

Supplementary Data

**Targeted offline two-dimensional HPLC and UHPLC-Orbitrap-MS
combined with molecular networking reveal the effect of processing
on chemical constituents of Xuetong (the stem of *Kadsura heteroclita*)**

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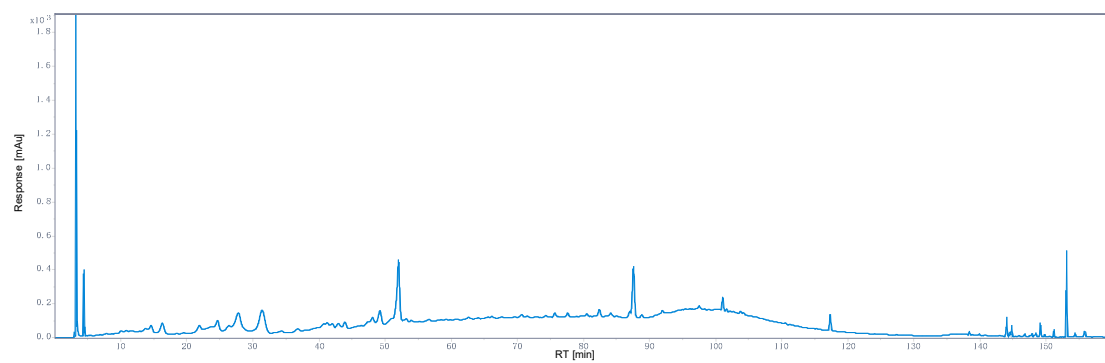


Figure S1. Optimized 1D HPLC chromatogram of Xueting.

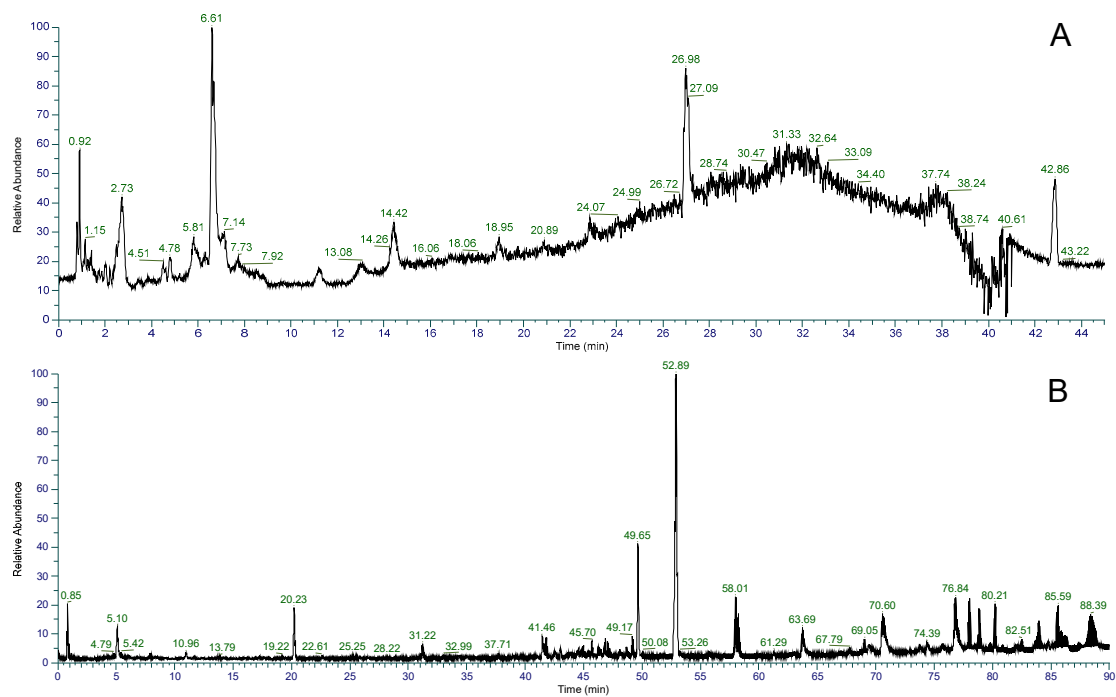


Figure S2. Total ion chromatogram (TIC) in the positive model of F1 (A) and F2 (B).

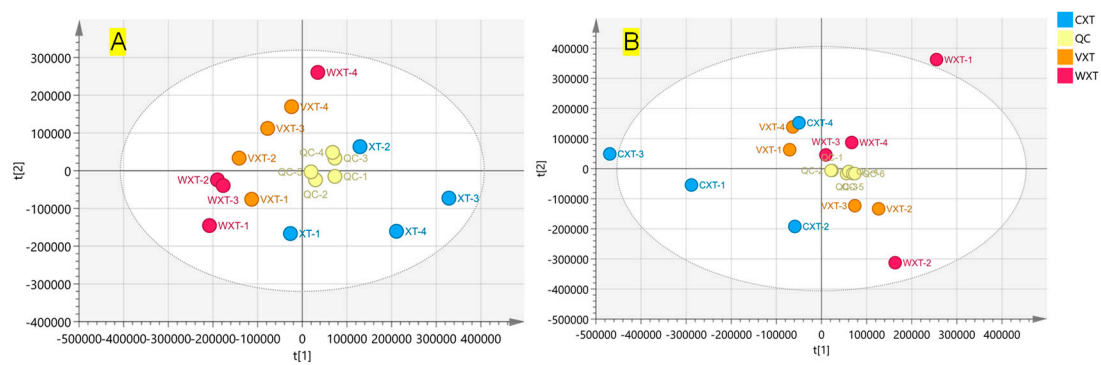


Figure S3. PCA scoring plot of ²D LC-MS data of F1 (A) and F2 (B).

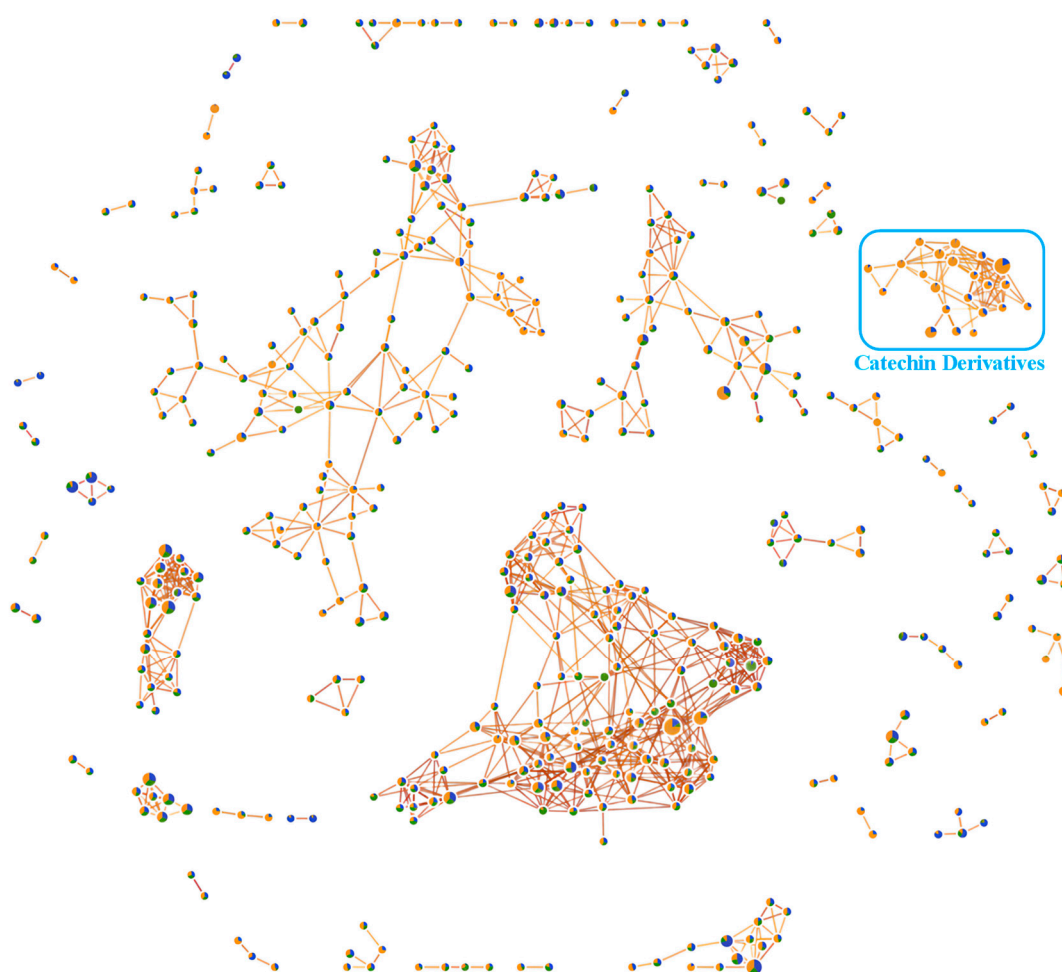


Figure S4. Molecular networking constructed by ^2D UHPLC-MS data of F1.

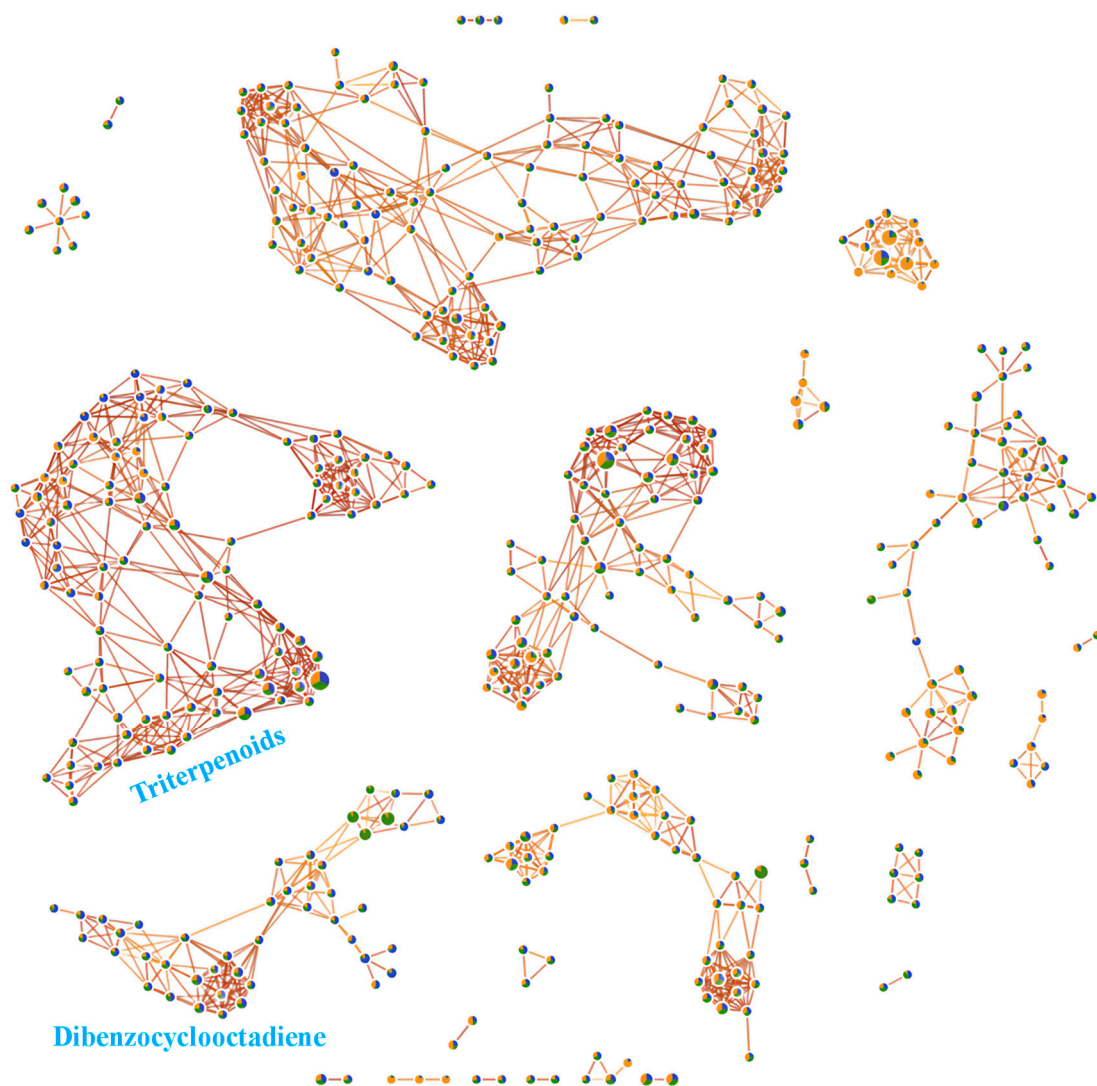


Figure S5. Molecular networking constructed by ²D UHPLC-MS data of F2 in positive mode.

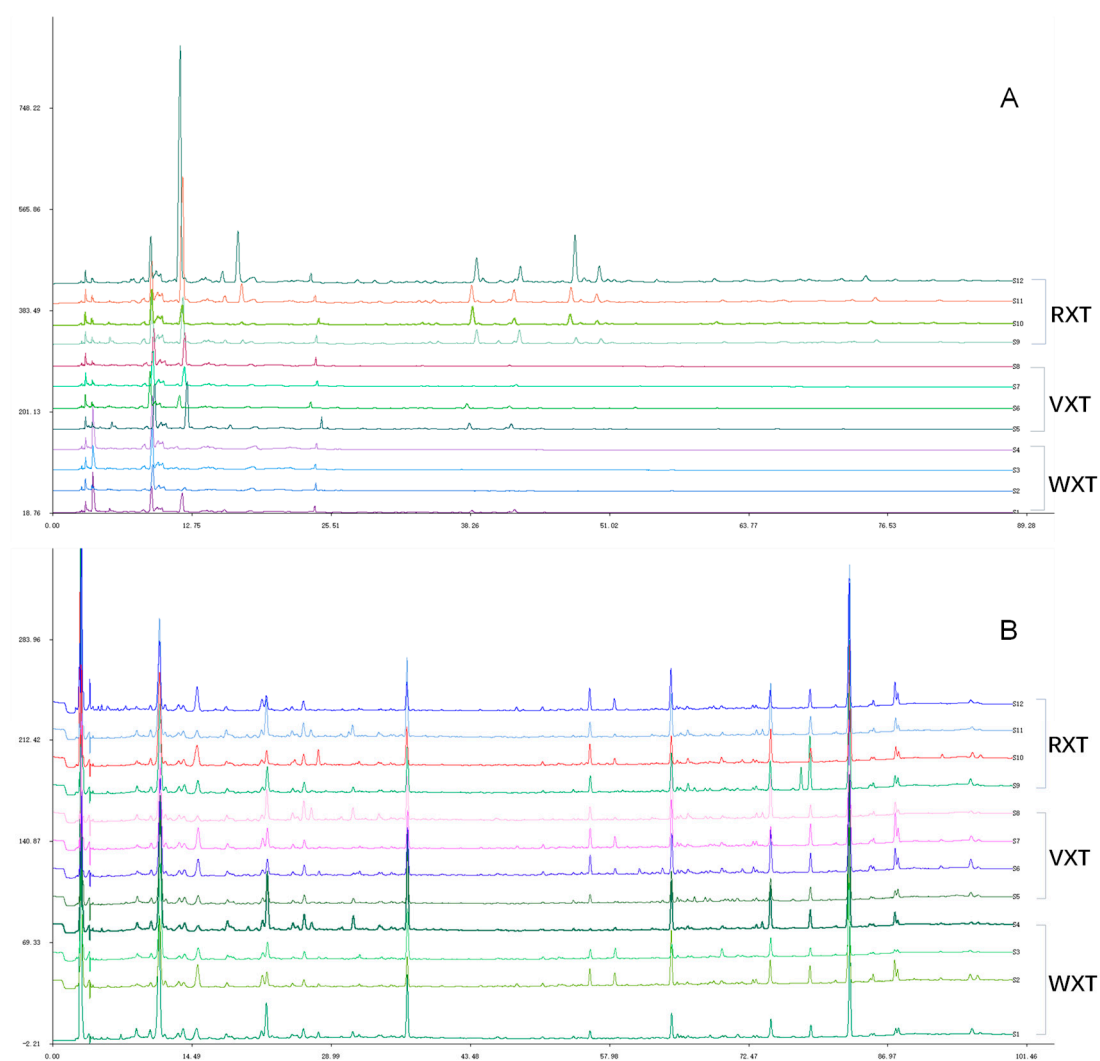


Figure S6. 2D HPLC Fingerprints of F1 (A) and F2 (B) of RXT (S9-S12), VXT (S5-S8), and WXT (S1-S4).

Table S1. Compounds identification of F1 by ²D UHPLC-MS analysis.

No.	RT (min)	Compound	Molecular formular	Adduct	Experimental m/z	Error (ppm)	MS ² fragment	Identification	Class
A1	0.847	Methyl 4-hydroxycinnamate	C ₁₀ H ₁₀ O ₃	[M-H] ⁻	177.05573	0.07	177.05565, 162.03217, 145.02946, 117.03455	mzVault	Phenol
A2	0.893	4-Hydroxybenzaldehyde isomer	C ₇ H ₆ O ₂	[M-H] ⁻	121.02954	0.31	121.02952, 92.02673, 79.95729, 65.03951	mzCloud	Phenol
A3	0.917	2,5-Dihydroxybenzaldehyde isomer	C ₇ H ₆ O ₃	[M-H] ⁻	137.02443	0.09	137.02434, 119.01384, 93.03458, 91.01890, 81.03451, 65.03977	mzCloud	Phenol
A4	1.028	Salicylic acid isomer	C ₇ H ₆ O ₃	[M-H] ⁻	137.02442	0.02	111.04506, 96.02216, 93.03450, 83.05022, 73.02946, 55.01877	mzCloud	Phenol
A5	1.040	4-Hydroxybenzaldehyde isomer	C ₇ H ₆ O ₂	[M-H] ⁻	121.02954	0.31	121.02948, 94.02981, 93.02066, 79.95729	mzCloud	Phenol
A6	1.140	6-Methoxysalicylic acid isomer	C ₈ H ₈ O ₄	[M-H] ⁻	167.03449	-2.95	152.01147, 139.04007, 123.04507, 108.02158, 109.02958, 93.03444, 91.01878, 81.03443	mzCloud	Phenol
A7	1.245	Ferulic acid	C ₁₀ H ₁₀ O ₄	[M-H] ⁻	193.05061	-0.11	134.03731, 117.03454, 106.04237, 89.03948	mzCloud	Phenol
A8	1.247	Esculetin	C ₉ H ₆ O ₄	[M-H] ⁻	177.01934	0.05	149.02451, 139.04018, 133.02953, 121.02973, 105.03458, 97.02988, 89.03970, 81.03442, 77.03954	mzVault	Phenol
A9	1.406	4-(Hydroxymethyl)benzoic acid	C ₈ H ₈ O ₃	[M-H] ⁻	151.04010	0.22	125.02448, 123.00883, 107.05023, 95.01379, 81.03458, 67.01893, 51.02399	mzCloud	Phenol
A10	1.422	Gentisic acid isomer	C ₇ H ₆ O ₄	[M-H] ⁻	153.01933	-0.01	109.02953, 91.01882, 81.03457, 79.01902, 69.03467, 65.03975	mzCloud	Phenol
A11	1.430	Catechol	C ₆ H ₆ O ₂	[M-H] ⁻	109.02957	0.62	91.01910, 81.03469, 67.97457	mzCloud	Phenol
A12	1.531	2,5-Dihydroxybenzaldehyde isomer	C ₇ H ₆ O ₃	[M-H] ⁻	137.02442	0.02	137.02435, 109.02945, 93.03448, 81.03451, 65.03967	mzCloud	Phenol
A13	1.759	L-(-)-3-Phenyllactic acid	C ₉ H ₁₀ O ₃	[M-H] ⁻	165.05574	0.14	147.04521, 119.05025, 101.03978, 91.05533, 72.99311	mzCloud	Phenol

A14	2.603	Ethyl gallate	C ₉ H ₁₀ O ₅	[M-H] ⁻	197.04555	0.02	203.08704, 197.04523, 137.02441, 125.02443, 111.04513, 95.05023, 83.01377, 71.01380, 59.01385, 57.03456	mzCloud	Phenol
A15	2.748	Schizzandriside isomer	C ₂₅ H ₃₂ O ₁₀	[M-H] ⁻	491.19176	-1.04	359.14868, 313.10718, 241.05029, 203.08678, 159.04492, 147.04500, 109.02937, 89.02428, 71.01375, 59.01377	Fragmentation pattern	Lignan
A16	2.939	Gallic acid	C ₇ H ₆ O ₅	[M-H] ⁻	169.01427	0.14	125.02435, 97.02922, 81.03447, 69.03459	mzCloud	Phenol
A17	2.983	2-(3,4-Dihydroxyphenyl)-2H-chromene-3,5,7-triol	C ₁₅ H ₁₂ O ₆	[M-H] ⁻	287.05631	0.69	259.06125, 243.06552, 219.06581, 201.05524, 175.03979, 159.04478, 137.02437, 125.02446, 121.02939, 109.02957, 83.01384, 57.03453	Network	Catechin
A18*	3.026	Catechin	C ₁₅ H ₁₄ O ₆	[M-H] ⁻	289.07167	-0.32	245.08131, 221.08116, 205.05016, 159.04437, 151.03947, 149.02394, 125.02407, 123.04477, 109.02924, 97.02929, 83.01350, 57.03448	Network, FISh	Catechin
A19	4.788	Salicylic acid isomer	C ₇ H ₆ O ₃	[M-H] ⁻	137.02443	0.09	108.02214, 93.03452, 68.01425, 65.99849	mzCloud	Phenol
A20	5.101	Protocatechuic acid	C ₇ H ₆ O ₄	[M-H] ⁻	153.01936	0.18	135.00888, 109.02959, 91.01911, 67.01893, 65.03970	mzCloud	Phenol
A21	5.278	Salicylic acid isomer	C ₇ H ₆ O ₃	[M-H] ⁻	137.02441	-0.05	108.02139, 93.03461, 65.01446	mzCloud	Phenol
A22	5.870	1- <i>O</i> -Vanilloyl- β -D-glucose	C ₁₄ H ₁₈ O ₉	[M-H] ⁻	329.08783	0.08	203.08685, 167.03494, 152.01146, 123.04514, 108.02159, 91.01911	mzVault	Phenol
A23	5.872	Vanillic acid	C ₈ H ₈ O ₄	[M-H] ⁻	167.03493	-0.31	152.01134, 123.04509, 108.02151	mzVault	Phenol
A24	6.012	4-{(1R,2S)-1,3-Dihydroxy-2-[4-(3-hydroxypropyl)-2-methoxyphenoxy]propyl}-2-methoxyphenyl- β -D-glucopyranoside	C ₂₆ H ₃₆ O ₁₂	[M+Na] ⁺	563.20964	-0.46	468.09744, 401.15884, 353.13516, 203.05185, 137.05393, 107.04855, 91.05409	mzCloud	Lignan

A25	6.032	Syringic acid	C ₉ H ₁₀ O ₅	[M-H] ⁻	197.04551	-0.19	182.02194, 166.99855, 138.03210, 123.00871, 95.01365, 67.01908, 61.98830	mzCloud	Phenol
A26	6.039	3,4,5-Trihydroxy-6-(hydroxymethyl)oxan-2-yl 3-hydroxy-4,5-dimethoxybenzoate	C ₁₅ H ₂₀ O ₁₀	[M+Na] ⁺	383.09491	0.11	221.04164, 202.05853, 185.04102, 124.01253	mzCloud	Phenol
A27	6.941	3,4'-Dihydroxypropiofenone-3-β-D-glucoside	C ₁₅ H ₂₀ O ₈	[M-H] ⁻	327.10957	3.15	203.08630, 147.04500, 101.02418, 89.02428, 71.01375, 59.01372	mzCloud	Phenol
A28*	7.930	Gallocatechin	C ₁₅ H ₁₄ O ₇	[M-H] ⁻	305.06601	-2.18	203.08698, 179.03506, 167.03516, 137.02415, 125.02447, 109.02922, 96.95994	Network	Catechin
A29	13.651	Gentisic acid isomer	C ₇ H ₆ O ₄	[M-H] ⁻	153.01933	-0.01	109.02940, 81.03468	mzCloud	Phenol
A30	18.878	Procyanidin B1 isomer	C ₃₀ H ₂₆ O ₁₂	[M-H] ⁻	577.13531	0.28	407.07584, 289.07230, 203.08670, 161.02477, 125.02428, 137.02422	Network, FISH	Catechin
A31	19.658	Rutin	C ₂₇ H ₃₀ O ₁₆	[M-H] ⁻	609.14628	0.28	300.02798, 271.02478, 255.02893, 243.02908, 227.03461,	mzCloud	Phenol
A32	19.830	Catechin 3- <i>O</i> -β-D-glucopyranoside isomer	C ₂₁ H ₂₄ O ₁₁	[M-H] ⁻	451.12402	-1.25	289.17166, 245.08141, 203.08759, 151.04019, 123.04498, 109.02909, 97.02923, 57.03423	Network, FISH	Catechin
A33	19.830	2-(3,4-Dihydroxyphenyl)-2H-chromene-3,5,7-triol-β-D-glucopyranoside	C ₂₁ H ₂₂ O ₁₁	[M-H] ⁻	449.10827	-1.48	287.05640, 259.06097, 243.06654, 229.05089, 203.03566, 201.05482, 177.02005, 175.04037, 165.01923, 149.02467, 121.02998, 109.02977, 83.01429	Network	Catechin
A34	20.457	Catechin 3- <i>O</i> -β-D-glucopyranoside isomer	C ₂₁ H ₂₄ O ₁₁	[M-H] ⁻	451.12392	-1.47	289.07117, 245.08128, 203.08871, 179.03555, 137.02428, 123.04485, 109.02930, 97.02939, 57.03455	Network, FISH	Catechin

A35	21.638	Procyanidin A2	C ₃₀ H ₂₄ O ₁₂	[M-H] ⁻	575.11973	0.40	423.07172, 407.07715, 361.07065, 325.07159, 309.04086, 307.06161, 297.03979, 285.03851, 167.03508, 165.05579, 150.03265, 125.02442, 109.02969, 83.01373, 71.01386, 61.98850	Network, FISh	Catechin
A36*	21.656	Procyanidol B4	C ₃₀ H ₂₆ O ₁₂	[M-H] ⁻	577.13513	-0.03	425.08759, 407.07602, 339.08646, 289.07159, 255.02930, 245.08206, 203.08826, 161.02443, 123.04505, 125.02433	Network, FISh	Catechin
A37	22.680	Procyanidin B1 isomer	C ₃₀ H ₂₆ O ₁₂	[M-H] ⁻	577.13541	0.45	407.07642, 289.07123, 203.08733, 166.05421, 161.02446, 125.02443, 123.04532	Network, FISh	Catechin
A38	24.490	Procyanidin	C ₃₀ H ₂₆ O ₁₃	[M-H] ⁻	593.13030	0.40	407.07584, 339.08524, 289.07104, 255.03032, 177.01932, 125.02413, 109.02939, 93.03460	Network	Catechin
A39	37.423	3-[2-(1,3-Benzodioxol-5-yl)-7-methoxy-1-benzofuran-5-yl]-3-hydroxypropyl hexopyranoside	C ₂₅ H ₂₈ O ₁₁	[M-H] ⁻	503.16120	10.56	221.06677, 203.08679, 179.05559, 161.04543, 143.03554, 119.03513, 113.02423, 89.02438, 71.01385, 59.01381	mzCloud	Phenol

*Verified by the reference standards.

Table S2. Lignans in F2 identified by ²D UHPLC-MS analysis.

No.	RT (min)	Compound	Molecular formular	Adduct	Calculated m/z	Experimental m/z	Error (ppm)	MS ² fragment	Identification
B1[#]	2.017	Isolarisiresinol 9-O-(4"-O-rhamnosyl)-xylopyranoside	C ₃₁ H ₄₂ O ₁₄	[M-H] ⁻	637.25018	637.25170	2.39	513.17438, 491.19366, 359.14883, 325.10928, 311.09177, 297.90210, 203.08755, 201.07138, 112.98578	FISh
B2[#]	4.518	Isolarisiresinol 9-O-(4"-O-xylopyranosyl)-xylopyranoside	C ₃₀ H ₄₀ O ₁₄	[M-H] ⁻	623.23453	623.23410	-0.69	491.19397, 359.14917, 341.13861, 203.08670, 201.07129, 109.02927, 71.01406	Network, FISh
B3	4.698	Schizandriside isomer	C ₂₅ H ₃₂ O ₁₀	[M-H] ⁻	491.19227	491.19151	-1.55	359.14883, 341.13797, 311.09225, 241.05109, 203.08752, 201.07120, 89.02441, 71.01388, 59.01380	Network, FISh
B4[*]	5.101	Schizandriside (Isolarisiresinol 9-O-β-D-xylopyranoside)	C ₂₅ H ₃₂ O ₁₀	[M-H] ⁻	491.19227	491.19142	-1.73	359.14941, 341.13928, 313.10901, 311.09369, 203.08755, 201.07181, 173.06128, 15904570, 109.03001, 89.02457, 71.01396, 59.01392	Network, FISh
B5	6.099	Schizandriside isomer	C ₂₅ H ₃₂ O ₁₀	[M-H] ⁻	491.19227	491.19154	-1.49	359.14923, 341.13818, 203.08734, 201.07153, 159.04575, 109.03043, 89.02482, 71.01411, 59.01386	Network, FISh
B6	8.342	Secoisolariciresinol-9-O-β-D-xylopyranoside	C ₂₅ H ₃₄ O ₁₀	[M-H] ⁻	493.20792	493.20720	-1.46	361.16437, 343.15414, 313.14450, 203.08699, 201.07120, 161.06088, 121.02970, 59.01384	Network
B7	9.368	Schizandriside isomer	C ₂₅ H ₃₂ O ₁₀	[M-H] ⁻	491.19227	491.19150	-1.57	341.13934, 311.12875, 281.08286, 203.08734, 201.07124, 121.02978, 71.01399	Network
B8	17.410	Schizandriside isomer	C ₂₅ H ₃₂ O ₁₀	[M-H] ⁻	491.19227	491.19150	-1.57	359.14923, 201.07161, 121.02980, 71.01411	Network, FISh
B9[#]	13.647	8-Hydroxyoxomatairesinol-β-D-glucopyranoside	C ₂₆ H ₃₀ O ₁₃	[M-H] ⁻	549.16136	549.16100	-0.66	387.10751, 369.09760, 343.11719, 203.08696, 201.07124, 121.02967, 83.01395	Network, FISh
B10[#]	17.236	6-Hydroxyhinokinin-6-O-(4"-O-xylopyranosyl)-β-D-glucopyranoside	C ₃₁ H ₃₆ O ₁₆	[M+HCOO] ⁻	709.19854	709.19819	-0.49	369.09717, 325.10892, 297.11258, 203.08678, 201.07196, 121.02959, 83.01393	Network, FISh

B11[#]	17.466	6-Hydroxyhinokinin-6- <i>O</i> -(4"- <i>O</i> -rhamnosyl)- β -D-glucopyranoside	C ₃₂ H ₃₈ O ₁₆	[M+HCOO] ⁻	723.21419	723.21402	-0.23	369.09753, 325.10886, 297.11261, 203.08679, 201.07166, 161.06067, 121.02974, 83.01382	Network, FISH
B12[#]	17.541	6-Hydroxyhinokinin-6- <i>O</i> -(4"- <i>O</i> -xylopyranosyl)- β -D-glucopyranoside isomer	C ₃₁ H ₃₆ O ₁₆	[M+HCOO] ⁻	709.19854	709.19846	-0.11	369.09668, 325.10849, 203.08716, 201.07149, 121.03005, 107.05068, 83.01434	FISH
B13[#]	18.746	6-Hydroxyhinokinin-6- <i>O</i> -(4"- <i>O</i> -rhamnosyl)- β -D-glucopyranoside isomer	C ₃₂ H ₃₈ O ₁₆	[M+HCOO] ⁻	723.21419	723.21414	-0.06	369.09775, 325.10883, 203.08732, 201.07095, 121.02969, 112.98572	FISH
B14[#]	18.902	6-Hydroxyhinokinin-6- <i>O</i> -(4"- <i>O</i> -xylopyranosyl)- β -D-glucopyranoside isomer	C ₃₂ H ₃₈ O ₁₆	[M-H] ⁻	663.19306	663.19298	-0.12	369.09796, 325.10696, 203.08701, 201.07106, 121.02971, 83.01402	FISH
B15	19.206	6-Hydroxyhinokinin-6- <i>O</i> - β -D-glucopyranoside isomer	C ₂₆ H ₂₈ O ₁₂	[M+HCOO] ⁻	577.15628	577.15786	2.741	369.09631, 325.10941, 203.08705, 201.07144, 201.05038, 121.03004, 82.93755, 79.96176	FISH
B16	20.020	6-Hydroxyhinokinin-6- <i>O</i> - β -D-glucopyranoside isomer	C ₂₆ H ₂₈ O ₁₂	[M+HCOO] ⁻	577.15628	577.15630	0.038	369.09641, 325.1913, 203.08659, 201.07159, 121.02929, 83.01390	FISH
B17[*]	20.230	6-Hydroxyhinokinin-6- <i>O</i> - β -D-glucopyranoside	C ₂₆ H ₂₈ O ₁₂	[M+HCOO] ⁻	577.15628	577.15594	-0.59	369.09729, 325.10919, 203.08707, 201.07124, 121.02929, 102.94852, 83.01415	FISH
B18	20.391	6-Hydroxyhinokinin-6- <i>O</i> - β -D-glucopyranoside isomer	C ₂₆ H ₂₈ O ₁₂	[M+HCOO] ⁻	577.15628	577.15610	-0.31	369.09619, 325.10788, 203.08705, 201.07150, 121.02946, 83.01378	FISH

B19	21.690	6-Hydroxyhinokinin-6- <i>O</i> - β -D-glucopyranoside isomer	C ₂₆ H ₂₈ O ₁₂	[M+HCOO] ⁻	577.15628	577.15625	-0.05	369.09802, 325.10593, 203.08701, 201.07144	FISh
B20[#]	23.931	6-Hydroxyhinokinin-6- <i>O</i> -xylopyranoside	C ₂₅ H ₂₆ O ₁₁	[M+HCOO] ⁻	547.14571	547.14548	-0.43	369.09683, 325.10901, 297.11273, 201.07121, 121.02987, 102.94897, 83.03649, 61.98861	FISh
B21[*]	31.203	6-Hydroxyhinokinin	C ₂₀ H ₁₈ O ₇	[M-H] ⁻	369.09798	369.09669	-3.48	325.10901, 297.11218, 203.08704, 210.07178, 175.07655, 135.04507, 121.02951, 107.05031, 121.02951, 83.01385	Network, FISh
B22	32.014	6-Hydroxyhinokinin isomer	C ₂₀ H ₁₈ O ₇	[M-H] ⁻	369.09798	369.09682	-3.13	325.10825, 297.11148, 150.03204, 121.02922, 107.05048, 83.01407	FISh
B23	32.867	6-Hydroxyhinokinin isomer	C ₂₀ H ₁₈ O ₇	[M-H] ⁻	369.09798	369.09689	-2.94	325.10767, 297.11118, 203.08760, 201.07083, 121.02984, 83.01392	Network
B24	35.958	Kadsuranin isomer	C ₃₀ H ₃₆ O ₁₁	[M+Na] ⁺	595.21498	595.21510	0.198	495.16284, 435.14282, 413.16025, 385.16501, 371.14883, 356.12485, 340.13058, 329.10776, 325.10776, 309.11310, 295.09689, 265.06646, 251.07033, 237.05473, 235.07753, 211.07497, 207.08000, 195.08055, 178.07729, 165.07006	In-house database
B25	36.919	Heteroclitalignan A	C ₃₁ H ₃₂ O ₁₁	[M+Na] ⁺	603.18368	603.18368	-0	543.16278, 523.31787, 481.14838, 439.13953, 421.12592, 399.14529, 391.11737, 357.13309, 355.11682, 327.12442, 311.09079, 295.09695, 281.07953, 267.06573, 251.06917, 237.05522, 223.07587, 209.05940, 195.07875, 181.06511, 167.08568, 165.06993, 141.06984, 105.03340, 95.04820, 91.11907	In-house database
B26	37.897	Heteroclitalignan A isomer	C ₃₁ H ₃₂ O ₁₁	[M+H] ⁺	581.20174	581.19937	-4.07	521.17908, 421.12628, 399.14212, 355.11795, 325.10736, 295.09613, 265.08633, 237.05487, 221.05995, 203.08492, 181.06520, 165.07037, 153.07050	Network

B27	38.328	Kadheterin C	C ₃₂ H ₃₈ O ₁₁	[M+Na] ⁺	621.23063	621.23042	-0.34	435.14227, 413.16199, 371.14893, 356.12540, 340.13068, 329.10205, 325.10739, 309.11633, 295.09641, 281.08008, 265.08668, 251.07018, 239.07088, 223.07661, 207.07967, 195.08189, 181.06421	In-house database
B28	38.770	Heilaohuguosu B	C ₂₈ H ₃₄ O ₁₀	[M+Na] ⁺	553.20442	553.20450	0.149	453.15149, 421.12650, 413.15985, 385.16528, 371.14877, 356.12552, 342.10904, 329.10214, 313.10657, 298.08383, 271.06104, 255.06587, 241.08595, 235.07523, 327.06929, 209.05911, 197.06021, 181.06396, 167.08559,	Network
B29	38.929	Heteroclitin Q	C ₃₁ H ₃₂ O ₁₁	[M+Na] ⁺	603.18368	603.18366	-0.04	481.14700, 421.12558, 357.13303, 355.11826, 342.10941, 325.10742, 295.09628, 299.09143, 265.08597, 251.06961, 237.05447, 195.08058, 181.06482, 165.07036, 105.03342, 69.97251	Network
B30	39.361	Heteroclitin Q isomer	C ₃₁ H ₃₂ O ₁₁	[M+Na] ⁺	603.18368	603.18376	0.129	481.14346, 421.12567, 399.14465, 355.11771, 325.10727, 315.08665, 295.09692, 265.08569, 251.07043, 235.07466, 225.05510, 205.06493, 181.06531, 165.07007, 153.07028, 95.04886	In-house database
B31	41.595	kadsurarin	C ₃₀ H ₃₆ O ₁₁	[M+Na] ⁺	595.21498	595.21489	-0.15	435.14108, 413.16095, 371.14859, 356.12433, 340.13080, 325.10736, 295.09747, 267.10196, 265.08646, 251.07066, 223.07506, 207.08054, 181.06485, 167.08620, 83.04925	Network
B32	42.469	Heteroclitalignan D	C ₃₂ H ₃₄ O ₁₁	[M+Na] ⁺	617.19933	617.19904	-0.47	435.14136, 413.16327, 382.14075, 371.14883, 369.13336, 356.12469, 340.13058, 329.10208, 325.10770, 309.11264, 295.09824, 265.08344, 251.07098, 239.07076, 235.07573, 223.07620, 209.05983, 181.06543, 165.06992	Network

B33	43.070	Kadsuphilol P	C ₃₁ H ₃₂ O ₁₀	[M+Na] ⁺	587.18877	587.18877	0.004	527.17328, 163.18716, 405.13052, 383.14841, 343.11743, 311.09103, 293.11780, 225.09149, 165.05473, 105.03346, 95.04912, 77.03860	Network
B34	43.861	Heteroclitalignan B	C ₃₁ H ₃₈ O ₁₁	[M+Na] ⁺	609.23063	609.23038	-0.41	435.14313, 413.16049, 371.14914, 369.13358, 356.12570, 340.13062, 329.10306, 325.10718, 309.11365, 295.09814, 267.10220, 251.07112, 235.07468, 223.07675, 211.07484, 197.06105, 181.06497	Network
B35	43.862	Angustifolin A	C ₃₆ H ₃₂ O ₁₀	[M+H] ⁺	625.20682	625.20420	-4.19	371.14880, 356.12656, 341.13928, 325.10880, 311.09406, 309.11301, 299.09155, 293.08084, 279.06561, 251.07156, 227.06944	Network
B36	44.056	Kadsuphilol R	C ₃₂ H ₃₈ O ₁₁	[M+Na] ⁺	621.23063	621.23029	-0.55	521.17639, 421.12579, 357.13391, 355.11880, 342.10873, 325.10764, 295.09616, 281.08093, 265.08594, 252.07791, 237.05470, 209.06021, 181.06511, 165.07004, 153.07071	Network
B37	44.277	Kadheterin F	C ₃₆ H ₃₄ O ₁₁	[M+H] ⁺	643.21739	643.21473	-4.13	435.14297, 413.16165, 371.14908, 356.12564, 340.13098, 325.10721, 309.11310, 295.09711, 265.08618, 251.07082, 235.07410, 223.07515, 205.06516, 181.06558, 165.07045, 153.06989	Network
B38	45.866	Kadangustin C	C ₃₄ H ₃₈ O ₁₁	[M+H] ⁺	623.24869	623.24602	-4.28	435.14227, 413.16199, 371.14893, 356.12540, 340.13068, 329.10205, 325.10739, 309.11633, 295.09641, 281.08008, 265.08688, 251.07018., 223.07616, 197.06071, 181.06421, 165.07036, 83.04895	Network
B39	46.020	Ananonin B (Arisanschinin D)	C ₃₂ H ₃₄ O ₁₀	[M+Na] ⁺	601.20442	601.20442	0.00	397.16541, 357.13339, 326.11493, 311.09146, 281.08136, 225.09006, 105.03345	Network

B40	46.119	9-Benzoyloxy-gomisin B	C ₃₅ H ₃₈ O ₁₁	[M+H] ⁺	635.24869	635.24601	-4.21	435.14120, 413.15955, 383.14618, 371.14896, 369.13327, 356.12506, 340.13074, 329.10233, 325.10739, 311.09018, 309.11322, 295.09708, 265.08658, 251.07109, 235.07503, 223.07457, 195.08087, 181.06485, 165.07045, 153.07028	Network
B41	46.276	Interiotherin C	C ₃₀ H ₃₆ O ₁₀	[M+Na] ⁺	579.22007	579.22008	0.022	397.16391, 367.15207, 357.13312, 342.10986, 326.11481, 311.09106, 299.09149, 283.09666, 281.08102, 241.04991, 225.05473, 210.06723, 195.08096, 165.06935, 137.50542, 85.30091	Network
B42	46.622	9-Benzoyloxy-gomisin B isomer	C ₃₅ H ₃₈ O ₁₁	[M+Na] ⁺	657.23063	657.23038	-0.38	435.14090, 413.16022, 371.14899, 369.13318, 356.12506, 340.13107, 329.10278, 325.10657, 307.09482, 295.09723, 281.08145, 267.10172, 251.07008, 235.07458, 223.07550, 207.08125, 195.08102, 181.06493, 165.06963, 155.08669	Network
B43	47.438	Schizanrin A	C ₃₁ H ₃₂ O ₈	[M+Na] ⁺	555.19894	555.19881	-0.23	473.25070, 448.07404, 385.16486, 376.12778, 353.13867, 343.11850, 323.12946, 316.09375, 295.13382, 285.07733, 277.08624, 265.08676, 249.09061, 241.05029, 225.05508, 211.07555, 205.06596, 197.05928, 169.06465, 165.07063, 155.04936, 141.06975, 137.05367	Network
B44	47.547	Intermedin A	C ₃₅ H ₄₀ O ₁₁	[M+H] ⁺	637.26434	637.26162	-4.26	435.14087, 413.16049, 371.14868, 356.12579, 340.13056, 329.10202, 325.10748, 309.11307, 295.09711, 277.08527, 251.07051, 235.07556, 223.07622, 211.07573, 205.06494, 181.06526, 167.08578	Network
B45	48.123	Tiegusanin I	C ₃₁ H ₃₈ O ₁₀	[M+Na] ⁺	593.23572	593.23582	0.173	403.13559, 397.13528, 371.14560, 367.15427, 366.14716, 357.13321, 326.11478, 327.12497, 311.09171, 299.09183, 283.09668, 281.08130, 253.08626, 225.09131, 195.08032, 165.07060	Network

B46	49.166	Kadsutherin	C ₂₇ H ₃₂ O ₇	[M+H] ⁺	469.22208	469.22198	-0.21	439.16458, 355.15393, 353.13953, 343.11862, 339.11932, 329.10486, 323.12927, 316.09296, 311.09116, 302.07889, 295.13376, 281.08099, 263.10718, 242.05716, 197.05928, 181.06578, 165.07108, 57.06989	Network
B47	49.167	Wuweizisu C	C ₂₂ H ₂₄ O ₆	[M+H] ⁺	385.16456	385.16449	-0.19	370.14236, 355.15408, 343.11633, 339.12241, 329.10272, 323.12824, 316.09384, 311.09042, 302.07803, 297.07559, 295.13342, 285.07629, 265.08554, 255.06467, 241.04951, 225.05473, 203.08502, 183.04431, 155.04915, 139.05423, 115.05396, 87.99991	Network
B48	49.445	Longipedunin C	C ₃₁ H ₃₂ O ₈	[M+Na] ⁺	555.19894	555.19880	-0.25	407.14511, 392.12369, 376.13040, 355.15469, 316.09244, 271.05771, 229.14876, 208.35350, 76.04242	In-house database
B49	8.125	Apigenin 5- <i>O</i> - β -D-glucopyranoside	C ₂₁ H ₂₀ O ₁₀	[M+H] ⁺	433.11292	433.11312	0.46	271.06058, 203.08655, 201.07161, 151.00345, 119.05008, 107.01387, 59.01387	Standard

*Verified by the reference standard.

#Potential new compound.

Table S3. Triterpenoids in F2 identified by ²D UHPLC-MS analysis.

No.	RT (min)	Compound	Molecular formular	Adduct	Calculated m/z	Experimental m/z	Error (ppm)	MS ² fragment	Identification
C1	37.735	Diosgenin	C ₂₇ H ₄₄ O ₅	[M+H] ⁺	415.32067	415.32064	-0.07	397.31039, 275.20145, 261.18533, 249.18600, 235.16922, 207.13870, 203.17947, 195.13800, 189.16403, 159.11723, 147.11670, 135.11687, 119.08570, 107.08548, 95.08562, 67.05434, 55.05431	mzCloud
C2	39.136	Heteroclitalactone E isomer	C ₃₂ H ₄₀ O ₇	[M+H] ⁺	537.28468	537.28458	-0.18	477.26184, 267.13898, 261.12683, 233.09544, 225.09183, 217.10025, 207.08101, 179.08626, 165.06972, 97.02840	In-house database
C3	39.877	Heteroclitalactone E isomer	C ₃₂ H ₄₀ O ₇	[M+H] ⁺	537.28468	537.28464	-0.07	477.26279, 303.17593, 267.13785, 261.12747, 233.09590, 221.13203, 207.11639, 193.10149, 179.08548, 165.06903, 109.06470, 81.06976	In-house database
C4	40.866	Kadsulactone A	C ₃₀ H ₄₂ O ₅	[M+H] ⁺	483.3105	483.31043	-0.14	465.29987, 447.28708, 325.21619, 307.20685, 299.20013, 269.15256, 247.16949, 229.06891, 209.13181, 197.13159, 195.11746, 183.11713, 169.10118, 157.10150, 145.10123, 131.08543, 119.08556, 105.06982, 91.05408, 81.06988, 67.05412, 55.05420	In-house database
C5*	41.465	Heteroclitalactone E	C ₃₂ H ₄₀ O ₇	[M+H] ⁺	537.28468	537.28461	-0.13	477.26328, 323.20352, 321.18585, 267.13904, 229.12352, 221.13287, 207.11754, 165.07094, 109.06471, 81.06989	In-house database
C6	41.473	Kadsuracoccinic acids B	C ₃₀ H ₄₈ O ₂	[M+H] ⁺	441.37271	441.37266	-0.10	441.36206, 423.36731, 269.23068, 215.18015, 203.17941, 189.16377, 175.14806, 159.11676, 147.11678, 133.10100, 119.08540, 107.08540, 95.08543, 81.06976, 67.05424, 55.05415	In-house database

C7	41.562	Schisandronic acid isomer	C ₃₀ H ₄₆ O ₃	[M-H ₂ O+H] ⁺	437.34141	437.34132	-0.20	394.29638, 381.28064, 325.21640, 295.24265, 269.22470, 253.19135, 227.18002, 211.14838, 183.11707, 171.11696, 157.10103, 133.10120, 109.10085, 95.08527, 81.06981, 67.05422, 55.05418	In-house database
C8	41.737	Kadsuphilactone B	C ₃₀ H ₄₂ O ₅	[M+Na] ⁺	505.29244	505.29240	-0.09	483.31702, 465.30322, 447.28894, 429.28149, 325.21423, 307.20721, 257.15317, 245.15498, 231.13722, 215.14392, 197.13275, 183.11734, 171.11656, 157.10138, 145.10144, 131.08571, 119.08553, 105.06984, 95.08540, 81.06995, 67.05414, 55.05429	In-house database, Clogp
C9	42.492	Heteroclitalactone E isomer	C ₃₂ H ₄₀ O ₇	[M+H] ⁺	537.28468	537.28461	-0.13	477.27325, 321.18469, 277.19513, 221.13269, 207.11688, 221.13269, 205.10124, 193.10095, 179.08415, 109.06488, 83.04926	In-house database
C10	42.595	seco-Coccinic acids A	C ₃₀ H ₄₈ O ₂	[M+H] ⁺	441.37271	441.37264	-0.15	441.37262, 423.36334, 327.26626, 269.22668, 215.17896, 211.14900, 199.14838, 183.11728, 171.11687, 157.10138, 145.101174, 131.08533, 119.08550, 109.10120, 95.08552, 81.06985, 69.06994, 67.05421, 55.05426	In-house database
C11	43.035	Schisanlactone B	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31544	-0.31	449.30402, 431.29419, 407.25052, 368.26950, 327.23160, 309.22192, 273.18607, 197.13293, 183.11653, 171.11649, 159.11684, 157.10091, 145.10086, 131.08559, 119.08542, 105.06973, 95.08540, 91.05412, 83.04903	In-house database
C12	43.101	seco-Coccinic acids B	C ₃₀ H ₄₈ O ₂	[M+H] ⁺	441.37271	441.37267	-0.08	423.36331, 217.19568, 203.17903, 189.16351, 175.14810, 159.11694, 147.11661, 135.11662, 133.10121, 119.08546, 107.08549, 95.08553, 81.06981, 69.06986, 55.05436	In-house database

C13	44.163	Lancilactone B isomer	C ₃₀ H ₃₈ O ₄	[M+H] ⁺	463.28428	463.28429	0.01	445.27213, 427.26266, 417.28210, 323.20120, 269.15332, 223.14847, 209.13257, 193.10144, 179.08534, 169.10094, 157.10155, 131.08630, 119.08526, 95.08555, 91.05418, 81.06976	In-house database
C14	44.459	Coccinetane A	C ₃₀ H ₄₈ O ₂	[M+H] ⁺	441.37271	441.37270	-0.01	441.37482, 423.36234, 241.19426, 215.18053, 203.17979, 189.16393, 161.13222, 147.11679, 135.11694, 119.08545, 107.08557, 95.08560, 81.06996, 67.05426, 55.05423	In-house database
C15	44.518	Schisanlactone A	C ₃₀ H ₄₀ O ₄	[M+H] ⁺	465.29993	465.29982	-0.25	447.29056, 429.27847, 419.29562, 401.28531, 381.27994, 333.22250, 325.21671, 307.20456, 227.14340, 209.13347, 197.13298, 185.13275, 171.11765, 157.10120, 143.08582, 131.08545, 119.08559, 105.06988, 95.08562, 67.05425	In-house database
C16*	44.519	Heteroclitalactone G	C ₃₂ H ₄₀ O ₆	[M+H] ⁺	521.28976	521.28973	-0.07	461.26819, 347.19397, 321.18286, 293.15329, 267.13950, 261.12772, 247.11252, 233.09689, 207.11732, 193.10144, 191.08554, 179.08574, 165.07040, 95.08575, 67.05442	In-house database
C17	44.823	Schisandronic acid isomer	C ₃₀ H ₄₆ O ₃	[M-H ₂ O+H] ⁺	437.34141	437.34140	-0.01	269.22723, 239.18098, 213.16458, 211.1448, 199.14888, 183.11719, 173.13269, 169.10101, 159.11731, 145.10132, 133.10132, 131.06525, 119.08547, 109.10099, 105.06967, 95.08561, 93.06961, 91.05417, 81.06977, 69.06992, 67.05430, 55.05419	In-house database
C18	45.494	Kadnanolactone A	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33118	-0.12	451.32639, 433.31030, 329.24698, 311.23950, 249.18552, 233.15399, 217.15897, 185.13261, 173.13138, 159.11646, 145.10133, 119.08548, 105.06979, 95.08548, 81.06988, 67.05428, 55.05422	In-house database
C19	45.976	Kadcotrione A	C ₃₀ H ₄₄ O ₅	[M+H] ⁺	485.32615	485.32610	-0.10	449.30045, 311.23740, 235.13596, 229.07407, 199.14845, 175.11281, 159.11755, 137.05989, 133.10135, 119.08554, 107.08523, 93.06986, 81.06969, 67.05437, 55.05432	In-house database, Clogp

C20	46.211	Schisanlactone B isomer	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31550	-0.18	449.30588, 431.29688, 421.29688, 413.28360, 407.29871, 389.24454, 327.23178, 309.22208, 299.20044, 287.19958, 273.18378, 211.14885, 197.13286, 185.13272, 183.11650, 171.11676, 157.10118, 145.10114, 131.08542, 119.08526, 105.06982, 95.06990, 81.06985, 67.05439, 55.05422	In-house database
C21	46.368	Kadsuphilactone B isomer	C ₃₀ H ₄₂ O ₅	[M+Na] ⁺	505.29244	505.29243	-0.03	447.28934, 429.27396, 419.29697, 311.23849, 309.22107, 283.24258, 231.24258, 229.15724, 215.14310, 197.13297, 185.13234, 157.10091, 145.10161, 143.08566, 131.08546, 119.08533, 105.06958, 95.08550, 81.05424, 67.05421, 55.05429	In-house database
C22	46.471	Schisanlactone B isomer	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31549	-0.20	449.30801, 431.29312, 407.29550, 353.24878, 327.23138, 309.22226, 223.14877, 199.14816, 183.11635, 171.11650, 157.10098, 145.10081, 131.08534, 119.08530, 105.06989, 95.08549, 81.06978	In-house database
C23	46.769	Schisandronic acid isomer	C ₃₀ H ₄₆ O ₃	[M-H ₂ O+H] ⁺	437.34141	437.34129	-0.26	394.28851, 369.36444, 355.25239, 325.21658, 285.18307, 271.16971, 239.17999, 227.18004, 211.14804, 185.13203, 171.11678, 157.10097, 145.10112, 133.10106, 119.08545, 109.10098, 95.08543, 81.06981, 69.06987, 55.05420	In-house database
C24	46.808	Lancilactone B	C ₃₀ H ₃₈ O ₄	[M+H] ⁺	463.28428	463.28419	-0.20	445.27322, 427.26498, 409.25333, 399.27155, 364.23996, 349.21796, 331.20584, 323.20111, 295.17053, 277.15897, 221.13222, 207.11702, 193.10178, 157.10097, 95.08553, 91.05454,	In-house database
C25*	46.835	<i>d</i> -Epigalbacin	C ₂₀ H ₂₀ O ₅	[M+H] ⁺	341.13835	341.13830	-0.14	219.10105, 201.09157, 163.07549, 135.04401, 105.06976, 79.05428, 65.03859	In-house database

C26	47.229	Schisanlactone B isomer	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31549	-0.20	449.30872, 431.29419, 413.29184, 407.29669, 397.20062, 327.23218, 309.22189, 285.11752, 271.17004, 213.16377, 211.14890, 183.11752, 171.11671, 157.10136, 145.10101, 119.08546, 105.06995, 95.06995, 67.05412	In-house database
C27	47.566	Lancilactone B isomer	C ₃₀ H ₃₈ O ₄	[M+H] ⁺	463.28428	463.28427	-0.03	445.27374, 427.26208, 417.27960, 403.26300, 323.20135, 305.19040, 269.15298, 249.12679, 223.14888, 209.13246, 179.08557, 143.08551, 119.08560, 105.06967, 93.06980, 91.05408	In-house database
C28	47.737	Kadcotrione C	C ₃₀ H ₄₄ O ₅	[M+H] ⁺	485.32615	485.32611	-0.08	467.31012, 449.30713, 432.30148, 329.24609, 311.23666, 293.33617, 277.38632, 235.16841, 217.16022, 203.14317, 189.16362, 175.11179, 159.11649, 147.11652, 133.10117, 119.08547, 107.08539, 93.06992, 81.06982, 67.05414, 55.05428	In-house database, Clogp
C29	48.098	Schisanlactone B isomer	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31540	-0.40	449.30386, 431.29663, 421.30890, 413.28549, 335.23602, 327.23041, 309.22247, 291.21341, 281.22766, 229.15894, 215.14157, 187.14819, 173.13276, 159.11687, 145.10097, 131.08575, 119.08552, 105.06970, 95.08546, 81.06998, 67.05432, 55.05437	In-house database
C30	48.277	Schisanlactone B isomer	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31550	-0.18	449.30472, 431.29684, 421.31100, 327.23398, 245.15417, 135.14607, 233.15520, 213.12813, 197.13268, 183.11661, 171.11652, 157.10158, 145.10129, 131.08517, 105.06973, 95.08550, 81.06989, 67.05418, 55.05426	In-house database
C31	49.447	Manwuweizic acid	C ₃₀ H ₄₆ O ₄	[M+H] ⁺	471.34688	471.34683	-0.12	229.06781, 201.16411, 181.12141, 161.13277, 147.11681, 133.10120, 121.10120, 105.06962, 95.08548, 81.06995, 67.05417, 55.05428	In-house database, Clogp

C32*	49.651	Heteroclitalactone A	C ₃₂ H ₄₆ O ₆	[M-AcOH+H] ⁺	467.31558	467.31544	-0.31	449.30508, 431.29385, 327.23016, 309.00072, 225.16359, 197.13284, 185.13219, 159.11713, 157.10107, 119.08538, 105.06979, 95.08540, 67.05432	In-house database
C33	50.119	Lancilactone B isomer	C ₃₀ H ₃₈ O ₄	[M+H] ⁺	463.28428	463.28430	0.03	445.27322, 427.26520, 417.27701, 403.26666, 323.20020, 305.18976, 269.15347, 251.14258, 223.14835, 207.11697, 179.08575, 157.10097, 131.08549, 119.08556, 105.06985, 95.08544, 91.05421, 79.05409, 67.05425	In-house database
C34	50.281	Kadsudilactone	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33115	-0.18	451.32159, 433.31146, 415.30280, 329.25015, 311.23874, 249.18491, 231.17496, 215.14276, 201.12810, 187.14821, 173.13268, 159.11687, 145.10130, 133.10120, 119.08540, 105.06979, 95.08556, 81.06995, 67.05421, 55.05418	In-house database
C35	50.728	Heteroclic acid	C ₃₂ H ₄₈ O ₅	[M+H] ⁺	513.35745	513.35691	-1.05	471.57932, 453.18756, 437.20123, 189.16437, 181.52179, 123.01650, 119.08614, 107.08605, 95.08551, 81.07011	In-house database
C36	51.901	Schisanlactone B isomer	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31494	-1.38	449.30505, 431.29422, 425.27612, 413.28247, 403.30542, 367.26151, 347.24570, 327.23166, 309.22220, 291.21036, 271.16812, 253.15875, 243.13928, 223.14784, 211.14748, 197.13156, 183.11630, 171.11665, 157.11688, 143.08517, 131.08546, 119.08540, 105.06972, 95.08539, 81.06983, 67.05424, 55.05419	In-house database
C37	52.753	Schisanlactone B isomer	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31564	0.12	431.29675, 327.23270, 285.17969, 274.45486, 167.17603, 233.15489, 215.14331, 185.13246, 173.13264, 159.11642, 145.10110, 131.08539, 119.08545, 105.06973, 95.08540, 81.06979, 67.05419, 55.05427	In-house database

C38*	52.893	Schisanlactone E	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33110	-0.29	451.32086, 433.31317, 329.24805, 285.18118, 231.17500, 215.14346, 187.14832, 173.13266, 159.11678, 145.10118, 133.10138, 119.08554, 105.06995, 95.08549, 93.06978, 79.05423, 67.05425	In-house database
C39	53.889	Schisanlactone E isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33113	-0.22	451.32144, 433.31253, 415.29794, 405.31619, 329.24683, 311.23801, 281.35046, 247.16980, 235.16972, 187.14838, 173.13261, 159.11671, 145.10129, 133.10139, 119.08567, 105.06984, 95.08555, 81.06987, 67.05429, 55.05429	In-house database
C40	54.147	Diosgenin isomer	C ₂₇ H ₄₄ O ₅	[M+H] ⁺	415.32067	415.32070	0.07	397.30835, 215.17924, 195.13792, 177.12723, 159.11687, 147.11667, 135.11684, 121.10114, 107.08546, 95.08651, 93.06987, 81.06990, 67.05422, 55.05429	mzCloud
C41	55.731	12 α -Acetoxycoccinic acid	C ₃₂ H ₄₈ O ₅	[M+H] ⁺	513.35745	513.35731	-0.27	435.32507, 351.31882, 325.24991, 313.25211, 201.16438, 187.14780, 159.11737, 145.10149, 133.10091, 119.08548, 105.06991, 95.08561, 91.05393, 67.05424	In-house database
C42	55.731	Neokadsuranic acid A	C ₃₀ H ₄₄ O ₃	[M+H] ⁺	453.33632	453.33630	-0.04	435.32581, 247.16937, 233.15306, 201.16391, 187.14807, 173.13268, 159.11682, 133.10117, 119.08536, 105.06982, 95.08550, 93.06988, 91.05406, 81.07000, 67.05428, 55.05437	In-house database
C43	58.010	Schisanlactone E isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33105	-0.39	247.16936, 235.16965, 217.15889, 173.13242, 145.10175, 131.08540, 119.08555, 95.08553, 81.06988, 55.05423	In-house database
C44*	58.247	Nigranoic acid	C ₃₀ H ₄₆ O ₄	[M+H] ⁺	471.34688	471.34672	-0.35	435.32303, 365.72641, 351.45129, 295.63046, 247.17046, 235.16968, 217.15926, 187.14874, 173.13228, 161.13283, 133.10150, 121.10109, 107.08549, 95.08549, 93.06977, 81.06979, 67.05428	In-house database

C45*	61.277	Heteroclitalactone F	C ₃₁ H ₄₆ O ₄	[M+H] ⁺	483.34688	483.34690	0.03	451.32382, 433.30942, 311.23730, 293.22510, 263.20319, 213.16460, 187.14856, 161.09625, 159.11644, 145.10141, 133.101110, 131.08565, 119.08542, 105.06983, 95.08553, 93.06982, 81.06989	In-house database
C46	61.433	Ursolic acid isomer	C ₃₀ H ₄₈ O ₃	[M-H ₂ O+H] ⁺	439.35706	439.35711	0.12	325.15579, 202.05374, 191.17990, 175.14894, 161.13344, 147.11685, 135.11726, 121.10152, 109.10143, 95.08568, 81.06994, 67.0544, 55.05437	mzCloud
C47*	63.706	Schisandronic acid	C ₃₀ H ₄₆ O ₃	[M+H] ⁺	455.35197	455.35186	-0.24	437.34320, 247.16879, 235.16888, 203.17966, 201.16307, 189.16406, 161.13226, 135.11647, 119.08535, 109.10106, 95.08546, 81.06982, 67.05418	In-house database
C48	64.478	Ursolic acid	C ₃₀ H ₄₈ O ₃	[M+H] ⁺	457.36762	457.36764	0.04	437.34320, 217.19547, 203.17960, 201.16365, 161.13228, 135.11688, 133.10121, 119.08540, 105.06985, 95.08543, 81.06990, 67.05422	mzCloud
C49	64.787	Oleanolic acid	C ₃₀ H ₄₈ O ₃	[M+H] ⁺	457.36762	457.36766	0.09	439.35944, 384.11993, 247.16879, 203.17966, 189.16406, 161.13226, 147.11685, 119.08535, 109.10106, 95.08546, 81.06982, 67.05418	mzCloud
C50	66.262	Cycloartenone	C ₃₀ H ₄₈ O	[M+H] ⁺	425.37779	425.37781	0.04	407.36716, 369.32123, 313.25238, 299.23941, 271.20551, 257.19089, 245.19131, 199.14749, 205.19518, 173.13274, 161.13269, 149.13242, 135.11697, 119.08544, 109.10108, 95.08548, 81.06992, 67.05428, 59.04921	In-house
C51	66.296	Schisanlactone E isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33119	-0.10	233.15594, 173.13187, 159.11713, 145.10181, 133.10092, 119.08538, 105.07013, 95.08530, 81.07006, 67.05432, 55.04543	In-house database

C52	69.364	Cholecalciferol		C ₂₇ H ₄₄ O ₅	[M+H] ⁺	385.34649	385.34640	-0.24	367.33630, 325.29276, 259.24451, 255.21155, 241.19572, 213.16348, 199.14818, 187.14865, 173.13260, 159.11690, 145.10147, 131.08531, 119.08538, 105.06983, 95.08555, 81.06987, 67.05420, 55.05425	mzCloud
C53	73.577	Coccinetane isomer	A	C ₃₀ H ₄₈ O ₂	[M+H] ⁺	441.37271	441.37267	-0.08	441.29883, 315.15802, 231.21091, 203.17947, 149.13249, 121.10101, 107.08559, 93.06988, 81.06994, 69.07001, 67.05431	In-house database
C54	73.769	Schisanlactone B isomer		C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31550	-0.18	449.30820, 431.29645, 327.22803, 309.22180, 273.18457, 247.17140, 213.12794, 197.13271, 171.11676, 157.10091, 133.10083, 119.08539, 105.06982, 95.08530, 81.06980, 67.05422	In-house database
C55	74.396	<i>seco</i> -Neokadsuranic acid A		C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33114	-0.20	451.31946, 433.31177, 329.24820, 323.17563, 231.17366, 219.13928, 203.14259, 173.13258, 159.11707, 145.10106, 133.10123, 119.08539, 107.08550, 95.08535, 81.06978, 67.05421	In-house database
C56	74.638	Schisanlactone B isomer		C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31554	-0.10	449.30487, 431.29623, 339.22504, 327.23236, 297.18668, 279.17505, 271.17145, 233.15407, 225.16556, 211.14836, 199.14915, 185.13300, 171.11629, 157.10127, 145.10104, 131.08592, 119.08540, 105.06982, 93.06972, 81.06994, 67.05424	In-house database
C57	76.757	<i>seco</i> -Neokadsuranic acid A isomer		C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33088	-0.76	249.18535, 213.16403, 203.14371, 185.13203, 159.11666, 145.10158, 119.08537, 95.08524, 81.07002, 67.05440	In-house database

C58	77.103	Schisanlactone B isomer	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31557	-0.03	431.299535, 327.23090, 275.16586, 267.17645, 247.16931, 233.15295, 215.14333, 197.13208, 159.11653, 145.10118, 131.08543, 119.08519, 105.06972, 95.08546, 81.06973, 67.05418, 55.05430	In-house database
C59	77.922	Schisanlactone B isomer	C ₃₀ H ₄₂ O ₄	[M+H] ⁺	467.31558	467.31552	-0.14	431.30060, 233.15482, 215.14354, 199.14844, 171.11671, 145.10120, 131.08566, 119.08562, 105.06995, 95.08537, 81.06998, 67.05435, 55.05434	In-house database
C60	78.010	<i>seco</i> -Neokadsuranic acid A isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33111	-0.27	451.32114, 433.31052, 405.31714, 337.25513, 331.98972, 311.23560, 293.22583, 249.18648, 235.16969, 213.16386, 187.14850, 173.13231, 159.11673, 145.10136, 133.10127, 119.08542, 105.06984, 95.08550, 81.06989, 67.05422, 55.05424	In-house database
C61	78.481	<i>seco</i> -Neokadsuranic acid A isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33112	-0.24	451.32047, 433.31009, 337.25394, 329.24799, 325.21521, 249.18748, 231.17618, 215.14371, 173.13261, 159.11707, 145.10112, 133.10115, 119.08546, 105.06960, 95.08549, 81.06986, 67.05422, 55.05449	In-house database
C62	78.860	<i>seco</i> -Neokadsuranic acid A isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33113	-0.22	451.31909, 433.31146, 329.24728, 311.23920, 293.22955, 235.16942, 199.14838, 173.13243, 159.11688, 145.10078, 133.10126, 119.08537, 105.06982, 95.08545, 81.06989, 67.05426, 55.05421	In-house database
C63	80.841	Cycloartenone isomer	C ₃₀ H ₄₈ O	[M+H] ⁺	425.37779	425.37788	0.21	407.36856, 365.19547, 262.21927, 219.17513, 215.17996, 205.19525, 191.17995, 173.13237, 161.13206, 149.13264, 135.11682, 121.10114, 109.10112, 95.08556, 81.06990, 67.05425, 55.05427	In-house database

C64	82.523	Changnanic acid	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33121	-0.05	159.11749, 145.10146, 133.10095, 121.10110, 119.08571, 107.08561, 95.08545, 81.06986, 67.05430, 55.05415	In-house database
C65	83.650	Kadsuranic acid A	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33119	-0.10	433.31342, 187.14520, 173.09567, 145.10164, 133.10136, 119.08549, 95.08588, 81.07011, 67.05442, 55.05437	In-house database
C66	83.847	Changnanic acid isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33116	-0.16	433.30722, 381.12277, 235.16847, 213.16411, 187.11156, 173.13301, 159.11716, 145.10136, 133.10123, 119.08538, 105.06974, 95.08532, 81.06977, 67.05440, 55.05443	In-house database
C67	84.264	Changnanic acid isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33117	-0.14	433.30972, 215.14201, 203.14308, 187.14720, 159.11707, 145.10155, 133.10129, 121.10150, 119.08580, 105.06951, 95.08566, 81.06997, 67.05434, 55.05433	In-house database
C68	85.036	Xuetongsu F	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33126	0.05	433.31827, 231.17477, 187.14911, 173.13203, 159.11852, 145.10162, 133.10100, 121.10139, 119.08587, 95.08561, 81.07014, 67.05412, 55.05414	In-house database
C69	86.301	Xuetongsu F isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33117	-0.14	451.32428, 433.31274, 415.29910, 311.23907, 273.18576, 217.15750, 187.14861, 173.13327, 159.11691, 145.10078, 133.10080, 131.08549, 119.08553, 105.06967, 95.08536, 81.06980, 67.05406, 55.05424	In-house database
C70	89.285	Xuetongsu F isomer	C ₃₂ H ₄₄ O ₄	[M+H] ⁺	469.33123	469.33115	-0.18	433.31396, 226.98375, 159.11813, 145.10107, 133.10144, 119.08553, 105.06990, 95.08557, 81.06971, 67.05448, 55.05437	In-house database

*Verified by the reference standard.