A Comparative Study on UHPLC-HRMS Profiles and Biological Activities of *Inula sarana* Different Extracts and Its Beta-Cyclodextrin Complex: Effective Insights for Novel Applications

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Supplementary Materials

Assays for Total Phenolic and Flavonoid Contents

The total phenolic content was determined by employing the methods given in the literature with some modification. Sample solution (0.25 mL) was mixed with diluted Folin–Ciocalteu reagent (1 mL, 1:9, v/v) and shaken vigorously. After 3 min, Na_2CO_3 solution (0.75 mL, 1%) was added and the sample absorbance was read at 760 nm after a 2 h incubation at room temperature. The total phenolic content was expressed as milligrams of gallic acid equivalents (mg GAE/g extract) (Uysal et al., 2017).

The total flavonoid content was determined using the $AlCl_3$ method. Briefly, sample solution (1 mL) was mixed with the same volume of aluminum trichloride (2%) in methanol. Similarly, a blank was prepared by adding sample solution (1 mL) to methanol (1 mL) without $AlCl_3$. The sample and blank absorbances were read at 415 nm after a 10 min incubation at room temperature. The absorbance of the

blank was subtracted from that of the sample. Rutin was used as a reference standard and the total flavonoid content was expressed as milligrams of rutin equivalents (mg RE/g extract) (Uysal et al., 2017).

Determination of Antioxidant and Enzyme Inhibitory Effects

Antioxidant (DPPH and ABTS radical scavenging, reducing power (CUPRAC and FRAP), phosphomolybdenum and metal chelating (ferrozine method)) and enzyme inhibitory activities (cholinesterase (Elmann's method), tyrosinase (dopachrome method), α-amylase (iodine/potassium iodide method), α -glucosidase (chromogenic PNPG method) and pancreatic lipase (*p*-nitrophenyl butyrate (p-NPB) method) were determined using the methods previously described by Uysal et al. (Uysal et al., 2017) and Grochowski et al. (Grochowski et al., 2017)

For the DPPH (1,1-diphenyl-2-picrylhydrazyl) radical scavenging assay: Sample solution was added to 4 mL of a 0.004% methanol solution of DPPH. The sample absorbance was read at 517 nm after a 30 min incubation at room temperature in the dark. DPPH radical scavenging activity was expressed as milligrams of trolox equivalents (mg TE/g extract).

For ABTS (2,2′-azino-bis(3-ethylbenzothiazoline) 6-sulfonic acid) radical scavenging assay: Briefly, ABTS+ was produced directly by reacting 7 mM ABTS solution with 2.45 mM potassium persulfate and allowing the mixture to stand for 12–16 in the dark at room temperature. Prior to beginning the assay, ABTS solution was diluted with methanol to an absorbance of 0.700 ± 0.02 at 734 nm. Sample solution was added to ABTS solution (2 mL) and mixed. The sample absorbance was read at 734 nm after a 30 min incubation at room temperature. The ABTS radical scavenging activity was expressed as milligrams of trolox equivalents (mg TE/g extract).

For CUPRAC (cupric ion reducing activity) activity assay: Sample solution was added to premixed reaction mixture containing $CuCl_2$ (1 mL, 10 mM), neocuproine (1 mL, 7.5 mM) and NH_4Ac buffer (1 mL, 1 M, pH 7.0). Similarly, a blank was prepared by adding sample solution (0.5 mL) to premixed reaction mixture (3 mL) without $CuCl_2$. Then, the sample and blank absorbances were read at 450 nm after a 30 min incubation at room temperature. The absorbance of the blank was subtracted from that of the sample. CUPRAC activity was expressed as milligrams of trolox equivalents (mg TE/g extract).

For FRAP (ferric reducing antioxidant power) activity assay: Sample solution was added to premixed FRAP reagent (2 mL) containing acetate buffer (0.3 M, pH 3.6), 2,4,6-tris(2-pyridyl)-S-triazine (TPTZ) (10 mM) in 40 mM HCl and ferric chloride (20 mM) in a ratio of 10:1:1 (v/v/v). Then, the sample absorbance was read at 593 nm after a 30 min incubation at room temperature. FRAP activity was expressed as milligrams of trolox equivalents (mg TE/g extract).

For phosphomolybdenum method: Sample solution was combined with 3 mL of reagent solution (0.6 M sulfuric acid, 28 mM sodium phosphate and 4 mM ammonium molybdate). The sample absorbance was read at 695 nm after a 90 min incubation at 95 °C. The total antioxidant capacity was expressed as millimoles of trolox equivalents (mmol TE/g extract).

For metal chelating activity assay: Briefly, sample solution was added to $FeCl_2$ solution (0.05 mL, 2 mM). The reaction was initiated by the addition of 5 mM ferrozine (0.2 mL). Similarly, a blank was prepared by adding sample solution (2 mL) to $FeCl_2$ solution (0.05 mL, 2 mM) and water (0.2 mL) without ferrozine. Then, the sample and blank absorbances were read at 562 nm after 10 min incubation at room temperature. The absorbance of the blank was sub-tracted from that of the sample. The metal

chelating activity was expressed as milligrams of EDTA (disodium edetate) equivalents (mg EDTAE/g extract).

For Cholinesterase (ChE) inhibitory activity assay: Sample solution (was mixed with DTNB (5,5-dithio-bis(2-nitrobenzoic) acid, Sigma, St. Louis, MO, USA) (125 μL) and AChE (acetylcholines-terase (Electric ell acetylcholinesterase, Type-VI-S, EC 3.1.1.7,Sigma)), or BChE (butyrylcholinesterase (horse serum butyrylcholinesterase, EC 3.1.1.8, Sigma)) solution (25 μL) in Tris–HCl buffer (pH 8.0) in a 96-well microplate and incubated for 15 min at 25 °C. The reaction was then initiated with the addition of acetylthiocholine iodide (ATCI, Sigma) or butyrylthiocholine chloride (BTCl, Sigma) (25 μL). Similarly, a blank was prepared by adding sample solution to all reaction reagents without enzyme (AChE or BChE) solution. The sample and blank absorbances were read at 405 nm after 10 min incubation at 25 °C. The absorbance of the blank was subtracted from that of the sample and the cholinesterase inhibitory activity was expressed as galanthamine equivalents (mgGALAE/g extract).

For Tyrosinase inhibitory activity assay: Sample solution was mixed with tyrosinase solution (40 μL, Sigma) and phosphate buffer (100 μL, pH 6.8) in a 96-well microplate and incubated for 15 min at 25 °C. The reaction was then initiated with the addition of L-DOPA (40 μL, Sigma). Similarly, a blank was prepared by adding sample solution to all reaction reagents without enzyme (tyrosinase) solution. The sample and blank absorbances were read at 492 nm after a 10 min incubation at 25 °C. The absorbance of the blank was subtracted from that of the sample and the tyrosinase inhibitory activity was expressed as kojic acid equivalents (mgKAE/g extract).

For α-amylase inhibitory activity assay: Sample solution was mixed with α-amylase solution (ex-porcine pancreas, EC 3.2.1.1, Sigma) (50 μL) in phosphate buffer (pH 6.9 with 6 mM sodium chloride) in a 96-well microplate and incubated for 10 min at 37 °C. After pre-incubation, the reaction was initiated with the addition of starch solution (50 μL, 0.05%). Similarly, a blank was prepared by adding sample solution to all reaction reagents without enzyme (α-amylase) solution. The reaction mixture was incubated 10 min at 37 °C. The reaction was then stopped with the addition of HCl (25 μL, 1 M). This was followed by addition of the iodine-potassium iodide solution (100 μL). The sample and blank absorbances were read at 630 nm. The absorbance of the blank was subtracted from that of the sample and the α-amylase inhibitory activity was expressed as acarbose equivalents (mmol ACE/g extract).

For α-glucosidase inhibitory activity assay: Sample solution was mixed with glutathione (50 μL), α-glucosidase solution (from Saccharomyces cerevisiae, EC 3.2.1.20, Sigma) (50 μL) in phosphate buffer (pH 6.8) and PNPG (4-N-trophenyl-α-D-glucopyranoside, Sigma) (50 μL) in a 96-well microplate and incubated for 15 min at 37 °C. Similarly, a blank was prepared by adding sample solution to all reaction reagents without enzyme (α-glucosidase) solution. The reaction was then stopped with the addition of sodium carbonate (50 μL, 0.2 M). The sample and blank absorbances were read at 400 nm. The absorbance of the blank was subtracted from that of the sample and the α-glucosidase inhibitory activity was expressed as acarbose equivalents (mmol ACE/g extract).

Table S1. Specialized metabolites in *Inula sarana* extracts.

No.	Identified/tentatively annotated compound	Molecular formula	Exact mass $[M-H]^-$	Fragmentation pattern in (-) ESI-MS/MS	t_R (min)	Δppm	Distribution
			Hydroxybenzoic, hydroxycinnamic and acylquinic acids, and derivatives				
1	Protocatechuic acid-*O*-hexoside	$C_{13}H_{16}O_9$	315.0722	315.0720 (2.9), 153.0181 (100), 109.0280 (51.4), 91.0176 (0.1), 81.0280 (51.4)	1.19	-0.135	2,3,4,5
2	Protocatechuic acid-*O*-hexoside isomer	$C_{13}H_{16}O_9$	315.0722	315.0725 (100), 153.0182 (30.0), 109.0285 (9.8), 108.0202 (90.5)	1.19	-0.135	2,3,4,5
3	Hydroxybenzoic acid-hexoside	$C_{13}H_{16}O_8$	299.0779	299.0776 (1.0), 137.0231 (100), 93.0330 (70.5)	1.29	1.235	5,6
4	Vanillic acid-*O*-hexoside	$C_{14}H_{18}O_9$	329.0890	329.0876 (1.9), 167.0339 (100), 152.0103 (24.0), 123.0437 (13.7), 108.0201 (38.5)	1.78	-0.776	2,4,5,6
5	Protocatechuic acid[a]	$C_7H_6O_4$	153.0182	153.0182 (15.4), 109.0280 (100), 91.0173 (0.9), 81.0329 (1.3)	2.04	0.211	2,4,5,6
6	Syringic acid 4-*O*-hexoside	$C_{15}H_{20}O_{10}$	359.0984	359.0988 (7.7), 197.0447 (100), 182.0211 (19.3), 166.9976 (8.0), 153.0545 (15.1), 138.0309 (26.4), 123.0074 (33.0)	2.28	1.198	2,4,5,6
7	Neochlorogenic (3-caffeoylquinic) acid[a]	$C_{16}H_{18}O_9$	353.0867	353.0881 (38.6), 191.0553 (100), 179.0340 (60.0), 173.0448 (3.1), 161.0233 (3.7), 135.0438 (47.4), 127.0386 (1.9), 111.0439 (1.2), 93.0331 (4.3), 85.0280 (8.7)	2.37	0.835	4,5,6
8	Caffeic acid-*O*-hexoside	$C_{15}H_{18}O_9$	341.0867	341.0864 (4.1), 179.0340 (100), 161.0230 (2.5), 135.0438 (59.9), 117.0329 (0.4)	2.43	-4.032	4,5,6
9	Caffeic acid-*O*-hexoside isomer	$C_{15}H_{18}O_9$	341.0867	341.0882 (1.5), 179.0339 (1.9), 135.0438 (100), 107.088 (0.8)	2.57	1.245	5,6
10	Gentisic acid-*O*-hexoside	$C_{13}H_{16}O_9$	315.0722	315.0726 (41.2), 153.0181 (86.6), 135.0072 (3.7), 109.0280 (100)	2.58	0.415	4,5,6
11	*p*-hydroxyphenylacetic acid-*O*-hexoside	$C_{14}H_{18}O_8$	313.0929	313.0928 (1.8), 151.0388 (100), 123.0079 (0.5), 109.0279 (3.6)	2.68	-0.386	5
12	Vanillic acid[a]	$C_8H_8O_4$	167.0350	167.0339 (91.0), 152.0103 (8.1), 123.0437 (100), 108.0199 (5.7), 95.0486 (7.7)	2.75	-6.478	5
13	Caffeoylgluconic acid	$C_{15}H_{18}O_{10}$	357.0827	357.0824 (11.4), 195.0502 (100), 179.0341 (44.5), 177.0397 (10.2), 135.0438 (42.1), 87.0072 (7.7), 59.0124 (1.1)	2.82	-0.812	5,6
14	*O*-caffeoyl hexose	$C_{15}H_{18}O_9$	341.0867	341.0880 (19.9), 281.0668 (100), 251.0561 (54.1), 221.0451 (52.8), 179.0340 (93.6), 161.0233 (60.7), 135.0438 (71.2), 107.0487 (2.0)	2.83	0.688	4,5
15	4-Hydroxybenzoic acid	$C_7H_6O_3$	137.0230	137.0231 (100), 108.0203 (8.6), 93.0331 (3.3)	2.83	-9.614	1,2,3,5,6,7,8,9
16	3-Hydroxybenzoic acid	$C_7H_6O_3$	137.0230	137.0230 (13.1), 108.0204 (0.6), 93.0330 (100)	2.83	-9.614	1,2,3,5,6,7,8,9
17	Hydroxybenzoic acid-hexoside	$C_{13}H_{16}O_8$	299.0779	299.0784 (1.4), 137.0230 (100), 93.0330 (51.9)	3.00	3.876	4,5,6

18	Caffeoylgluconic acid isomer	$C_{15}H_{18}O_{10}$	357.0827	357.0818 (4.7), 195.0654 (100), 135.0438 (5.7), 59.0123 (12.2)	3.41	-2.604	5
19	*O*-caffeoyl hexose isomer	$C_{15}H_{18}O_{9}$	341.0867	341.0878 (28.9), 281.0667 (71.9), 251.0560 (40.5), 221.0450 (37.8), 179.0340 (100), 161.0233 (42.9), 135.0438 (73.4), 107.0484 (0.6)	3.12	0.600	4,5
20	Quinic acid	$C_{7}H_{12}O_{6}$	191.0561	191.0553 (100), 173.0445 (1.8), 155.0339 (0.4), 127.0387 (3.7), 111.0437 (1.5), 93.0331 (6.8), 85.0280 (19.5)	3.19	-4.404	4,5,6
21	Chlorogenic (5-caffeoylquinic) acid[a]	$C_{16}H_{18}O_{9}$	353.0867	353.0878 (4.0), 191.0553 (100), 179.0341 (1.4), 173.0448 (0.6), 161.0235 (1.6), 135.0438 (0.7), 127.0389 (2.0), 111.0437 (0.8), 93.0330 (3.1), 85.0279 (7.5)	3.19	-0.100	1,2,3,4,5,6
22	*p*-coumaric acid[a]	$C_{9}H_{8}O_{3}$	163.0389	163.0388 (13.2), 135.0438 (8.5), 119.0488 (100)	3.34	-7.958	5
23	4-Caffeoylquinic acid	$C_{16}H_{18}O_{9}$	353.0867	353.0883 (31.7), 191.0554 (41.6), 179.0340 (66.2), 173.0445 (100), 161.0231 (2.7), 135.0439 (48.1), 127.0386 (1.5), 111.0437 (3.4), 93.0330 (20.6), 85.0279 (7.2)	3.37	1.401	1,2,3,4,5,6
24	Caffeic acid[a]	$C_{9}H_{8}O_{4}$	179.0338	179.0340 (19.0), 135.0438 (100), 117.0331 (0.8), 107.0487 (1.5)	3.55	-5.485	2,4,5,6
25	Gentisic acid[a]	$C_{7}H_{6}O_{4}$	153.0182	153.0181 (77.3), 135.0074 (30.5), 109.0280 (100), 91.0174 (5.2), 81.0331 (0.5)	3.86	0.141	4,5
26	5-*p*-Coumaroylquinic acid	$C_{16}H_{18}O_{8}$	337.0929	337.0934 (8.6), 191.0553 (100), 173.0445 (7.0), 163.0390 (5.8), 127.0387 (1.0), 119.0489 (4.0), 111.0437 (3.1), 93.0330 (15.1), 85.0279 (4.5)	3.96	1.363	4,5,6
27	*p*-Hydroxyphenylacetic acid	$C_{8}H_{8}O_{3}$	151.0401	151.0388 (100), 136.0153 (8.6), 123.0438 (78.8), 107.0486 (87.2)	3.47	-8.391	2,4,5
28	5-Feruloylquinic acid	$C_{17}H_{20}O_{9}$	367.1035	367.1039 (16.3), 193.0503 (5.4), 191.0553 (100), 173.0446 (11.6), 135.0392 (0.3), 134.0360 (10.1), 111.0437 (0.4), 93.0330 (25.6), 85.0279 (4.7)	4.40	1.075	4,5,6
29	1-Caffeoyl-3-hydroxy-dihydrocaffeoylquinic acid	$C_{25}H_{26}O_{13}$	533.1301	533.1312 (28.3), 371.0987 (59.7), 353.0876 (5.2), 335.0779 (6.7), 335.0776 (2.9), 197.0447 (2.9), 191.0552 (14.7), 197.0448 (3.8), 179.0341 (13.7), 173.0444 (34.3), 161.0229 (5.0), 153.0544 (12.5), 135.0438 (100), 111.0435 (2.8), 93.0330 (10.0), 85.0279 (4.0)	4.43	2.187	5,6
30	*m*-Coumaric acid[a]	$C_{9}H_{8}O_{3}$	163.0389	163.0389 (8.9), 135.0438 (2.0), 119.0488 (100)	4.56	-1.127	5
31	Syringic acid (caffeoyl)-hexoside	$C_{24}H_{26}O_{13}$	521.1301	521.1305 (83.4), 359.0974 (1.1), 323.0775 (20.2), 263.0554 (1.3), 203.0349 (0.7), 179.0340 (14.8), 161.0233 (54.2), 135.0438 (100)	4.65	0.818	4,5,6
32	Hydroxyisopropanoic acid-*O*-(coumaroyl)-hexoside	$C_{21}H_{32}O_{12}$	475.1821	475.1814 (47.8), 429.1766 (100), 325.1150 (3.0), 265.0935 (9.8), 235.0821 (1.6), 205.0708 (16.9), 163.0600 (56.5), 119.0336 (8.9)	5.00	-1.535	2,4,5,6

33	Syringic acid (caffeoyl)-hexoside	$C_{24}H_{26}O_{13}$	521.1301	521.1303 (100), 359.0989 (5.4), 323.0774 (20.9), 203.0345 (0.6), 197.0448 (38.1), 182.0207 (4.4), 179.0341 (21.3), 166.9977 (3.4), 161.0232 (64.7), 151.0392 (0.7), 135.0438 (28.6), 123.0437 (9.0), 123.0077 (1.3)	5.09	0.472	4,5,6
34	Gentisic acid-(caffeoyl)-hexoside	$C_{22}H_{22}O_{12}$	477.1038	477.1042 (76.8), 323.0775 (44.3), 315.0722 (2.2), 221.0452 (5.2), 179.0340 (9.1), 161.0233 (45.2), 153.0182 (100),135.0439 (12.2), 133.0282 (16.2), 109.0280 (88.7)	5.17	0.359	4,5,6
35	Caffeic acid-(hydroxyisovaleryl)-hexoside	$C_{20}H_{26}O_{11}$	441.1402	441.1404 (78.7), 341.0864 (2.3), 323.0775 (11.1), 281.0667 (6.5), 251.0556 (4.4), 221.0457 (6.0), 179.0342 (15.4), 161.0232 (100), 135.0437 (18.4), 133.0281 (29.4),	5.37	0.397	5,6
36	Caffeic acid-*O*-(salicyl)-hexoside	$C_{22}H_{22}O_{11}$	461.1089	461.1099 (2.3), 323.0776 (47.3), 221.0454 (8.6), 179.0341 (18.5), 161.0233 (78.9), 137.0231 (40.7), 135.0438 (17.0), 133.0281 (32.2), 93.0330 (50.4)	5.40	2.072	2,3,4,5,6
37	Vanillic acid-4-*O*-(6-*O*-caffeoyl)-hexoside	$C_{23}H_{24}O_{12}$	491.1195	491.1197 (100), 323.0776 (35.2), 221.0452 (6.2), 179.0341 (17.4), 167.0339 (27.9), 161.0233 (66.1), 152.0103 (25.2), 135.0438 (21.8), 123.0438 (5.4), 108.0202 (15.2)	5.52	0.388	4,5,6
38	3,4-Dicaffeoylquinic acid[a]	$C_{25}H_{24}O_{12}$	515.1195	515.1201 (77.6), 353.0882 (46.7), 335.0771 (10.4), 299.0554 (12.7), 227.0715 (2.0), 203.0344 (45.4), 191.0555 (33.8), 179.0341 (65.6), 173.0446 (100), 161.0234 (11.9), 135.0439 (75.0), 111.0436 (6.5), 93.0330 (28.7), 85.0279 (3.2)	5.59	0.137	4,5,6
39	1,5-Dicaffeoylquinic acid[a]	$C_{25}H_{24}O_{12}$	515.1195	515.1198 (100), 353.0883 (16.5), 335.0791 (6.6), 191.0552 (31.2), 179.0340 (56.6), 173.0445 (58.9), 161.0233 (16.5), 135.0438 (54.4), 111.0435 (3.3), 93.0330 (15.6), 85.0280 (4.6)	5.70	0.584	1,2,3,4,5,6
40	3,5-Dicaffeoylquinic acid[a]	$C_{25}H_{24}O_{12}$	515.1195	515.1205 (17.0), 353.0881 (87.0), 191.0553 (100), 179.0304 (48.1), 161.0231 (5.1), 111.0434 (2.0), 93.0333 (4.0), 85.0280 (6.6)	5.85	1.904	1,2,3,4,5,6
41	4,5-dicaffeoylquinic acid	$C_{25}H_{24}O_{12}$	515.1195	515.1201 (75.6), 353.0882 (56.3), 203.0342 (3.8), 191.0553 (37.3), 179.0340 (65.6), 173.0445 (100), 135.0438 (76.4), 127.0385 (2.8), 111.0436 (4.9), 593.0330 (25.2), 85.0280 (5.6)	6.22	1.089	1,2,3,4,5,6
42	Salicylic acid[a]	$C_7H_6O_3$	137.0230	1537.0231 (9.8), 108.0203 (1.5), 93.0330 (100)	6.28	-9.611	1,3,4,5,6,7,8,9
43	Caffeoyl-(salicyl)-hexoside isomer	$C_{22}H_{22}O_{11}$	461.1089	461.1091 (45.5), 323.0776 (28.4), 221.0448 (2.1), 179.0342 (5.4), 161.0234 (29.2), 137.0231 (100), 133.0281 (12.8), 135.0437 (7.3), 93.0331 (58.7)	6.58	0.359	5

44	3-Caffeoyl-5-*p*-coumaroylquinic acid	$C_{25}H_{24}O_{11}$	499.1246	499.1256 (17.2), 353.0880 (54.1), 337.0930 (23.9), 191.0552 (100), 179.0338 (8.7), 173.0446 (17.5), 163.0389 (25.8), 161.0231 (8.1), 135.0439 (7.6), 119.0487 (19.5), 111.0437 (6.8), 93.0330 (12.2), 85.0280 (6.7)	6.50	0.351	4,5
45	4-*p*-Coumaroyl-5-caffeoylquinic acid	$C_{25}H_{24}O_{11}$	499.1246	499.1244 (24.5), 353.0884 (6.5), 337.0933 (61.2), 191.0554 (13.2), 179.0341 (2.2), 173.0445 (100), 163.0390 (19.4), 127.0389 (0.7), 111.0438 (4.4), 93.0330 (23.5), 85.0279 (2.1)	6.92	-0.330	4,5
46	3,4,5-Tricaffeoylquinic acid	$C_{34}H_{30}O_{15}$	677.1512	677.1517 (100). 515.1199 (42.6), 353.0882 (47.7), 335.0778 (0.8), 203.0350 (0.9), 191.0554 (47.9), 179.0341 (68.0), 173.0446 (92.1), 161.0233 (25.3), 135.0439 (81.2), 111.0437 (5.6), 93.0331 (25.1), 85.0278 (4.3)	7.77	0.793	5
				Caffeoylhexaric acids			
47	Caffeoylhexaric acid	$C_{15}H_{16}O_{11}$	371.0620	371.0611 (3.6), 209.0296 (100), 191.0189 (20.5), 179.0338 (1.5), 173.0088 (0.5), 147.0285 (3.7), 135.0436 (3.4), 129.0180 (3.7), 111.0073 (1.4), 85.0279 (42.4)	1.31	0.150	5,6
48	Caffeoylhexaric acid isomer	$C_{15}H_{16}O_{11}$	371.0620	371.0610 (3.6), 209.0296 (100), 191.0189 (24.0), 179.0338 (0.7), 173.0075 (1.5), 147.0285 (3.0), 135.0435 (2.2), 129.0180 (3.9), 111.0072 (1.7), 85.0279 (45.7)	2.02	-2.653	4,5,6
49	Caffeoylhexaric acid isomer	$C_{15}H_{16}O_{11}$	371.0620	371.0639 (2.9), 209.0296 (100), 191.0188 (22.2), 179.0339 (0.6), 173.0083 (0.8), 147.0290 (3.5), 135.0437 (0.9), 129.0179 (4.3), 111.0071 (1.7), 85.0279 (37.6)	2.43	5.243	4,5,6
50	Caffeoylhexaric acid isomer	$C_{15}H_{16}O_{11}$	371.0620	371.0620 (3.8), 209.0297 (100), 191.0190 (21.7), 179.0343 (2.2), 147.0290 (1.8), 135.0442 (4.5), 129.0178 (2.5), 111.0074 (2.2), 85.0279 (38.0)	2.67	-0.012	5,6
51	Dicaffeoylhexaric acid	$C_{24}H_{22}O_{14}$	533.0937	533.0928 (11.3), 371.0624 (95.2), 353.0526 (1.5), 209.0297 (100), 191.0190 (29.1), 179.0347 (3.6), 173.0080 (1.0), 147.0287 (4.5), 135.0438 (5.7), 5129.0178 (5.3), 111.0072 (3.5), 85.0279 (54.8),	3.77	-1.704	5,6
52	Dicaffeoylhexaric acid isomer	$C_{24}H_{22}O_{14}$	533.0937	533.0879 (11.6), 371.0622 (79.9), 353.0491 (1.6), 335.0787 (0.4), 209.0297 (100), 191.0188 (23.6), 179.0341 (6.7), 161.0230 (0.8), 147.0284 (4.4), 135.0438 (9.8), 129.0178 (8.0), 85.0278 (53.1)	4.12	-10.858	5,6
53	Dicaffeoylhexaric acid isomer	$C_{24}H_{22}O_{14}$	533.0937	533.0975 (11.4), 371.0612 (67.6), 353.0490 (3.5), 209.0297 (100), 191.0189 (27.6), 173.0343 (35.0), 147.0286 (4.3), 135.0438 (29.0), 129.0179 (7.0), 111.0076 (4.0), 85.0279 (50.5)	4.70	-3.905	5,6

54	Dicaffeoylhexaric acid isomer	$C_{24}H_{22}O_{14}$	533.0937	533.0974 (9.3), 371.0618 (71.1), 353.0514 (3.0), 209.0297 (100), 191.0190 (22.7), 173.0445 (5.3), 161.0234 (2.2), 147.0287 (3.7), 135.0438 (7.2), 129.0184 (4.5), 111.0072 (3.0), 85.0279 (47.2)	4.88	-13.485	5,6
55	Dicaffeoylhexaric acid isomer	$C_{24}H_{22}O_{14}$	533.0937	533.0895 (10.6), 371.0622 (82.6), 353.0504 (2.5), 179.0342 (2.9), 161.0231 (1.0), 209.0279 (100), 191.0190 (24.90), 147.0284 (4.0), 135.0439 (7.3), 129.0180 (4.5), 111.0073 (3.7), 85.0279 (48.3)	5.16		5,6
56	Tetracaffeoylhexaric acid	$C_{42}H_{34}O_{20}$	857.1571	857.1796 (48.2), 695.1470 (57.2), 533.1164 (13.2), 371.0606 (2.9), 209.0297 (100), 191.0189 (46.5), 179.0340 (0.5), 173.0080 (2.3), 161.0230 (7.8), 147.0287 (9.4), 135.0438 (34.4), 129.0179 (20.3), 111.0074 (5.7), 85.0279 (71.4)	5.21	1.673	5
57	Tricaffeoylhexaric acid	$C_{33}H_{28}O_{17}$	695.1254	695.1260 (27.7), 533.0943 (32.1), 371.0623 (17.2), 353.0498 (1.5), 209.0297 (100), 191.0189 (15.8), 179.0340 (3.9), 173.0079 (1.1), 161.0230 (0.5), 147.0285 (3.2), 135.0438 (7.1), 129.0179 (5.8), 111.0076 (2.6), 85.0279 (39.4)	5.89	0.874	4,5,6
58	Tricaffeoylhexaric acid isomer	$C_{33}H_{28}O_{17}$	695.1254	695.1265 (26.4), 533.0944 (37.2), 371.0623 (18.8), 209.0296 (100), 191.0189 (19.3), 179.0337 (3.3), 173.0087 (1.1), 161.0235 (3.0), 147.0284 (5.4), 135.0440 (5.7), 129.0181 (5.7), 111.0072 (3.5), 85.0279 (43.4)	6.33	1.665	5,6
59	Tricaffeoylhexaric acid isomer	$C_{33}H_{28}O_{17}$	695.1254	695.1255 (28.0), 533.0934 (31.7), 371.0620 (17.0), 209.0296 (100), 191.0188 (16.0), 179.0341 (4.2), 173.0447 (1.5), 161.0233 (2.0), 147.0283 (3.7), 135.0437 (7.2), 129.0179 (6.5), 111.0073 (1.9), 85.0279 (41.8)	6.46	0.255	5,6
60	Tetracaffeoylhexaric acid isomer	$C_{42}H_{34}O_{20}$	857.1571	857.1584 (40.0), 695.1299 (8.6), 533.0965 (4.2), 371.0623 (13.8), 209.0297 (100), 191.0188 (15.7), 179.0340 (3.8), 173.0086 (0.9), 161.0233 (7.1), 147.0283 (4.1), 129.0181 (6.1), 111.0073 (1.4), 85.0279 (43.3)	7.48	1.544	4,5,6
61	Isobutanyl-tricaffeoylhexaric acid-hexoside	$C_{43}H_{44}O_{23}$	927.2201	927.2217 (100), 765.1890 (71.1), 603.1569 (18.8), 441.1046 (0.6), 423.0937 (1.8), 341.0883 (24.4), 323.0780 (10.0), 279.0721 (42.8), 261.0617 (13.9), 179.0340 (58.7), 173.0081 (5.6), 161.0233 (20.7), 147.0285 (6.4), 135.0438 (79.8), 129.0180 (18.3), 111.0072 (8.8)	7.72	1.811	4,5,6
62	2-Methylbutanyl/isovaleryl-dicaffeoylhexaric acid	$C_{29}H_{30}O_{15}$	617.1512	617.1533 (14.9), 455.1205 (100), 293.0881 (46.8), 191.0188 (56.6), 179.0336 (4.1), 147.0288 (15.8), 135.0438 (14.2), 129.0178 (18.2), 111.0072 (5.1), 85.0279 (95.5)	7.91	3.446	5,6

63	2-Methylbutanyl/isovaleryl-dicaffeoylhexaric acid isomer	$C_{29}H_{30}O_{15}$	617.1512	617.1553 (14.9), 455.1199 (100), 293.0881 (44.6), 191.0190 (58.0), 179.0336 (12.3), 147.0288 (13.0), 135.0438 (22.2), 129.0181 (12.6), 111.0073 (3.4), 85.0279 (80.8)	8.22	-2.862	5
64	2-Methylbutanyl/isovaleryl-tricaffeoylhexaric acid-hexoside	$C_{44}H_{46}O_{23}$	941.2357	941.2369 (100), 779.2042 (63.1), 617.1731 (18.5), 455.1232 (2.1), 341.0880 (25.0), 323.0880 (8.5), 293.0880 (35.5), 191.0190 (41.6), 179.0340 (63.8), 161.0233 (17.1), 147.0285 (6.6), 135.0438 (73.5), 129.0180 (17.9), 85.0279 (84.4)	8.32	1.264	5
65	Isobutanyl-tricaffeoylhexaric acid	$C_{37}H_{34}O_{18}$	765.1672	765.1685 (45.2), 603.1365 (46.8), 441.1043 (31.6), 279.0722 (86.2), 191.0189 (64.7), 179.0338 (10.4), 173.0077 (5.3), 161.0233 (6.7), 147.0286 (10.8), 135.0439 (26.9), 129.0180 (12.4), 111.0073 (5.8), 85.0279 (100)	8.52	1.598	4,5,6
66	2-Methylbutanyl/isovaleryl-tricaffeoylhexaric acid	$C_{38}H_{36}O_{18}$	779.1829	779.1848 (45.6), 617.1522 (34.2), 455.1199 (26.3), 293.0882 (68.5), 191.0189 (61.9), 179.0340 (12.1), 173.0079 (4.1), 161.0233 (7.7), 147.0287 (11.2), 135.0438 (24.1), 129.0180 (14.4), 111.0075 (6.5), 85.0279 (100)	9.15	2.391	4,5,6
67	2-Methylbutanyl/isovaleryl-tricaffeoylhexaric acid isomer	$C_{38}H_{36}O_{18}$	779.1829	779.1839 (46.2), 617.1521 (38.7), 455.1202 (29.3), 293.0880 (74.5), 191.0189 (67.8), 179.0339 (14.2), 173.0083 (5.1), 161.0235 (7.3), 147.0287 (13.3), 135.0438 (24.2), 129.0179 (14.0), 85.0279 (100)	9.22	1.300	4,5,6
				Flavonoids			
68	Quercetin 7-*O*-rutinoside	$C_{27}H_{30}O_{16}$	609.1461	609.1467 (81.4), 301.0356 (100), 283.0255 (1.4), 271.0255 (0.5), 255.0293 (2.8), 237.0195 (0.8), 227.0341 (2.3), 133.0287 (2.7)	4.64	0.824	2,3,4,5,6
69	Rutin[a]	$C_{27}H_{30}O_{16}$	609.1461	609.1467 (100), 301.0353 (36.4), 300.0278 (68.6), 271.0249 (31.0), 255.0299 (14.5), 243.0299 (8.1), 178.9975 (3.0), 163.0030 (1.8), 151.0027 (5.4), 121.0285 (1.7), 107.0127 (2.1)	5.09	-0.879	1,2,3,4,5,6
70	Eryodictiol *O*-rutinoside	$C_{27}H_{32}O_{15}$	595.1668	595.1677 (64.8), 287.0563 (75.5), 269.0434 (0.7), 175.0022 (4.0), 151.0025 (100), 135.0438 (54.3), 125.0227 (4.4), 107.0124 (19.1)	5.11	1.372	4,5,6
71	Isoquercitrin[a]	$C_{21}H_{20}O_{12}$	463.0882	463.0887 (100), 301.0346 (35.6), 300.0278 (79.7), 271.0250 (36.7), 255.0296 (14.1), 243.0299 (9.2), 227.0349 (2.9), 178.9982 (2.6), 161.0232 (2.4), 151.0027 (6.4), 121.0285 (1.5), 107.0126 (2.3)	5.18	1.081	1,2,3,4,5,6
72	Luteolin 7-*O*-neohesperidoside/rutinoside	$C_{27}H_{30}O_{15}$	593.1512	593.1521 (75.1), 285.0406 (100), 256.0368 (0.6), 239.0346 (0.7), 217.0513 (0.7), 199.0394 (1.8), 151.0023 (2.9), 133.0281 (4.2), 107.0124 (1.4)	5.21	1.529	2,4,5,6

73	Patuletin *O*-rutinoside	$C_{28}H_{32}O_{17}$	639.1567	639.1574 (100), 331.0457 (32.0), 330.0385 (67.5), 316.00224 (11.0), 315.0151 (20.4), 287.0201 (21.7), 271.0250 (4.7), 259.0247 (4.6), 243.0300 (3.8), 231.0297 (4.3), 215.0345 (4.5), 175.0028 (4.4), 165.9899 (4.6), 139.0025 (2.6), 136.9864 (1.0)	5.23	1.154	1,2,3,4,5,6
74	Hyperoside[a]	$C_{21}H_{20}O_{12}$	463.0882	463.0888 (100), 301.0353 (45.3), 300.0278 (81.8), 271.0250 (34.8), 255.0297 (15.9), 243.0297 (10.3), 227.0343 (2.1), 199.0389 (0.9), 178.9982 (3.4), 163.0023 (1.1), 151.0024 (5.9), 121.0278 (0.8), 107.0123 (2.2)	5.28	1.254	1,2,3,4,5,6
75	Luteolin 7-*O*-glucoside[a]	$C_{21}H_{20}O_{11}$	447.0933	447.0934 (100), 285.0404 (91.2), 256.0375 (4.7), 227.0347 (2.1), 211.0394 (1.0), 199.0396 (1.7), 175.0388 (1.4), 151.0024 (5.2), 133.0281 (4.8), 107.0124 (3.5)	5.39	0.348	2,4,5
76	Patuletin *O*-hexoside	$C_{22}H_{21}O_{13}$	493.0988	493.0993 (100), 331.0457 (30.5), 330.0385 (62.0), 315.0152 (20.2), 287.0200 (20.1), 271.0247 (4.4), 259.0242 (3.7), 243.0303 (2.8), 199.0912 (1.3), 187.0393 (2.2), 175.0026 (2.6), 165.09899 (3.6), 139.0024 (2.7)	5.44	1.087	2,3,4,5,6
77	Quercetin 3-*O*-acetylhexoside	$C_{23}H_{22}O_{13}$	505.0995	505.0995 (100), 463.0868 (1.7), 301.0350 (38.0), 300.0277 (96.2), 271.0250 (45.7), 255.0299 (18.1), 243.0298 (10.6), 227.03406 (2.9), 178.9974 (2.7), 163.0032 (1.9), 151.0025 (6.5), 121.0283 (1.3), 107.01234 (2.2)	5.60	1.378	4,5,6
78	Kaempferol 3-*O*-rutinoside[a]	$C_{27}H_{30}O_{15}$	593.1512	593.1520 (100), 285.0404 (85.0), 284.0329 (47.6), 255.0404 (38.5), 227.0347 (27.5), 211.0401 (2.5), 151.0023 (0.9), 135.0071 (0.9), 107.0129 (1.1)	5.63	1.360	2,3,4,5,6
79	Nepetin *O*-glucoside[a]	$C_{22}H_{22}O_{12}$	477.1038	477.1041 (100), 315.0489 (15.6), 300.0282 (9.6), 299.0201 (14.6), 285.0395 (1.7), 271.0249 (2.3), 255.0311 (0.5), 243.0296 (2.0), 227.0338 (0.9), 133.0283 (15.4)	5.66	0.526	2,4,5,6
80	Nepetin *O*-rutinoside	$C_{28}H_{32}O_{16}$	623.1618	623.1627 (100), 315.0513 (49.7), 300.0278 (27.9), 271.0252 (31.7), 243.0298 (16.6), 255.0302 (3.9), 227.0343 (2.0), 215.0349 (6.7), 165.9896 (5.0), 133.0283 (1.9)	5.77	1.544	2,3,4,5,8
81	Kaempferol 3-*O*-glucoside[a]	$C_{21}H_{20}O_{11}$	447.0932	447.0936 (100), 285.0398 (25.1), 284.0328 (57.7), 255.0299 (42.3), 227.0346 (42.8), 211.0402 (1.8), 151.0028 (2.7), 107.0125 (0.6)	5.86	0.706	2,4,5
82	Isorhamnetin 3-*O*-glucoside[a]	$C_{22}H_{22}O_{12}$	477.1042	477.1042 (100), 315.0508 (25.6), 314.0437 (41.9), 300.0276 (16.2), 299.0199 (18.0), 271.0250 (28.7), 255.0303 (2.7), 243.0297 (13.8), 215.0348 (7.2), 199.0392 (2.3), 178.9978 (1.4), 151.0033 (0.4), 133.0282 (2.4)	6.03	0.253	2,5

83	Chrysoeriol *O*-hexoside	$C_{22}H_{22}O_{11}$	461.1089	461.1096 (100), 446.0861 (22.6), 299.0560 (9.2), 284.0316 (5.8), 283.0251 (18.2), 255.0299 (54.5), 227.0346 (0.6), 163.0026 (0.8), 151.0024 (0.7)	6.29	1.356	2,4,5
84	Cirsiliol *O*-hexoside	$C_{23}H_{24}O_{12}$	491.1195	491.1200 (100), 329.0670 (9.1), 313.0358 (76.7), 299.0195 (2.3), 270.0172 (39.6), 298.0123 (11.8), 257.0086 (3.0), 242.0219 (2.5), 229.0141 (0.8), 136.9871 (1.3), 133.0283 (0.3)	6.92	1.020	2,3,4,5,8
85	Spinacetin	$C_{17}H_{14}O_8$	345.0616	345.0617 (99.4), 330.0384 (100), 315.0150 (45.8), 287.0201 (10.9), 271.0246 (1.5), 259.0248 (3.1), 243.0298 (2.7), 231.0297 (5.2), 215.0344 (3.1), 165.9897 (6.3), 149.0233 (9.6), 139.0388 (4.0), 136.9865 (2.1)	7.23	0.346	2,4,5
86	Luteolin[a]	$C_{15}H_{10}O_6$	285.0405	285.0406 (100), 267.0278 (0.2), 241.0511 (0.6), 217.0503 (1.0), 199.0389 (1.8), 151.0027 (4.6), 133.0282 (22.4), 121.0280 (0.7), 107.0123 (3.6)	7.57	0.346	2,4,5
87	Quercetin[a]	$C_{15}H_{10}O_7$	301.0354	301.0354 (100), 273.0411 (3.08), 257.0453 (1.24), 229.0506 (0.91), 178.9979 (21.66), 151.0024 (48.25), 121.0280 (13.33), 107.0123 (15.03)	7.59	0.180	2,4,5
88	Patuletin (6-methoxyquercetin)	$C_{16}H_{12}O_8$	331.0464	331.0463 (100), 316.0227 (64.3), 287.0198 (11.2), 271.0249 (6.0), 259.0251 (3.0), 243.0305 (2.6), 181.0133 (5.9), 165.9897 (18.0), 139.0025 (11.3), 136.9868 (2.0), 121.0282 (2.9)	7.70	1.086	2,3,4,5
89	Nepetin (6-methoxyluteolin)	$C_{16}H_{12}O_7$	315.0514	315.0513 (84.4), 300.0277 (100), 271.0250 (0.6), 255.0302 (1.3), 243.0296 (1.8), 227.0344 (1.6), 201.0189 (3.4), 165.9899 (1.4), 136.9868 (9.0), 109.9994 (0.6)	7.74	0.965	2,3,4,5
90	Axillarin	$C_{17}H_{14}O_8$	345.0616	345.0618 (98.7), 330.0384 (100), 315.0150 (48.8), 287.0199 (13.2), 271.0233 (0.4), 259.0250 (3.6), 243.0298 (3.2), 231.0293 (5.1), 215.0345 (4.8), 175.0023 (3.7), 165.9894 (6.3), 149.0233 (11.3), 139.0389 (5.1), 136.9864 (0.7), 109.9993 (3.8)	8.25	0.172	2,3,4,5,8
91	Cirsiliol	$C_{17}H_{14}O_7$	329.0677	329.0670 (77.2), 314.0437 (100), 299.0198 (54.3), 271.0248 (12.4), 255.0311 (0.6), 243.0302 (3.1), 227.0355 (2.6), 215.0345 (11.6), 199.0397 (1.3), 165.9898 (10.1), 136.9865 (2.8), 133.0282 (5.2), 109.9995 (6.1)	8.38	0.985	1,2,3,4,5,7,8,9
92	Naringenin	$C_{15}H_{12}O_5$	271.0612	271.0614 (100), 227.0716 (1.0), 177.0183 (10.4), 151.0025 (69.6), 125.0232 (0.7), 119.0488 (55.8), 107.0124 (17.2)	8.58	-0.468	2,3,4,5
93	Apigenin[a]	$C_{15}H_{10}O_5$	269.0457	269.0456 (100), 225.0556 (1.7), 201.0556 (0.7), 151.0025 (5.3), 117.0331 (18.4), 107.0124 (4.8)	8.62	0.050	2,4,5

94	Quercetagetin-3,6,3'(4')-trimethyl ether	$C_{18}H_{16}O_8$	359.0772	359.0776 (100), 344.0540 (97.5), 329.0305 (82.6), 314.0065 (2.7), 301.0355 (3.1), 286.0121 (11.2), 258.018 (10.0), 230.0221 (6.3), 214.0262 (2.5), 165.9897 (7.0), 164.9818 (10.7), 163.0395 (2.9), 149.0230 (2.8), 148.0152 (2.2), 136.9867 (2.7), 109.9994 (5.9)	8.69	1.029	1,2,3,4,5,8,9
95	Kaempferol[a]	$C_{15}H_{10}O_6$	285.0405	285.0404 (100), 257.0450 (0.7), 239.0347 (0.9), 227.0350 (0.8), 211.0400 (1.1), 178.9920 (0.1), 151.0025 (1.7), 107.0123 (1.1)	8.80	0.031	2,4,5
96	Hispidulin (scutellarein-6-methyl ether)[a]	$C_{16}H_{12}O_6$	299.0563	299.0562 (58.8), 284.0327 (100), 255.0309 (0.9), 227.0348 (2.6), 211.0396 (2.1), 165.9897 (0.3), 139.0023 (0.7), 136.9867 (12.3), 109.9996 (0.3)	8.84	0.230	1,2,3,4,5,8,9
97	Chrysoeriol[a]	$C_{16}H_{12}O_6$	299.0562	299.0562 (100), 284.0327 (87.4), 256.0376 (19.5), 227.0349 (2.9), 211.0388 (0.4), 151.0026 (3.0), 107.0126 (2.1)	8.93	0.330	1,2,3,4,5,8,9
98	6-Methoxykaempferol	$C_{16}H_{12}O_7$	315.0512	315.0514 (100), 300.0278 (63.2), 271.0250 (42.3), 255.0297 (9.4), 243.0298 (39.0), 227.0344 (2.0), 181.0134 (2.1), 165.9898 (9.6), 139.0022 (3.3), 136.9868 (1.7), 109.9995 (5.4)	8.96	1.156	1,2,3,4,5,8,9
99	Isorhamnetin[a]	$C_{16}H_{12}O_7$	315.0512	315.0514 (100), 300.0277 (50.0), 271.0249 (8.1), 227.0341 (1.1), 151.0023 (6.3), 107.0123 (8.1), 63.0224 (5.5)	9.11	1.060	1,2,3,4,5,8
100	Jaceosidin (6-hydroxyluteolin-6,3'-dimethyl ether)[a]	$C_{17}H_{14}O_7$	329.0677	329.0671 (74.8), 314.0436 (100), 299.0200 (48.4), 271.0250 (18.6), 255.0305 (0.9), 243.0297 (4.4), 227.0351 (2.6), 215.0343 (12.2), 165.9898 (10.0), 136.9857 (1.9), 133.0280 (6.5), 109.9995 (5.3)	9.50	1.289	1,2,3,4,5,6,7,8,9
101	Quercetagetin-3,6,3'(4')-trimethyl ether	$C_{18}H_{16}O_8$	359.0772	359.0776 (100), 344.0540 (97.5), 329.0305 (82.6), 314.0065 (2.7), 301.0355 (3.1), 286.0121 (11.2), 258.0168 (10.0), 230.0221 (6.3), 214.0262 (2.5), 165.9897 (7.0), 164.9818 (10.7), 163.0395 (2.9), 149.0230 (2.8), 136.9867 (2.7), 109.9994 (5.9)	9.68	1.029	1,2,3,4,5
102	Quercetagetin-3,6,3'(4')-trimethyl ether	$C_{18}H_{16}O_8$	359.0772	359.0777 (100), 344.0540 (76.5), 329.0306 (53.8), 314.0085 (2.7), 301.0356 (13.7), 286.0120 (21.9), 258.071 (17.8), 230.0217 (9.5), 214.0270 (2.5), 165.9903 (2.5), 163.0391 (0.7), 148.0162 (2.2), 136.9873 (0.5), 109.9999 (2.2)	9.77	1.279	1,2,3,4,5
103	Cirsimaritin (6-hydroxyapigenin-6,7-dimethyl ether)	$C_{17}H_{14}O_6$	313.0719	313.0721 (100), 298.0484 (53.2), 283.0249 (50.1), 269.0457 (3.5), 255.0295 (11.5), 227.0348 (4.2), 163.0026 (13.6), 135.0073 (4.0), 117.0332 (9.9)	10.39	1.082	2,3,4,5,8
104	Eupatilin/santin	$C_{18}H_{16}O_7$	343.0812	343.0825 (81.6), 328.0590 (100), 313.0357 (59.0), 298.0122 (11.8), 285.0407 (2.9), 270.0171 (43.7), 257.0095 (3.2), 242.0216 (3.7), 214.0265 (4.7), 198.0306 (0.7), 186.0314 (7.6), 164.9819 (1.8), 136.9866 (1.1), 133.0281 (3.1), 123.0437 (3.3)	11.04		1,2,3,4,5,6,9

105	Casticin quercetagetin-tetramethyl ether	$C_{19}H_{18}O_8$	373.0932	373.0932 (100), 358.0696 (75.5), 343.0461 (71.5), 328.0232 (4.8), 315.0508 (2.1), 312.9998 (6.3), 300.0279 (13.1), 285.0042 (32.5), 257.0091 (20.0), 241.0140 (3.6), 229.0140 (7.9), 213.0185 (4.0), 185.0233 (1.0), 164.9821 (0.8), 163.0389 (0.8), 148.0158 (0.9)	11.33	0.347	1,2,3,4,5
	Tentatively annotated compound	**Molecular formula**	**Exact mass $[M+H]^+$**	**Fragmentation pattern in (+) ESI-MS/MS**	**t_R (min)**	**Δ ppm**	**Distribution**
				Sesquiterpene lactones and derivatives			
106	Dehydrocostus lactone[a]	$C_{15}H_{18}O_2$	231.1376	231.1375 (74.8), 213.1270 (19.6), 203.1432 (19.6), 195.1166 (10.6), 189.0906 (5.9), 185.1322 (100), 175.0751 (21.2), 159.1166 (29.2), 143.0853 (26.5), 131.0854 (30.9), 119.0856 (8.3), 105.0701 (29.6), 103.0545 (3.4), 95.0859 (26.1), 93.0703 (8.1), 91.0546 (14.2), 81.0704 (11.2), 67.0549 (4.4), 55.0551 (3.6)	8.51	-1.672	1,2,3,4,5,6,7,8,9
107	Hydroxyalantolactone	$C_{15}H_{20}O_3$	249.1480	249.1479 (46.9), 231.1375 (26.7), 213.1268 (11.9), 203.1426 (7.5), 185.1321 (16.7), 175.1470 (0.8), 177.1270 (21.7), 159.1167 (5.9), 143.0853 (5.5), 131.0854 (5.9), 119.0856 (7.9), 105.0701 (10.9), 97.0651 (100), 91.0546 (5.7), 79.0548 (5.8), 67.0549 (3.3), 55.0186 (1.9)	9.04	-1.971	1,2,3,4,5,6,7,8,9
108	Isoalantolactone[a]	$C_{15}H_{20}O_2$	233.1533	233.1532 (81.1), 215.1427 (55.6), 205.1584 (51.9), 197.1323 (21.9), 187.1478 (100), 161.1322 (20.3), 159.1166 (22.8), 147.1166 (48.6), 145.1166 (37.9), 133.1011 (23.1), 131.0855 (40.4), 119.0856 (32.1), 117.0700 (13.7), 105.0702 (55.4), 95.0859 (30.1), 91.0547 (28.9), 81.0704 (26.9), 79.0548 (14.2), 67.0549 (12.9), 55.0550 (8.8)	9.74	-1.357	1,2,3,4,5,6,7,8,9
109	Partenolide[a]	$C_{15}H_{20}O_3$	249.1482	249.1476 (40.5), 231.1376 (100), 213.1268 (73.4), 203.1427 (41.7), 195.1165 (19.5), 185.1322 (81.4), 173.0960 (30.2), 145.1003 (72.9), 131.0857 (46.3), 119.0856 (28.7), 105.0703 (47.0), 91.0546 (29.3), 81.0704 (17.9), 67.0550 (8.9), 55.0550 (3.3)	10.09	-1.329	1,2,3,4,5,6,7,8,9
110	Dehydroalantolactone	$C_{15}H_{18}O_2$	231.1376	231.1376 (99.5), 213.1271 (29.3), 203.1432 (6.6), 185.1323 (100), 175.0752 (17.3), 157.1010 (24.2), 143.0854 (30.8), 131.0855 (36.9), 119.0855 (12.7), 105.0702 (29.9), 95.0859 (54.1), 91.0546 (21.9), 81.0704 (20.6), 67.0550 (10.7), 55.0550 (6.8)	10.62	-1.412	1,2,3,4,5,6,7,8,9

111	Curcumene	$C_{15}H_{22}$	203.1792	203.1792 (100), 175.1481 (5.6), 161.1324 (18.9), 159.1165 (0.7), 147.1166 (59.6), 135.1167 (5.9), 133.1011 (27.7), 121.1012 (14.1), 119.0856 (31.1), 109.1014 (49.7), 95.0859 (49.7), 93.0704 (12.2), 81.0704 (29.9), 79.0549 (6.7), 67.0549 (13.4), 55.0551 (6.9)	11.38	-0.922	1,2,3,4,5,6,7,8,9
112	Curcumene isomer	$C_{15}H_{22}$	203.1792	203.1790 (100), 175.1477 (5.21), 161.1321 (8.35), 133.1010 (12.99), 121.1012 (13.70), 107.0857 (27.57), 95.0859 (40.15), 93.0703 (12.33), 81.0704 (18.96), 67.0549 (9.90), 55.0550 (4.07)	11.69	-1.069	1,2,3,4,5,6,7,8,9
113	Alantolactone[a]	$C_{15}H_{20}O_2$	233.1533	233.1530 (59.5), 215.1426 (60.4), 205.1583 (3.8), 197.1321 (19.7), 187.1478 (100), 159.1165 (30.4), 147.1165 (27.5), 133.1010 (27.3), 119.0856 (26.7), 117.0700 (12.6), 161.1322 (38.2), 145.1009 (38.8), 131.0854 (46.3), 117.0700 (12.6), 105.0701 (90.1), 95.0859 (36.2), 91.0546 (40.1), 81.0704 (39.9), 79.0548 (20.5), 67.0549 (14.2), 55.0550 (11.0)	15.74	-1.443	1,2,3,4,5,6,7,8,9
114	Farnesene	$C_{15}H_{24}$	205.1948	205.1947 (54.0), 163.1475 (8.6), 149.1323 (68.5), 135.1166 (39.1), 121.1012 (100), 107.0857 (44.9), 97.1014 (2.8), 95.0859 (49.7), 81.0704 (58.9), 71.0862 (2.5), 69.0705 (27.1), 55.0551 (16.7)	18.82	-1.449	1,2,3,4,5,6,7,8,9

[a] compare to reference standard; 1-n-hexane extract; 2-ethyl acetate extract; 3-DCM extract; 4-ethanol extract; 5-70% ethanol extract; 6-water extract; 7-n-hexane/β-CD; 8-ethyl acetate/β-CD; 9-DCM/β-CD.

Table S2. Secondary metabolites in *Inula sarana* extracts assayed by UHPLC-ESI-MS/MS in positive ion mode.

No.	Identified/tentatively annotated compound	Molecular formula	Exact mass $[M+H]^+$	Fragmentation pattern in (+) ESI-MS/MS	Δppm
			Hydroxybenzoic, hydroxycinnamic and acylquinic acids, and derivatives		
5	Protocatechuic acid[a]	$C_7H_6O_4$	155.0338	155.0339 (15.5), 137.0232 (20.1), 111.0443 (100), 93.339 (57.0), 65.0393 (53.3)	0.095
7	Neochlorogenic (3-caffeoylquinic) acid[a]	$C_{16}H_{18}O_9$	355.1023	163.0387 (100), 145.0285 (7.6), 135.0439 (14.9), 117.0337 (9.6), 89.0390 (5.7)	-
12	Vanillic acid[a]	$C_8H_8O_4$	169.0495	169.0482 (18.7), 151.0388 (24.2), 125.0597 (60.4), 111.0443 (100), 93.0339 (78.6), 65.0393 (69.9)	-1.747
24	Caffeic acid[a]	$C_9H_8O_4$	181.0495	181.0494 (2.2), 163.0387 (100), 145.0283 (14.7), 135.0440 (21.6), 117.0336 (15.9), 89.0391 (15.4)	-0.858
15	4-Hydroxybenzoic acid	$C_7H_6O_3$	139.0389	139.0387 (10.4), 111.0442 (100), 93.0339 (59.7), 65.0393 (62.6)	-1.874
16	3-Hydroxybenzoic acid	$C_7H_6O_3$	139.0389	139.0389 (13.1), 121.0285 (6.4), 111.0444 (57.6), 95.0495 (100), 93.0340 (4.0), 65.0393 (9.6)	-0.580
21	Chlorogenic (5-caffeoylquinic) acid[a]	$C_{16}H_{18}O_9$	355.1023	163.0387 (100), 145.0282 (9.0), 135.0439 (12.7), 117.0336 (8.1), 89.0391 (6.7)	-
23	4-Caffeoylquinic acid[a]	$C_{16}H_{18}O_9$	355.1023	163.0387 (100), 145.0286 (7.7), 135.0438 (13.5), 117.0336 (7.0), 89.0392 (6.3)	-
27	p-Hydroxyphenylacetic acid	$C_8H_8O_3$	153.0546	153.0547 (2.3), 135.0439 (41.1), 107.0494 (100), 95.0495 (6.5)	0.518
38	3,4-Dicaffeoylquinic acid[a]	$C_{25}H_{24}O_{12}$	517.1340	163.0387 (100), 145.0284 (10.1), 135.0439 (18.2), 117.0336 (10.7), 89.0389 (9.0)	-
40	3,5-Dicaffeoylquinic acid[a]	$C_{25}H_{24}O_{12}$	517.1340	163.0387 (100), 145.0283 (11.1), 135.0439 (17.7), 117.0337 (11.6), 89.0391 (9.4)	-
41	4,5-Dicaffeoylquinic acid	$C_{25}H_{24}O_{12}$	517.1340	163.0387 (100), 145.0282 (11.4), 135.0440 (17.5), 117.0336 (11.6), 89.0389 (6.8)	-
			Flavonoids		
68	Quercetin 7-*O*-rutinoside	$C_{27}H_{30}O_{16}$	611.1606	611.1591 (17.4), 465.1018 (16.8), 303.0481 (100), 285.0391 (2.9), 257.0434 (1.1)	-2.522
69	Rutin[a]	$C_{27}H_{30}O_{16}$	611.1606	611.1583 (1.5), 465.1015 (11.6), 303.0492 (100), 257.0427 (2.2), 229.0492 (3.0), 165.0180 (1.5), 153.0178 (2.8), 137.0230 (2.8)	-3.863
71	Isoquercitrin	$C_{21}H_{20}O_{12}$	465.1028	465.1022 (2.5), 303.0495 (100), 285.0380 (0.6), 274.0459 (0.5), 257.0429 (1.9), 229.0499 (3.5), 165.0180 (2.0), 137.0236 (4.0), 153.0183 (3.9),	0.059
72	Luteolin 7-*O*-neohesperidoside/rutinoside	$C_{27}H_{30}O_{15}$	595.1657	595.1639 (17.4), 449.1064 (29.0), 287.0542 (100), 153.0179 (4.4), 135.0439 (1.4)	-3.136

73	Patuletin *O*-rutinoside	$C_{28}H_{32}O_{17}$	641.1712	641.1681 (1.1), 486.1123 (13.2), 333.0595 (100), 318.0362 (22.7), 273.0385 (1.6), 261.0360 (0.3), 244.0366 (1.9), 169.0126 (0.5), 137.0231 (1.1),	4.891
74	Hyperoside	$C_{21}H_{20}O_{12}$	465.1028	465.1028 (5.6), 303.0495 (100), 285.0379 (0.5), 274.0461 (0.3), 257.0439 (1.5), 229.0490 (2.8), 165.0182 (1.4), 137.0235 (2.6), 153.0182 (8.0),	-1.123
75	Luteolin 7-*O*-glucoside[a]	$C_{21}H_{20}O_{11}$	449.1078	449.1066 (10.9), 287.0543 (100), 269.0439 (2.3), 241.0498 (0.3), 153.0181 (0.9), 121.0284 (1.1)	-2.756
76	Patuletin *O*-hexoside	$C_{22}H_{22}O_{13}$	495.1133	495.1104 (1.5), 333.0595 (100), 318.0362 (18.6), 290.0414 (1.90, 273.0380 (1.9), 261.0396 (0.6), 244.0359 (2.2), 169.0127 (0.9), 137.0230 (2.0)	-5.811
78	Kaempferol 3-*O*-rutinoside[a]	$C_{27}H_{30}O_{15}$	595.1657	595.1697 (1.6), 449.1062 (11.6), 287.0542 (100), 241.0506 (0.2), 231.0646 (0.4), 213.0541 (1.3), 165.0174 (1.8), 153.0182 (3.1), 121.0285 (2.1)	-3.863
79	Nepetin *O*-hexoside	$C_{22}H_{22}O_{12}$	479.1184	479.1164 (14.6), 317.0650 (100), 302.0415 (43.6), 135.0444 (0.5), 137.0235 (2.2)	4.200
80	Nepetin *O*-rutinoside	$C_{28}H_{32}O_{16}$	625.1763	625.1724 (0.9), 479.1175 (13.1), 317.0649 (100), 302.0414 (23.9), 274.0450 (1.5), 256.0363 (0.4), 229.0490 (1.1), 147.0650 (1.4), 129.0545 (3.6)	-6.320
81	Kaempferol 3-*O*-glucoside[a]	$C_{21}H_{20}O_{11}$	449.1078	449.1052 (25.3), 287.0544 (100), 153.0182 (2.1)	-5.896
82	Isorhamnetin 3-*O*-glucoside[a,b]	$C_{22}H_{22}O_{12}$	479.1184	479.1188 (1.4), 317.0649 (100), 302.0415 (6.5), 274.0463 (3.9), 246.0512 (1.8), 229.0493 (3.3), 165.0182 (0.3), 153.0181 (7.4)	-0.005
83	Chrysoeriol *O*-hexoside	$C_{22}H_{22}O_{11}$	463.1234	463.1225 (18.1), 301.0699 (100), 286.0465 (34.7), 258.0518 (11.4), 229.0491 (0.3), 168.0050 (3.3)	-2.133
84	Cirsiliol *O*-hexoside	$C_{23}H_{24}O_{12}$	493.1340	493.1330 (16.9), 331.0802 (100), 315.0491 (10.4), 301.0326 (1.8), 298.0462 (5.4), 273.0387 (12.0)	
85	Spinacetin	$C_{17}H_{14}O_{8}$	347.0761	347.0755 (100), 332.0518 (31.6), 317.0289 (4.8), 289.0338 (7.6), 261.0391 (5.4), 233.0438 (0.5), 168.0051 (8.4)	-1.942
86	Luteolin[a]	$C_{15}H_{10}O_{6}$	287.0550	287.0544 (100), 269.0435 (0.8), 241.0490 (0.9), 231.0660 (0.1), 213.0550 (0.3), 203.0340 (0.2), 153.0182 (10.5), 137.0234 (1.5), 135.0441 (3.6),	-2.106
87	Quercetin[a]	$C_{15}H_{10}O_{7}$	303.0499	303.0492 (100), 285.1217 (5.5), 257.0446 (1.7), 229.0493 (8.2), 153.0183 (7.9), 137.0233 (5.9)	-2.538
88	Patuletin (6-methoxyquercetin)	$C_{16}H_{12}O_{8}$	333.0605	333.0597 (100), 318.0364 (28.1), 273.0381 (2.7), 168.0051 (0.7), 137.0235 (3.3),	-2.413
89	Nepetin (6-methoxyluteolin)	$C_{16}H_{12}O_{7}$	317.0656	317.0651 (100), 302.0418 (17.5), 274.0467 (30.8), 203.0336 (0.8), 153.0180 (0.9), 178.0869 (2.9), 132.0809 (3.5)	-1.637
90	Axillarin	$C_{17}H_{14}O_{8}$	347.0761	347.0738 (100), 332.0518 (13.5), 317.0293 (2.7), 289.0336 (11.7), 168.0052 (1.6), 137.0233 (1.2)	-0.205
91	Cirsiliol	$C_{17}H_{14}O_{7}$	331.0803	331.0806 (100), 315.0493 31.10), 301.0337 (1.1), 273.0389 (1.6), 245.0435 (0.1), 163.0179 (1.1), 137.0218 (0.1), 136.0147 (0.2)	-1.901
93	Apigenin[a]	$C_{15}H_{10}O_{5}$	271.0601	271.0597 (100), 243.0635 (0.5), 229.0477 (0.3), 163.0383 (0.7), 153.0182 (10.1), 121.0285 (1.4), 119.0493 (5.5)	8.61

94	Quercetagetin 3,6,3'(4')-trimethyl ether	$C_{18}H_{16}O_8$	361.0918	361.0915 (100), 346.0676 (30.3), 331.0446 (1.4), 316.0229 (0.2), 257.0435 (2.1), 229.0493 (11.9), 168.0052 (7.0), 163.0385 (0.9), 139.0028 (0.3)	1.112
96	Hispidulin (scutellarein-6-methyl ether)[a]	$C_{16}H_{12}O_6$	301.0707	301.0700 (100), 286.0465 (24.0), 258.0517 (28.7), 229.0494 (1.9), 168.0050 (1.1), 121.0295 (0.4),	-0.372 -2.075
99	Isorhamnetin[a]	$C_{16}H_{12}O_7$	317.0656	317.0650 (100), 302.0430 (4.2), 153.0182 (6.5)	-1.827
100	Jaceosidin (6-hydroxyluteolin-6,3'-dimethyl ether)[a,b]	$C_{17}H_{14}O_7$	331.0812	331.0803 (100), 316.0570 (35.6), 301.0335 (7.4), 273.0388 (9.1), 245.0439 (6.7), 168.0051 (12.1)	-2.746
101	Quercetagetin 3,6,3'(4')-trimethyl ether	$C_{18}H_{16}O_8$	361.0918	361.0909 (100), 346.0675 (24.3), 331.0426 (2.4), 316.0219 (0.3), 257.0440 (3.1), 229.0493 (18.3), 169.0131 (5.3), 137.0226 (0.5), 119.0493 (0.4)	-2.448
103	Cirsimaritin (6-hydroxyapigenin-6,7-dimethyl ether)a,[b]	$C_{17}H_{14}O_6$	315.0863	315.0857 (100), 299.0546 (29.3), 285.0388 (1.4), 271.0597 (9.0), 242.0569 (2.4), 153.0182 (0.6)	-1.887

Table S3. The equations, range and R^2 values of standard compounds in the biological activity assays

Assays	**Equation**	**Range**	**R^2**
Total phenolic content (for Gallic acid)	Absorbance (y): 0.2199 x (µg gallic acid)	0-5 µg	0.9993
Total flavonoid content (for Rutin)	Absorbance (y): 0.1274 x (µg rutin)+0.0506	0-20 µg	0.9968
DPPH radical scavenging (for Trolox)	Absorbance: 14.135x (µg trolox)+1.5632	0-5 µg	0.9944
ABTS radical scavenging (for Trolox)	Absorbance: 12.054x (µg trolox)-1.9894	0-2.5 µg	0.9800
CUPRAC (for Trolox)	Absorbance: 0.1328x (µg trolox)+0.002	0-2.5 µg	0.9993
FRAP (for Trolox)	Absorbance: 0.3166x (µg trolox)+0.003	0-2.5 µg	0.9999
Phosphomolybdenum (for Trolox)	Absorbance: 0.062x (µg trolox)-0.027	0-100 µg	0.9998
Metal chelating (for EDTA)	Absorbance: 13.314x (µg EDTA)-3.5881	0-4 µg	0.9786
AChE inhibition (for Galanthamine)	Absorbance: 185.44x (µg galanthamine)+0.5502	0-0.2 µg	0.9962
BChE inhibition (for Galanthamine)	Absorbance: 187.96x (µg galanthamine)-0.1896	0-0.2 µg	0.9917
Tyrosinase inhibition (for Kojic acid)	Absorbance: 1.5235x (mg kojic acid)+0.0055	0-0.3 mg	0.9981
Amylase inhibition (for Acarbose)	Absorbance: 2.0654x (µg acarbose)+4.0458	0-50 µg	0.9543
Glucosidase inhibition (for Acarbose)	Absorbance: 2.1183 (µg acarbose)-02336	0-50 µg	0.9410

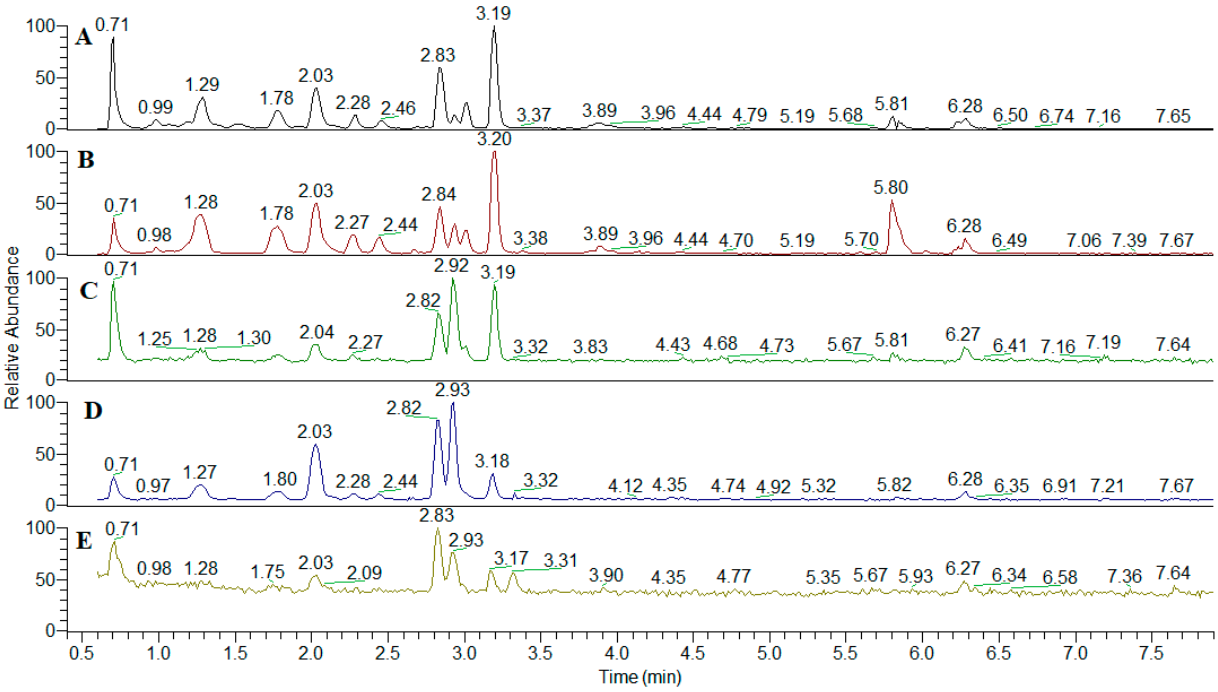

Figure S1. Extracted ion chromatograms of hydroxybenzoic and hydroxycinnamic acids and their derivatives; **A**—ethanol/water extract; **B**—ethanol extract; **C**—dichloromethane extract; **D**—ethyl acetate extract; **E**—hexane extract.

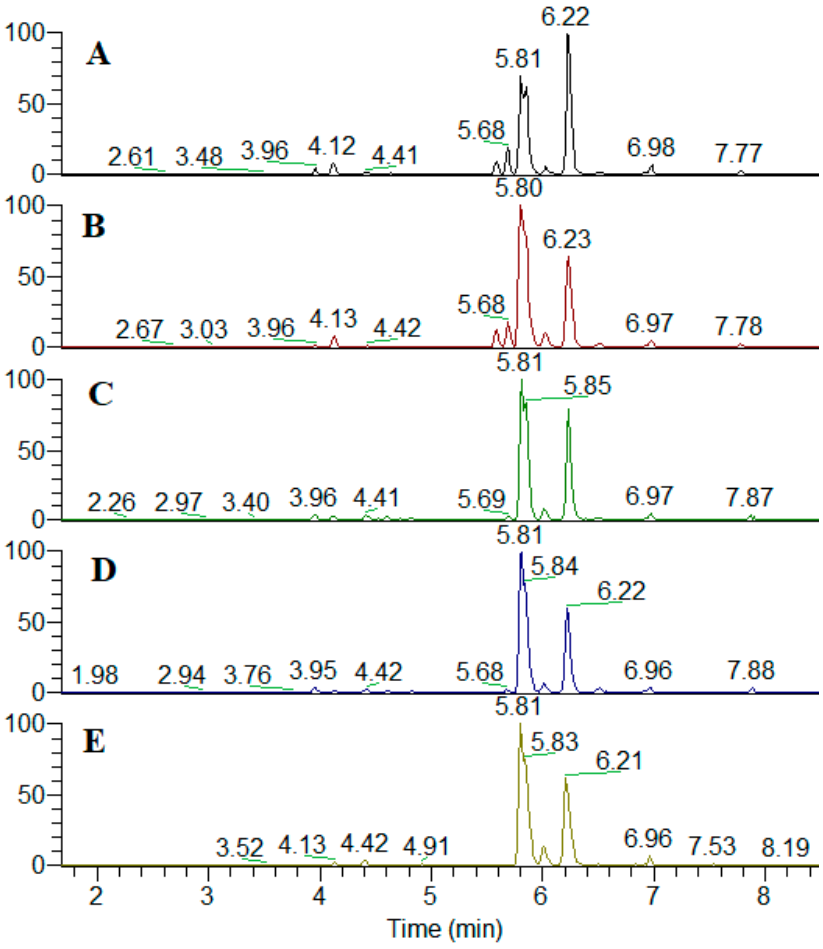

Figure S2. Extracted ion chromatograms of acylquinic acids; **A**—ethanol/water extract; **B**—ethanol extract; **C**—dichloromethane extract; **D**—ethyl acetate extract; **E**—hexane extract.

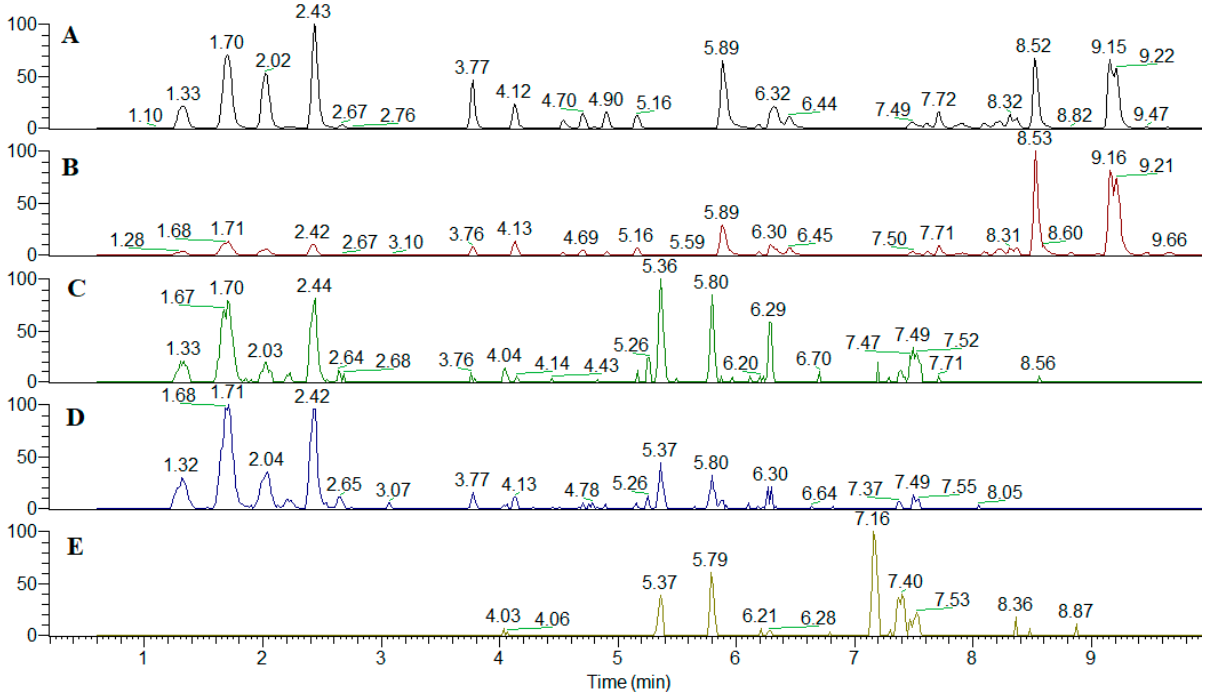

Figure S3. Extracted ion chromatograms of caffeoylhexaric acids; **A**—ethanol/water extract; **B**—ethanol extract; **C**—dichloromethane extract; **D**—ethyl acetate extract; **E**—hexane extract.

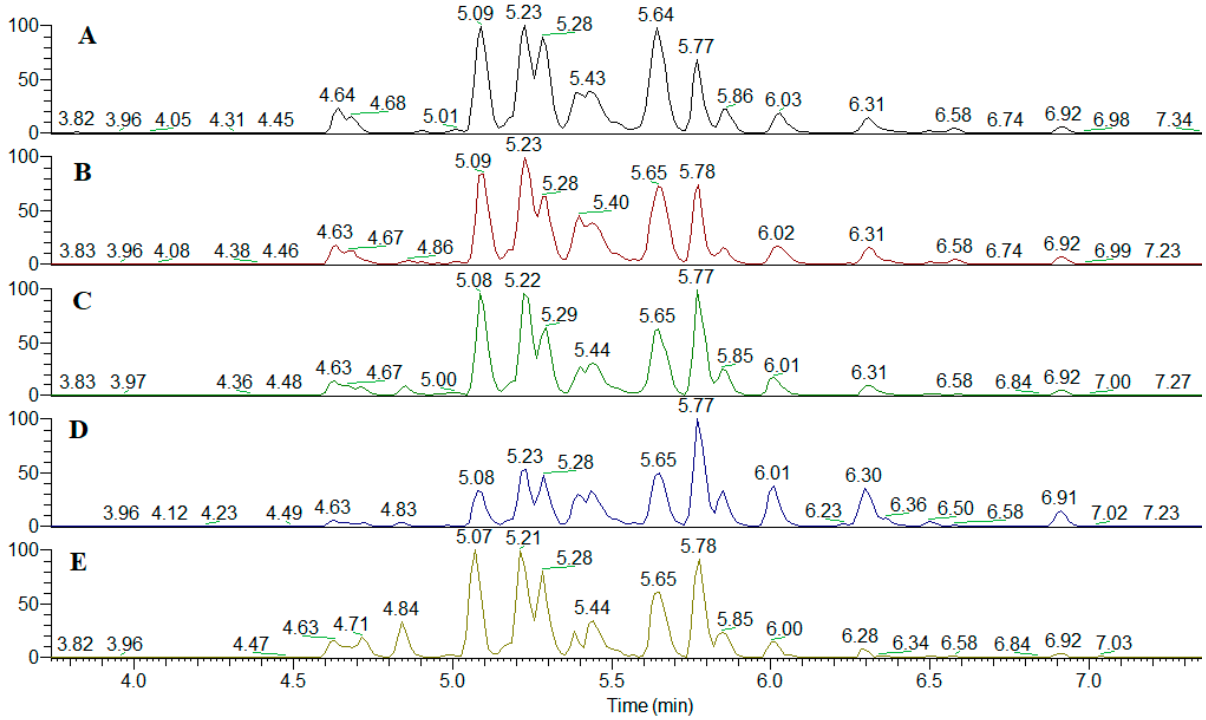

Figure S4. Extracted ion chromatograms of flavonoid glycosides; **A**—ethanol/water extract; **B**—ethanol extract; **C**—dichloromethane extract; **D**—ethyl acetate extract; **E**—hexane extract.

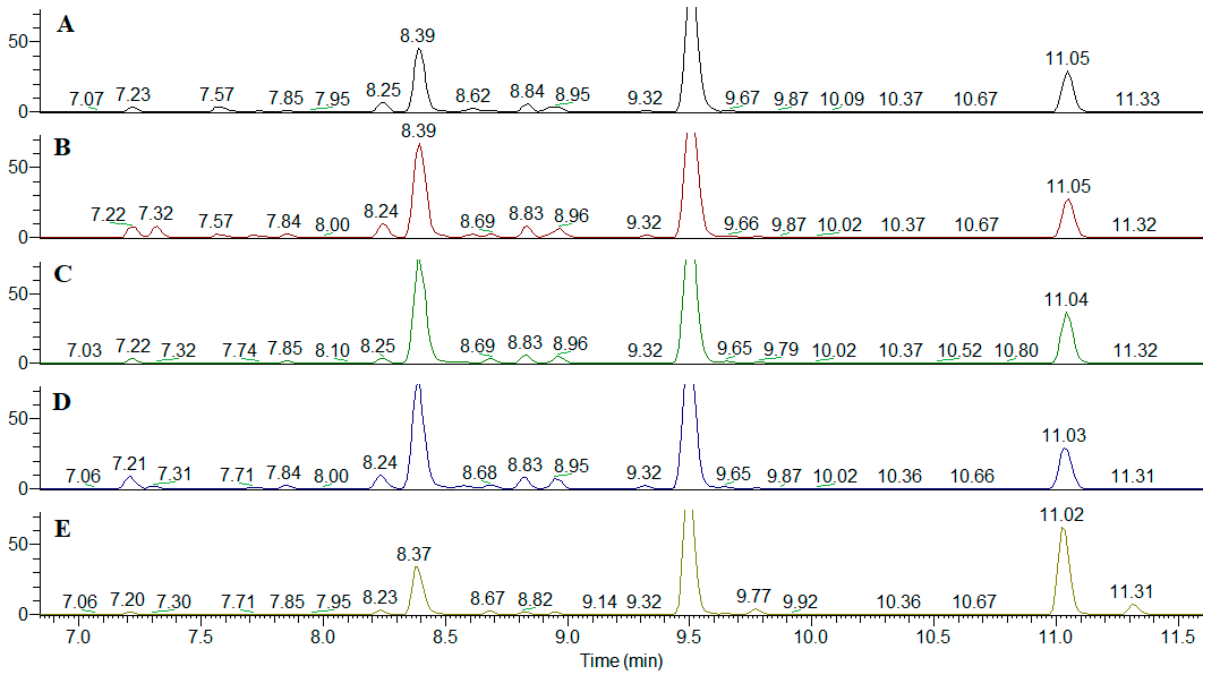

Figure S5. Extracted ion chromatograms of flavonoid aglycons; **A**—ethanol/water extract; **B**—ethanol extract; **C**—dichloromethane extract; **D**—ethyl acetate extract; **E**—hexane extract.

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