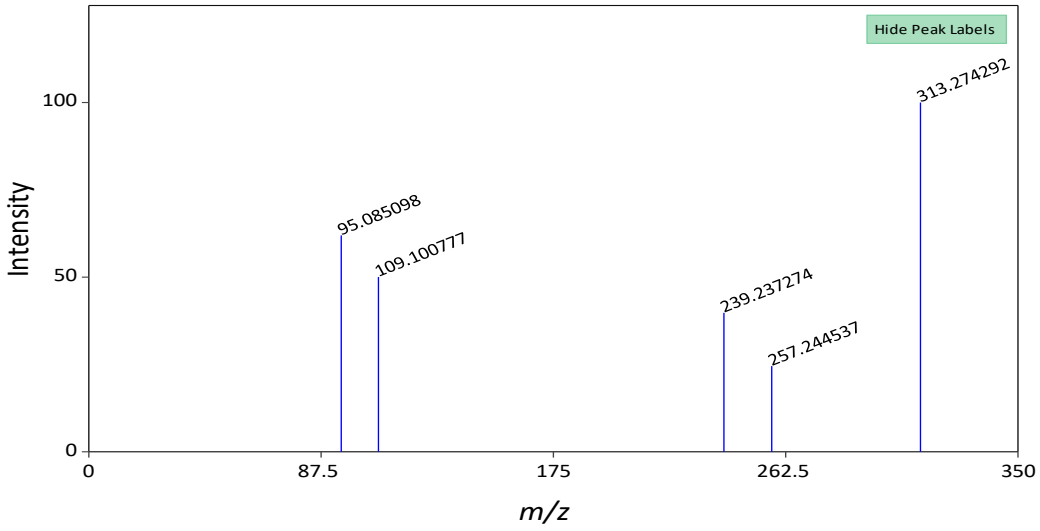

Fig.S28. Secondary mass spectrum of the monopalmitin (Compound 11) standard retrieved from PubChem.

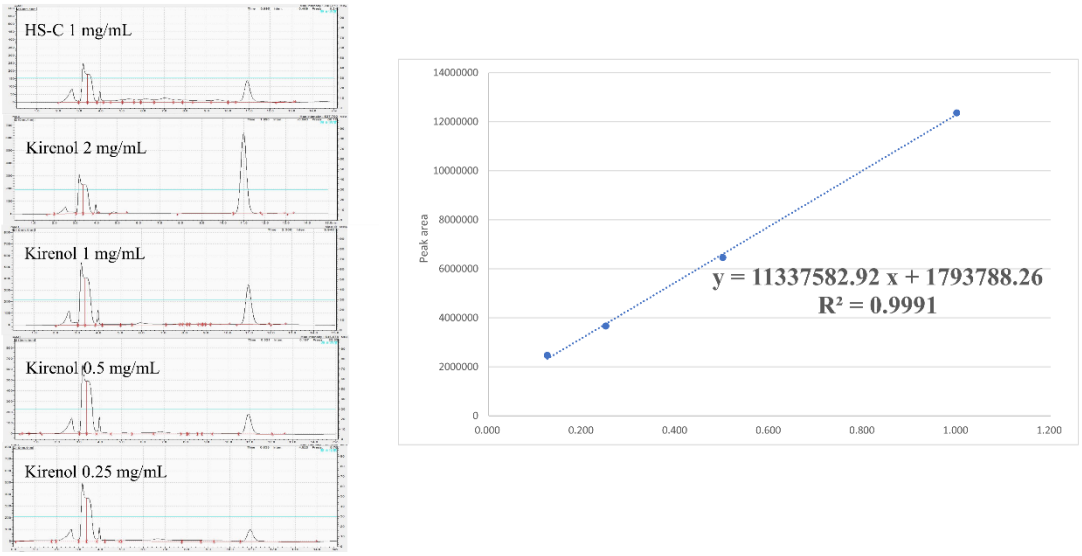

Figure S29. Standard plot of kirenol.

Table S1.

Information on the identification of 11 components of HS-C.

	Name	m/z	RT[min]	Δm/ppm	Major fragment ion	Reference	mzCloud sore (%)
1	Ent-2*β*,15,16-trihydroxypimar-8(14)-en-18-oic acid	$[M-H]^-$351.2177	14.03	0.00	$[M-H-CH_2O]^-$321.2069	[1]	-
2	Ent-15-oxo-2*β*,16,19-trihydroxypimar-8(14)-ene	$[M+H]^+$337.2369	18.59	-1.19	$[M+H-H_2O]^+$319.2266 $[M+H-2H_2O]^+$301.2147 $[M+H-3H_2O]^+$283.2047	[2]	-
3	Ent-15,16-dihydroxypimar-1,8(14)-dien-3-one	$[M+H]^+$319.2265	18.63	-0.94	$[M+H-H_2O]^+$301.2160 $[M+H-2H_2O]^+$283.2045	[1]	-
4	Kirenol	$[M+H]^+$339.2524	18.97	-1.77	$[M+H-H_2O]^+$321.2416 $[M+H-2H_2O]^+$303.2295 $[M+H-3H_2O]^+$285.2196	[3]	-
5	Siegesbeckic acid	$[M-H]^-$335.2227	19.12	-0.30	$[M-H-CH_2O]^-$305.2122 $[M-H-CH_2O-2OH]^-$271.2065	[4]	-
6	Eicosapentaenoic acid	$[M+H]^+$303.2314	19.63	-1.32	$[M+H-H_2O]^+$285.2206 $[M+H-2H_2O]^+$267.2099	[6]	89

7	Quercetin	$[M+H]^+$303.0499	19.87	1.98	$[M+H-H_2O]^+$285.2206 $[M+H-2H_2O]^+$267.2099 $[M+H-H_2O-CO]^+$257.2253 $[M+H-2CO-H_2O]^+$229.1595 $[M+H-2CO-H_2O-O]^+$213.1627	[5]	97.6
8	Oxydipropyl dibenzoate	$[M+H]^+$343.1539	27.26	-0.29	$[M+H-C_{10}H_{12}O_3]^+$163.0752	[6]	87.8
9	Dodecyl hydrogen sulphate	$[M-H]^-$265.148	32.27	0.38	$[M-H-C_{12}H_{25}]^-$96.9600 $[M-H-C_{12}H_{25}-OH]^-$79.9572	[6]	99.8
10	4-dodecylbenzenesulfonic acid	$[M-H]^-$325.1843	37.69	0.00	$[M-H-C_{10}H_{22}]^-$183.0119	[6]	97.2
11	Monopalmitin	$[M+H]^+$31.2848	28.28	1.51	$[M+H-H_2O]^+$313.2732	[8]	-

Table S2.

Calculation of kirenol content in HS-C.

Name	Concentration (mg/mL)	Peak area
HS-C	1	8879778
Kirenol	2	24606513
Kirenol	1	12862721
Kirenol	0.5	7305618
Kirenol	0.25	4916237

Reference

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