

Supplementary information

Protective mechanism of *Polygonum perfoliatum* L. extract on chronic alcoholic liver injury based on UHPLC-QExactive Plus mass spectrometry lipidomics and MALDI-TOF/TOF mass spectrum imaging

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Figure S1 Total ion chromatograms (TIC) of compounds detection in *P. perfoliatum* extract

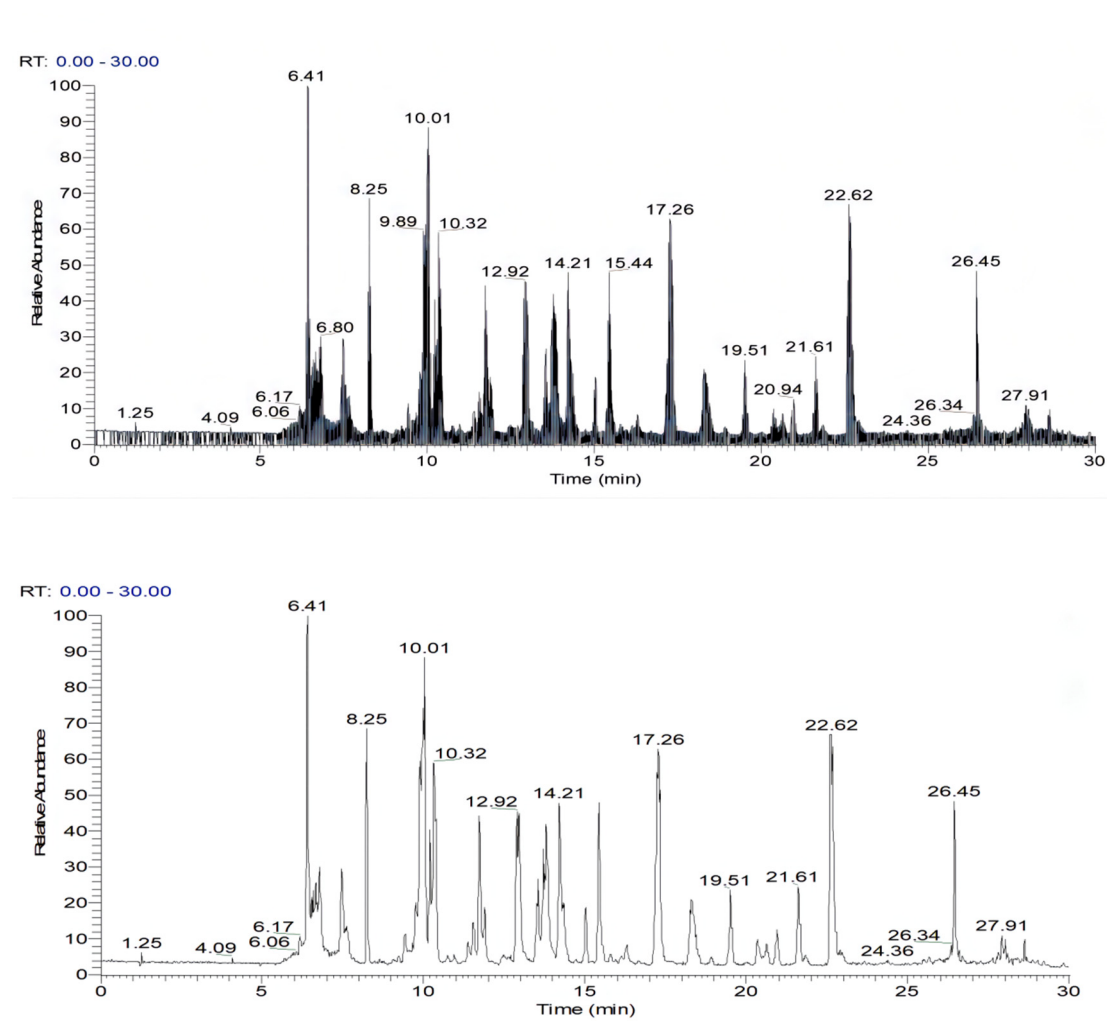


Table S1 Compounds identified by UHPLC-MS in negative ion mode

No.	t/min	Compound	Molecular formula	Estimated value (m/z)	Error	Secondary mass spectrometry (m/z)
1	6.17	Gallocatechin	C ₁₅ H ₁₄ O ₇	305.7069	1.98	287.1098, 261.0209, 219.3217, 179.0732, 167.1120
2	6.41	Catechinic acid	C ₁₅ H ₁₄ O ₆	289.5927	4.32	245.4611, 203.1266, 179.3412, 151.9015
3	8.25	Chlorogenic Acid	C ₁₆ H ₁₈ O ₉	351.1774	2.19	191.1088
4	10.01	Epicatechin	C ₁₅ H ₁₄ O ₆	288.7415	1.02	245.6725, 203.0728, 179.1927, 151.0307
5	10.32	Sanitol-7-O-rhamnose-3-O-glucoside	C ₂₇ H ₃₀ O ₁₅	596.4124	-0.39	284.1092, 285.0802
6	12.92	Rutin	C ₂₇ H ₃₀ O ₁₆	607.1754	1.64	300.1011, 301.2016
7	14.21	Kaempferol-3-O-neocyanin	C ₂₇ H ₃₀ O ₁₅	592.122	3.22	284.2922, 285.1650
8	17.26	Isoquercitrin	C ₂₁ H ₂₀ O ₁₂	462.9188	2.55	300.1213, 301.2090
9	19.51	Kaempferol rutin	C ₂₇ H ₃₀ O ₁₅	591.5722	4.11	284.3731, 285.4232
10	21.61	Quercitrin	C ₂₁ H ₂₀ O ₁₁	448.2144	2.68	300.2901, 301.2884
11	22.62	Quercetin	C ₁₅ H ₁₀ O ₇	301.9162	3.77	273.1736, 229.8021, 179.0902, 151.1877
12	26.46	Kaempferol	C ₁₅ H ₁₀ O ₆	284.2505	2.89	255.2334, 227.0519, 181.2976

Table S2 MS/MS fragmentation of each identified compound

NO.	Metabolite	Formula	Measured m/z	MASS accuracy (ppm)	Secondary mass spectrometry (m/z)
1	Stearoyl-L-Carnitine	C ₂₅ H ₄₉ NO ₄	426.3421	-2.03	85.0100, 60.0182, 84.0147, 86.0118
2	6-Aminohexanoate	C ₆ H ₁₂ NO ₂	131.3162	-0.79	115.0772, 114.0931, 97.0673, 69.0712
3	Linoleic acid	C ₁₈ H ₃₂ O ₂	280.3325	-0.91	264.2402, 245.2264, 97.1009
4	PC(16:0/18:1)	C ₄₂ H ₈₂ NO ₈ P	703.4683	1.49	506.4024, 406.1626, 281.1215, 224.0020
5	LPE(20:3)	C ₂₅ H ₄₆ NO ₇ P	503.3612	-0.95	440.2333, 214.0486, 152.9958, 78.9591
6	Bexarotene	C ₂₄ H ₂₈ O ₂	348.5070	-0.71	279.1367, 251.1056, 227.1778
7	Ginkgolide B	C ₂₀ H ₂₄ O ₁₀	424.4803	1.35	368.1410, 367.1388, 125.0237, 113.0234
8	Abietic acid	C ₂₀ H ₃₀ O ₂	302.2624	-0.97	257.2265, 149.1325, 123.1169, 121.1012
9	SM(d18:1/18:0)	C ₄₁ H ₈₃ N ₂ O ₆ P	730.5561	-1.06	184.0749, 104.1077, 86.0971
10	SM(d18:0/16:0)	C ₃₉ H ₈₁ N ₂ O ₆ P	704.4763	-0.11	619.4890, 464.3328, 239.2369, 74.0964