Supplementary materials

Hybrid multidimensional data acquisition and data-processing strategy for comprehensive characterization of known, unknown and isomeric compounds from the Compound Danzhi Tablet by UPLC-TWIMS-QTOFMS

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[1] *These authors contributed equally to this work.*

Contents

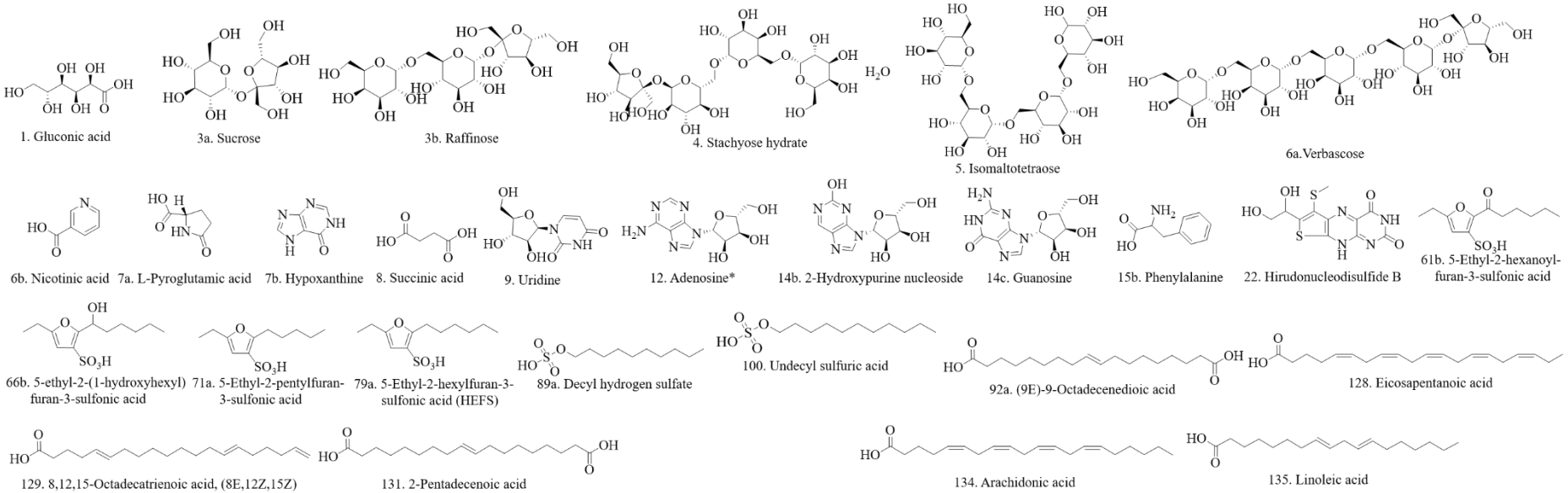


Fig.S1 Structures of the representative chemical components identified from DZT. (*compared with a reference standard.)

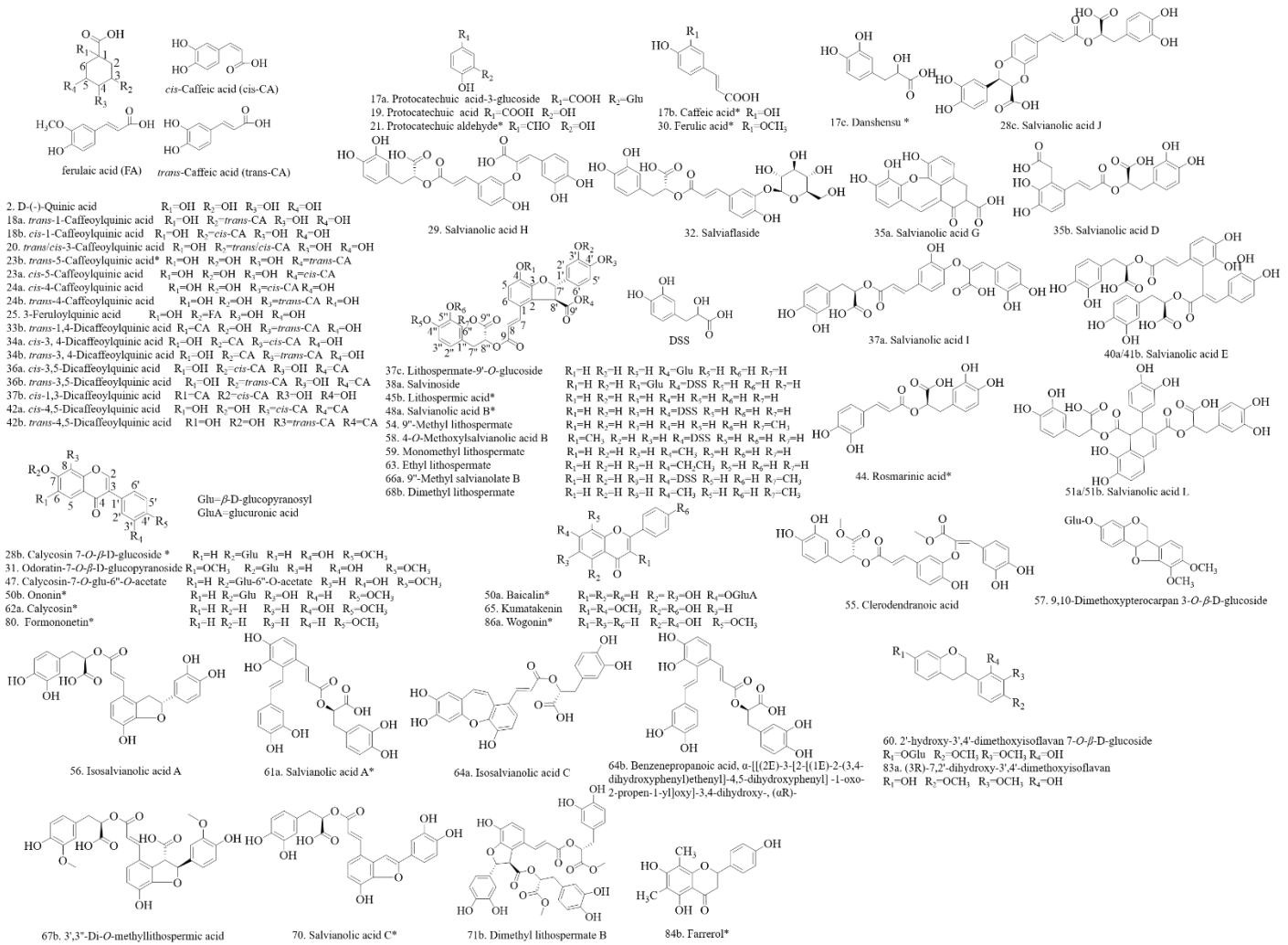
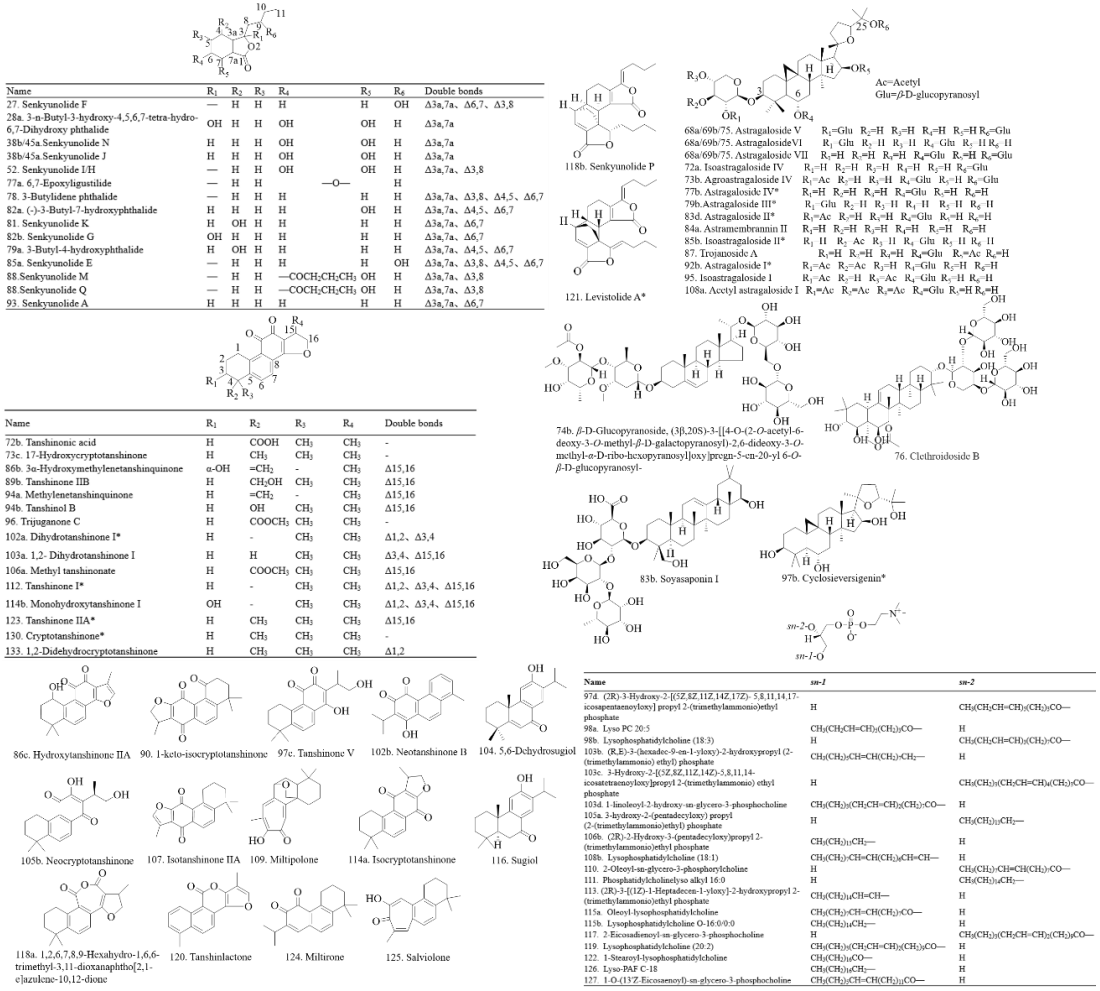


Fig. S1 (Continued).



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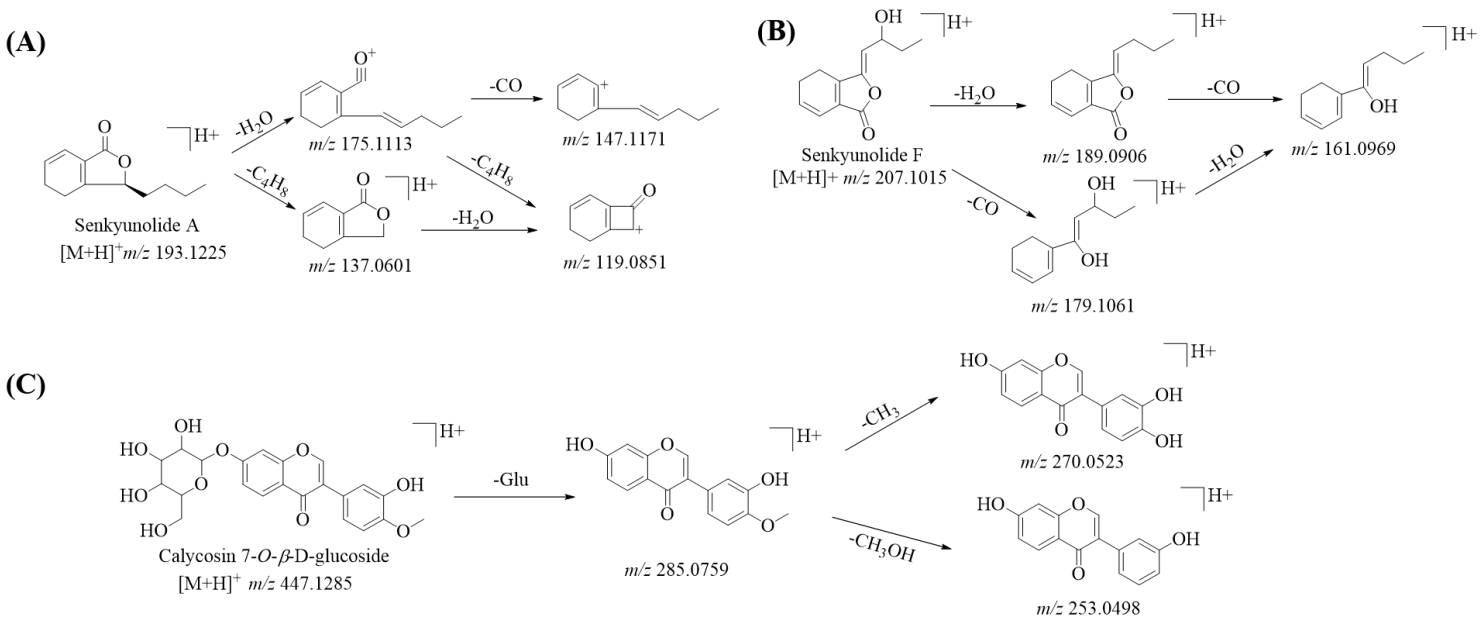

Fig. S2 The fragmentation pathway of senkyunolide A (A), senkyunolide F (B)and calycosin 7-*O*-*β*-D-glucoside(C) in positive ion mode.

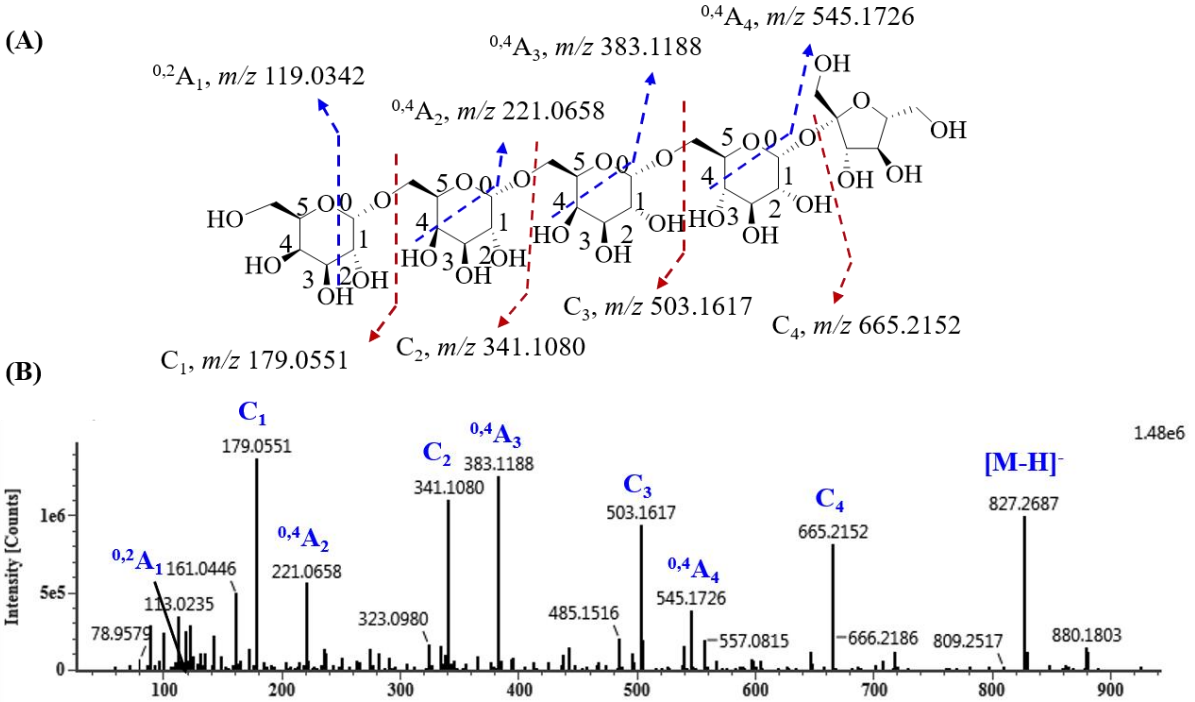

Fig. S3 The fragmentation pathway (A) and MS/MS spectrum (B) of verbascose in negative ion mode.

Table S1. The list of identified compounds in DZT sample based on UPLC-TWIM-QTOFMS.

Peak No.	compound No.	Rt (min)	Formula	Molecular ion	Error (ppm)	Fragment ions	Drift time (ms)	Identification	Original sources
1	1	0.86	$C_6H_{12}O_7$	195.0514 $[M-H]^-$	4.5	177.0382, 159.0298, 141.0196, 129.0179, 111.0080, 99.0078, 87.0083, 75.0081, 71.0130, 57.0326	1.73	Gluconic acid	LC
2	2	0.93	$C_7H_{12}O_6$	191.0553 $[M-H]^-$	-4.9	173.0455, 155.0338, 131.0339, 109.0299, 85.0293	1.76	D- (-)-Quinic acid	LC/SM
3				343.1241 $[M+H]^+$	0.8	203.0523, 185.0420	4.08		
	3a	0.96	$C_{12}H_{22}O_{11}$	341.1082 $[M-H]^-$	-1.6	323.0980, 281.0878, 221.0660, 179.0552, 161.0445, 143.0351, 119.0342, 101.0240	2.81	Sucrose	LC/SM/AM
	3b	0.96	$C_{18}H_{32}O_{16}$	527.1604 $[M+Na]^+$	0.7	365.1056, 347.0943	5.97	Raffinose	LC/SM/AM
				503.1615 $[M-H]^-$	0.5	341.1089, 323.0796, 59.0121	3.98		
4	4	1.03	$C_{24}H_{44}O_{22}$	683.2282 $[M-H]^-$	1.2	341.1089	5.17	Stachyose hydrate	LC/AM
5	5	1.22	$C_{24}H_{42}O_{21}$	665.2147 $[M-H]^-$	1.05	485.1514，383.1199，221.0664，179.0561	4.75	Isomaltotetraose	LC/AM
6	6a	1.33	$C_{30}H_{52}O_{26}$	827.2687 $[M-H]^-$, 873.2743 $[M+HCOOH-H]^-$	-0.1	665.2152, 647.2038, 545.1726, 503.1617, 485.1516, 383.1188, 341.1080, 323.0980, 221.0658, 179.0551, 161.0446, 119.0342	6.52	Verbascose	LC/AM
	6b	1.35	$C_6H_5NO_2$	124.0392 $[M+H]^+$	2.5	106.0289, 96.0442, 84.9612, 80.0494	2	Nicotinic acid	PA
7	7a	1.81	$C_5H_7NO_3$	130.0509 $[M+H]^+$	0.1	113.9643, 102.0537, 84.0426, 72.9366	-	L-Pyroglutamic acid	HN
				128.0344 $[M-H]^-$	1.4	-	-		
	7b	1.83	$C_5H_4N_4O$	137.0467 $[M+H]^+$	3.1	119.0352, 110.0347, 94.0398, 82.0397, 67.0279	2.07	Hypoxanthine	PA/HN
				135.0312 $[M-H]^-$	0	92.03	-		
8	8	2.21	$C_4H_6O_4$	117.0182 $[M-H]^-$	-5	99.0107, 73.0284	-	Succinic acid	SM
9	9	2.43	$C_9H_{12}N_2O_6$	267.0594 $[M+Na]^+$	2.24	211.1075, 136.0619	2.45	Uridine	PA/HN
				243.0626 $[M-H]^-$	1.2	226.0375, 216.0742, 203.1020, 200.0558	2.19		

10				407.1165 $[M+Na]^+$	1.1	245.0630, 227.0528, 203.0523, 164.0342, 132.0723	4.58		
	10	3.13	$C_{14}H_{24}O_{12}$	383.1189 $[M-H]^-$	-0.2	341.1080, 323.0977, 203.0533, 179.0537, 161.0460, 143.0336, 119.0346, 101.0254	3.21	AD-383A	LC
11				407.116 $[M+Na]^+$	-0.2	245.0623, 227.0526, 203.0530	4.50		
	11	3.41	$C_{14}H_{24}O_{12}$	383.1189 $[M-H]^-$	-1.7	341.1087, 323.0953, 179.0570, 161.0450, 135.0303, 113.0252, 101.0250	3.18	AD-383B	LC
12				268.1036 $[M+H]^+$	1.7	253.1552, 225.0874, 207.0765, 184.0503, 161.0694, 136.0620, 119.0354, 94.0404, 70.0646	3.49		
	12	3.75	$C_{10}H_{13}N_5O_4$	312.0941 $[M+HCOOH-H]^-$	-2.6	134.0476, 107.0369	-	Adenosine*	PA/HN
13				407.1153 $[M+Na]^+$	-1.6	245.0622, 227.0518, 203.0525, 185.0419	4.56		
	13	3.84	$C_{14}H_{24}O_{12}$	383.1187 $[M-H]^-$	-0.6	341.1084, 323.0973, 221.0593, 179.0572, 161.0448, 149.0495, 119.0360, 101.0254	3.20	AD-383C	LC
14	14a	3.92	$C_{16}H_{26}O_{14}$	441.1245 $[M-H]^-$	-1.5	341.1087, 221.0688, 179.0568, 161.0460, 119.0349, 101.0242	3.36	ID-441A	LC
	14b	3.94	$C_{10}H_{12}N_4O_5$	267.0734 $[M-H]^-$	-0.3	253.0839, 179.0548, 149.0460, 135.0301, 108.0191	2.39	2-Hydroxypurine nucleoside	PA/HN
	14c	3.94	$C_{10}H_{13}N_5O_5$	284.0998 $[M+H]^+$	2.9	269.0887, 152.0571, 135.0304, 110.0347, 86.0954	-	Guanosine	LC/PA/AM
				282.0844 $[M-H]^-$	0.2	150.0424, 133.0160, 108.0200, 66.0093	2.53		
15				465.1225 $[M+Na]^+$	1.1	447.1611, 429.1640, 303.0664, 285.0567, 203.0525	5.05		
	15a	4.11	$C_{16}H_{26}O_{14}$	441.1245 $[M-H]^-$	-1.4	341.1081, 281.1276, 179.0555, 161.0449, 143.0350, 119.0307, 101.0240	3.31	ID-441B	LC
	15b	4.17	$C_{10}H_{13}NO_2$	180.1027 $[M+H]^+$	1	162.0914, 136.0767, 119.0484, 97.9697, 91.0561	2.49	Phenylalanine	LC/PA/HN
16	16	4.29	$C_{16}H_{26}O_{14}$	441.1245 $[M-H]^-$	-1.8	341.1080, 323.0974, 179.0557, 161.0446, 143.0340, 119.0341, 101.0228	3.27	ID-441C	LC
17	17a	4.98	$C_{13}H_{16}O_9$	315.0697 $[M-H]^-$	-2.5	153.0169, 128.0347, 109.0280	2.86	Protocatechuic acid-3-glucoside	SM/LC
	17b	4.99	$C_9H_8O_4$	181.0505 $[M+H]^+$	5	163.0409, 135.0452, 119.0490	2.48	Caffeic acid*	SM

				179.0338 [M-H]$^-$	-4.6	161.0231, 151.0409, 135.0446, 123.0446, 109.0279, 91.0571	1.71		
	17c	4.99	$C_9H_{10}O_5$	197.0459 [M-H]$^-$	-2.83	179.0334, 173.0224, 152.9044, 135.0439, 123.0452, 109.0304, 72.9919	1.91	Danshensu*	SM
18	18a	5.26	$C_{16}H_{18}O_9$	353.0876 [M-H]$^-$	-3.3	191.0564	2.88	*cis*-1-Caffeoylquinic acid	LC
	18b	5.26	$C_{16}H_{18}O_9$	353.0876 [M-H]$^-$	-3.3	191.0564	3.24	*trans*-1-Caffeoylquinic acid	LC
19	19	5.55	$C_7H_6O_4$	153.0183 [M-H]$^-$	5	109.0284	-	Protocatechuic acid	SM/LC
20				377.0854 [M+Na]$^+$	2.8	359.0748, 215.0515, 197.0415, 185.0198, 179.0148,	-		
	20	5.79	$C_{16}H_{18}O_9$			163.0397, 145.0288		*cis/trans*-3-Caffeoylquinic acid	LC
				353.0885 [M-H]$^-$	-2.3	191.0571, 179.0358,161.0224, 135.0453	2.88		
21	21	6.27	$C_7H_6O_3$	137.0236 [M-H]$^-$	-2.8	108.011	1.37	Protocatechuic aldehyde*	SM
22	22	6.39	$C_{11}H_{10}N_4O_4S_2$	325.0058 [M-H]$^-$	-4.9	306.9959, 291.9714, 278.9647, 263.9798, 232.0069	2.79	Hirudonucleodisulfide B	HN
23	23a	6.68	$C_{16}H_{18}O_9$	353.0875 [M-H]$^-$	-2.6	191.0573,	2.87	*cis*-5-Caffeoylquinic acid	LC/AM
				377.0855 [M+Na]$^+$	0.3	359.0728, 331.0789, 259.1086, 215.0525, 197.0411,	-		
	23b	6.68	$C_{16}H_{18}O_9$			185.0208, 179.0331, 163.0394, 145.0278		*trans*-5-Caffeoylquinic acid*	LC/AM
				353.0875 [M-H]$^-$	-2.6	191.0573	3.24		
24	24a	6.88	$C_{16}H_{18}O_9$	353.0875 [M-H]$^-$	-3	191.0559, 179.0343, 173.0458, 135.0454	2.88	*cis*-4-Caffeoylquinic acid	LC
				377.0846 [M+Na]$^+$	0.9	359.0739, 331.0812, 215.0506, 197.0404, 179.0339,	-		
	24b	6.88	$C_{16}H_{18}O_9$			163.0373, 145.0292		*trans*-4-Caffeoylquinic acid	LC
				353.0875 [M-H]$^-$	-3	191.0550, 179.0337, 173.0453, 161.0235, 135.0452	3.28		
25				391.1004 [M+Na]$^+$	1.1	373.0888, 345.0919, 292.6082, 215.0542, 177.0542, 145.0291, 117.0309	3.26		
	25	7.35	$C_{17}H_{20}O_9$					3-Feruloylquinic acid	LC
				367.1025 [M-H]$^-$	-2.1	191.0554, 173.0453, 155.0349, 134.0369, 93.0342, 71.0126	3.65		
26	26	7.76	$C_{25}H_{24}O_{12}$	515.1203 [M-H]$^-$	0.5	353.0873, 191.0552, 179.0343, 173.0457, 135.0451	4.34	*trans*-1,3- Dicaffeoylquinic acid	LC

27	27	8.66	$C_{12}H_{14}O_3$	207.1029 $[M+H]^+$	1.8	189.0886, 179.1047, 163.1108, 84.9593	-	Senkyunolide F	LC
28	28a	8.84	$C_{12}H_{18}O_5$	265.1036 $[M+Na]^+$	3.7	247.0946, 225.0734, 219.0660, 207.0984, 135.0432	-	3-n-butyl-3-hydroxy-4,5,6,7-tetrahydro-6,7-dihydroxy phthalide	LC
				241.1086 $[M-H]^-$	-3.5	223.0931, 205.0860, 197.1190, 179.1082, 155.0350, 141.0924, 123.0817, 111.0450, 92.0209	2.37		
	28b	8.86	$C_{22}H_{22}O_{10}$	447.1285 $[M+H]^+$	-0.1	285.0759, 270.0523, 253.0498, 225.05488, 213.0552, 197.0604, 169.0662, 157.0664, 137.0235, 81.0334	6.09		
				445.1134 $[M-H]^-$, 491.119 $[M+HCOOH-H]^-$	-0.2	430.0920, 329.1375, 311.0611, 297.0382, 295.0618, 283.0603, 268.0368, 253.0511, 239.0336, 227.0359, 219.0679, 211.0349, 135.0078	4.94	Calycosin 7-*O*-*β*-D-glucoside*	AM
				561.1004 $[M+Na]^+$	1.5	461.1087, 381.0575, 363.0484, 319.0601, 185.0208, 135.0422	6.81		
	28c	8.96	$C_{27}H_{22}O_{12}$	537.1046 $[M-H]^-$	1.5	493.1132, 383.0727, 359.0764, 341.0656, 313.0697, 295.0610, 253.0872, 225.0520, 197.0447, 185.0237, 179.0336, 173.0251, 161.0240, 135.0442, 109.0290, 72.9911	4.27	Salvianolic acid J	SM
29				561.0999 $[M+Na]^+$	-1.4	381.0576, 319.0579, 297.0703, 279.0629, 261.0541, 221.0426	6.85		
	29	9.03	$C_{27}H_{22}O_{12}$	537.1036 $[M-H]^-$	-0.5	493.1158, 359.0780, 341.0706, 313.0712, 295.0603, 277.0514, 267.0650, 253.0902, 197.0470, 185.0239, 179.0339, 173.0229, 161.0246, 135.0459, 109.0280,	4.23	Salvianolic acid H	SM
30	30	9.13	$C_{10}H_{10}O_4$	193.0507 $[M-H]^-$	-4.8	178.0262, 165.0581, 149.0606, 134.0372, 121.0275, 93.0330	1.8	Ferulic acid*	LC/AM
31				477.1402 $[M+H]^+$	2.3	315.0877, 300.0613, 283.0592, 255.0648, 227.0710, 167.0355, 136.0608, 120.0841	-		
	31	9.25	$C_{23}H_{24}O_{11}$	521.1296 $[M+HCOOH-H]^-$	-0.8	477.1390, 409.0649, 313.0715, 298.0491, 287.0936, 269.0450, 257.0846, 167.0330	4.28	Odoratin-7-*O*- -D-glucopyranoside	AM

32	32	9.35	$C_{24}H_{26}O_{13}$	521.1297 $[M-H]^-$	-0.7	359.0772, 341.0861, 323.0775, 309.0402, 295.0606, 283.0619, 197.0440, 179.0339, 161.0232, 135.0453, 123.0447, 72.9925	4.28	Salviaflaside	SM
33	33a	9.47	$C_{25}H_{24}O_{12}$	515.1203 $[M-H]^-$	0.5	353.0876	-	di-Caffeoylquinic acid isomer	LC
	33b	9.47		515.1203 $[M-H]^-$	-0.8	353.0876, 335.0771, 317.0676, 299.0650, 255.0667, 203.0344, 191.0556, 179.0341, 173.0457, 161.0246, 135.0450	4.24	*trans*-1,4-Dicaffeoylquinic acid	
34				539.117 $[M+Na]^+$	0.5	377.0807, 359.0724, 197.0389	-		
	34a	9.53	$C_{25}H_{24}O_{12}$	515.1203 $[M-H]^-$	-0.8	353.0880, 191.0547, 179.0338, 173.0453, 161.0232, 135.0440	4.41	*cis*-3,4-Dicaffeoylquinic acid	LC
	34b	9.53	$C_{25}H_{24}O_{12}$	515.1203 $[M-H]^-$	-0.8	179.0351, 161.0246	4.89	*tans*-3,4-Dicaffeoylquinic acid	CX
35	35a	9.65	$C_{18}H_{12}O_7$	339.0497 $[M-H]^-$	-4	321.0418, 295.0599, 277.0488, 267.0664, 252.0414, 225.0552, 185.0232, 173.0250, 161.0291, 159.0469, 145.0294, 109.0304	2.96	Salvianolic acid G	SM
	35b	9.67	$C_{20}H_{18}O_{10}$	417.0816 $[M-H]^-$	-2.7	373.0923, 197.0461, 179.0335, 175.0386, 157.0279, 135.0438, 109.0288, 72.9926	3.48	Salvianolic acid D	SM
36	36a	9.71	$C_{25}H_{24}O_{12}$	515.1188 $[M-H]^-$	-1.4	191.0571, 179.0351, 135.0451	4.26	*cis*-3,5-Dicaffeoylquinic acid	LC
	36b	9.71	$C_{25}H_{24}O_{12}$	539.118 $[M+Na]^+$	3.7	521.1060, 493.1117, 377.0824, 359.0730, 331.0793, 317.0849, 197.0407, 179.0342, 163.0379, 145.0252, 135.0454	-	*trans*-3,5-Dicaffeoylquinic acid	
				515.1188 $[M-H]^-$	-1.4	353.0877, 335.0771, 191.0548, 179.0335, 161.0236, 135.0438	4.24		
37	37a	9.78	$C_{27}H_{22}O_{12}$	537.1029 $[M-H]^-$	-1.7	339.0496, 321.0393, 313.1100, 295.0600, 267.0649, 197.0449, 185.0246, 179.0335, 161.0222, 159.0455, 135.0438, 109.0288, 72.9930	4.55	Salvianolic acid I	SM

	37b	9.78	$C_{25}H_{24}O_{12}$	539.118 $[M+Na]^+$	3.7	521.1060, 493.1117, 377.0824, 359.0730, 331.0793, 317.0849, 197.0407, 179.0342, 163.0379, 145.0252, 135.0454	-	*cis*-1,3-Dicaffeoylquinic acid	LC
	37c	9.80	$C_{33}H_{32}O_{17}$	699.1552 $[M-H]^-$	-0.9	655.1628, 519.0926, 457.1106, 321.0393, 295.0598, 277.0505	-	Lithospermate-9'-*O*-glucoside	DS
38				903.1959 $[M+Na]^+$	-	723.1520, 521.1081, 323.0542	10.18		
	38a	9.86	$C_{42}H_{40}O_{21}$	879.1992 $[M-H]^-$	-3.4	681.1523, 519.0925, 501.1020, 483.0920, 457.1142, 339.0505, 321.0393, 295. 0602, 279.0296, 267.0656, 197.0435, 185.0242, 179.0349, 173.0239, 161.0263, 135.0452, 109.0297, 72.9921	6.69	Salvinoside	SM
	38b	9.87	$C_{12}H_{18}O_4$	249.1100 $[M+Na]^+$	1	209.1156, 191.1039, 163.1081, 153.0573, 147.1150	-	Senkyunolide N/Senkyunolide J	LC
39				903.1963 $[M+Na]^+$	-1.3	741.1398, 723.1525, 705.1424, 561.1001, 543.1040, 525.0981, 499.1222, 481.1071, 362.0387, 323.0539, 295.0590, 181.0492	10.2		
	39	9.95	$C_{42}H_{40}O_{21}$	879.1992 $[M-H]^-$	-3.4	835.1957, 717.1469, 699.1542, 681.1523, 655.1652, 637.1571, 621.1002, 561.1033, 519.0926, 501.1040, 493.1135, 483.0930, 475.1153, 457.1131, 339.0505, 321.0393, 295. 0602, 277.0504, 249.0564, 197.0452, 185.0245, 179.0349, 173.0243, 159.0450, 135.0454, 123.0450, 109.0307, 72.9940	6.69	Salvinoside isomer I	SM
40	40a	10.04	$C_{36}H_{30}O_{16}$	717.1451 $[M-H]^-$	-0.2	519.0932, 339.0510, 335.0538, 321.0406, 295.0610, 291.0633	5.26	Salvianolic acid E	SM
	40b	10.05	$C_{36}H_{30}O_{16}$	741.1426 $[M+Na]^+$	-2	561.0993, 543.0878, 381.0560, 363.0483, 319.0570, 295.0599, 279.0641, 221.0428, 163.0383	8.48	salvianolic acid E isomer	SM
				717.1451 $[M-H]^-$	-0.2	519.0934, 339.0510, 321.0406, 295.0610, 279.0298, 277.0501, 265.0499, 249.0553, 221.0602, 197.0458,	5.86		

41						185.0245, 179.0350, 161.0247, 135.0452, 123.0452, 109.0298, 72.9932			
	41	10.17	$C_{42}H_{40}O_{21}$	879.1994 $[M-H]^-$	-3.4	699.1522, 681.1523, 655.1799, 519.0935, 501.1033, 483.0916, 457.1146, 339.0505, 321.0393, 295. 0602, 277.0500, 197.0469, 179.0340, 161.0227, 135.0443, 109.0287, 72.9927	6.84	Salvinoside isomer II	SM
42				539.1179 $[M+Na]^+$	3.4	497.1396, 377.0817, 359.0723, 185.0238, 179.0346, 163.0392, 145.0301, 135.0459	-		
	42a	10.17	$C_{25}H_{24}O_{12}$	515.1191 $[M-H]^-$	-0.8	353.0877, 191.0548, 179.0330, 173.0456, 161.0236, 135.0440	4.39	*cis*-4,5-Dicaffeoylquinic	LC
	42b	10.17		515.1191 $[M-H]^-$	-0.8	353.0877, 191.0548, 179.0330, 173.0456	-	*trans*-4,5-Dicaffeoylquinic acid	
43	43	10.25	$C_8H_{16}O_4S$	207.0702 $[M-H]^-$	-5	79.9562	2.14	Unknown	PA
44				383.0744 $[M+Na]^+$	1.7	357.1635, 343.1059, 221.0407, 185.0230, 163.0393, 145.0266, 135.0446	5.17		
	44	10.33	$C_{18}H_{16}O_8$	359.075 $[M-H]^-$	-2.1	197.0446, 179.0339, 161.0234, 151.0402, 135.0439, 123.0454, 109.0292, 72.9922	2.94	Rosmarinic acid*	SM
45	45a	10.41	$C_{12}H_{18}O_4$	249.1103 $[M+Na]^+$	2.3	231.1358, 209.1159, 163.1111	-	Senkyunolide N/Senkyunolide J	LC
				539.1196 $[M+H]^+$	1.1	547.1145, 517.1084, 381.0629, 363.0488, 337.0653, 319.0580, 281.0419, 163.0385	6.51		
	45b	10.43	$C_{27}H_{22}O_{12}$	537.1033 $[M-H]^-$	-0.8	493.1168, 383.0768, 339.0506, 313.0721, 295.0603, 277.0495, 267.0652, 225.0544, 197.0460, 185.0233, 179.0338, 173.0231, 159.0440, 145.0292, 135.0440, 109.0284	4.67	Lithospermic acid *	SM
46	46	10.65	$C_{23}H_{36}O_{12}$	527.2115 $[M+Na]^+$	1.8	483.2148, 437.1775, 395.1667, 351.1784, 335.0950, 317.0837, 275.0791, 233.1133, 131.0505, 103.0543	-	LD-503	LC

				503.213 [M-H]$^-$, 549.2181 [M+HCOOH-H]$^-$	-0.4	341.1084, 221.0685, 191.0550,161.0456, 149.0452, 131.0351, 113.0244, 101.0238, 89.0234, 85.0294, 71.0127, 59.0125	4.6		
47				489.1394 [M+H]$^+$	0.8	285.0762, 270.0526, 253.0492, 225.0538, 197.0583, 169.0635, 137.0244	-		
	47	10.9	$C_{24}H_{24}O_{11}$	533.1301 [M+HCOOH-H]$^-$	0	283.0616, 268.0374	5.34	Calycosin-7-*O*-glc-6''-*O*-acetate	AM
48						561.1005, 543.0890, 517.1114, 381.0571, 363.0471, 337.0677, 319.0577, 295.0613, 279.0626, 251.0708, 221.0407, 203.0333, 181.0499, 161.0415, 139.0381, 135.0449			
	48a	10.91	$C_{36}H_{30}O_{16}$	719.1608 [M+H]$^+$, 741.1427 [M+Na]$^+$	0.2		8.61	Salvianolic acid B*	SM
				717.1458 [M-H]$^-$	0.3	519.0956, 339.0520, 321.0414, 295.0613, 277.0499	5.85		
	48b	10.91	$C_{36}H_{30}O_{16}$	717.1455 [M-H]$^-$	0.3	537.1032，519.0930, 493.1148, 339.0502, 321.0411, 295.0613, 279.0300, 277.0499, 249.0548, 229.0141, 197.0460, 185.0243, 179.0344, 135.0450, 109.0294	5.91	Salvianolic acid B isomer I	SM
49	49	10.95	$C_{12}H_{20}O_5S$	275.0948 [M-H]$^-$	0.2	257.0842, 195.1381, 184.9905, 165.1280, 135.0280, 121.0289, 80.9632, 79.9562	2.67	5-Ethyl-2-(1-hydroxyhexyl) furan-3-sulfonic acid isomer I	PA
50				447.0918 [M+H]$^+$, 469.0754 [M+Na]$^+$	0.8	431.1417, 382.1012, 331.1571, 293.0408, 271.0605, 237.0813, 229.1936, 211.0639, 121.1010	5.48		
	50a	10.98	$C_{21}H_{18}O_{11}$	445.077 [M-H]$^-$	-1.4	269.0441, 251.0336, 241.0487, 223.0397, 213.0519, 197.0597, 181.0608, 169.0672, 113.0246, 85.0294	3.98	Baicalin*	SM/AM
				431.1335 [M+H]$^+$	-0.3	291.0632, 269.0810, 255.2027,227.1799	5.85		
	50b	11.01	$C_{22}H_{22}O_9$	429.1179 [M-H]$^-$, 475.1243 [M+HCOOH-H]$^-$	-0.6	267.0654, 252.0417, 223.0391, 208.0522, 135.0074, 132.0211, 91.0195	4.77	Ononin*	AM
51	51a	11.19	$C_{36}H_{30}O_{16}$	717.1437 [M-H]$^-$	2.6	519.0927, 321.0400	5.08	Salvianolic acid L/isomer	SM
	51b	11.19		717.1437 [M-H]$^-$	2.6	519.0928, 339.0513, 321.0400	5.55	Salvianolic acid L/isomer	

52	52	11.3	$C_{12}H_{16}O_4$	247.0946 $[M+Na]^+$	0.8	207.1015, 189.09057, 171.0817, 161.09687, 143.0848, 119.0846, 105.0692, 91.0533	3.65	Senkyunolide I/Senkyunolide H	LC
53	53	11.37	$C_{36}H_{30}O_{16}$	719.1613 $[M+H]^+$, 741.1483 $[M+Na]^+$	1	561.1012, 543.0861, 517.1089, 381.0580, 362.0398, 337.0674, 319.0595, 295.0602, 233.0634, 221.0431, 135.0445	5.56	Salvianolic acid B isomer II	SM
				717.1457 $[M-H]^-$	0.2	559.0833, 537.1035, 519.0935, 515.0954, 493.1139, 339.0507, 335.0538, 321.0402, 295.0614, 291.0632, 185.0245	5.56		
54	54	11.4	$C_{28}H_{24}O_{12}$	551.1196 $[M-H]^-$	0.3	507.1292, 463.1431, 327.0882, 309.0773, 294.0534, 283.0979, 277.0508, 266.0559, 197.0459, 185.0243, 179.0352, 159.0442, 145.0288, 135.0457, 123.0443, 108.0204, 72.9925	-	9''-Methyl lithospermate	SM
55	55	11.58	$C_{29}H_{26}O_{12}$	565.1356 $[M-H]^-$	0.7	519.0918, 409.0873, 385.0907, 367.0822, 339.0499, 321.0395, 293.04489, 277.0488, 245.0451, 229.0127, 197.0442, 185.0244, 179.0340, 173.0235, 135.0444, 109.0278, 72.9913	4.94	Clerodendranoic acid	SM
56	56	11.64	$C_{26}H_{22}O_{10}$	495.1265 $[M+H]^+$, 517.1110 $[M+Na]^+$	1	337.0695, 319.0557, 297.0756, 279.0663, 269.0842, 251.0681, 233.0574, 221.0415, 205.0610, 163.0399, 135.0431	-	Isosalvianolic acid A	SM
				493.1123 $[M-H]^-$	-0.3	313.0721, 295.0603, 277.0495, 267.0652, 225.0544, 197.0458, 185.0233, 179.0338, 173.0231, 159.0440, 145.0296, 135.0440, 109.0284, 72.9934	4.16		
57	57	11.69	$C_{23}H_{26}O_{10}$	463.1608 $[M+H]^+$, 485.1429 $[M+Na]^+$	1	301.1072, 286.0819, 273.1114, 269.0800, 253.0450, 241.0847, 191.0698, 167.0708, 152.0468, 147.0442, 134.0363, 123.0440, 105.0340, 78.0461	5.56	9,10-Dimethoxypterocarpan 3-*O*-*β*-D-glucoside	AM

				507.1506 [M+HCOOH-H]$^-$	-0.4	299.0915, 284.0684, 269.0446, 241.0505, 225.1143, 197.0547, 181.1306	5.1		
58									
				755.1607 [M+Na]$^+$	3.1	575.1140, 557.1040, 531.1276, 446.1271, 395.0732, 377.0637, 359.0486, 351.0833, 333.0766, 309.0730, 277.0434, 265.0812	-		
	58	11.97	$C_{37}H_{32}O_{16}$					4-*O*-Methoxylsalvianolic acid B	SM
				731.1617 [M-H]$^-$	0.3	551.1202, 533.1089, 519.0937, 353.0654, 335.0548, 320.0323, 309.0766, 294.0536, 276.0404, 197.0455, 185.0248, 179.0347, 135.0452, 108.0208	6.08		
59									
				553.1358 [M+H]$^+$	1.9	521.1079, 355.0801, 323.0550, 295.0609, 277.0502, 267.0655, 253.0499, 249.0554, 221.0600, 153.0547	-		
	59	12.02	$C_{28}H_{24}O_{12}$					Monomethyl lithospermate	SM
				551.1193 [M-H]$^-$	-0.3	519.0925, 353.0666, 339.0509, 321.0398, 295.0613, 277.0507, 231.0295, 197.0420, 135.0449, 109.0291	4.62		
60				465.1766 [M-H]$^-$, 487.1594 [M+Na]$^+$	1.4	325.0997, 293.2119, 275.2001, 257.1903, 229.1919, 180.0425, 167.0680, 139.1115, 109.0982	5.9		
	60	12.07	$C_{23}H_{28}O_{10}$					2'-hydroxy-3',4'-dimethoxyisoflavan 7-*O*-*β*-D-glucoside	AM
				463.1603 [M-H]$^-$	-0.9	301.1070, 286.08341, 271.05968	-		
61									
	61a	12.18	$C_{26}H_{22}O_{10}$	493.1133 [M-H]$^-$	-0.9	313.0721, 295.0603, 277.0495, 267.0652, 225.0544, 185.0233, 179.0338, 173.0231, 159.0440, 135.0440, 109.0284, 72.9931	4.12	Salvianolic acid A*	SM
	61b	12.18	$C_{12}H_{18}O_5S$	273.0791 [M-H]$^-$	-4.1	257.0849,243.0692,204.0095, 188.9867, 175.0075, 111.0451, 95.9500, 80.9643, 79.9566	2.69	5-Ethyl-2-hexanoylfuran-3-sulfonic acid	PA
62				285.0776 [M+H]$^+$, 307.0594 [M+Na]$^+$	0.2	270.0565, 253.0502, 242.0575, 225.0550, 197.0587, 169.0654, 137.0240, 81.0323	3.59		
	62a	12.32	$C_{16}H_{12}O_5$					Calycosin*	AM
				283.061 [M-H]$^-$	-3.4	268.0379, 240.0360, 225.1502, ,211.0389, 135.0074	2.69		
	62b	12.37	$C_{12}H_{20}O_5S$	275.0948 [M-H]$^-$	0.2	257.0835, 243.0679, 214.0290, 204.0085, 188.9851, 175.0062, 159.9829, 111.0443, 79.9560	2.72	5-Ethyl-2-(1-hydroxyhexyl) furan-3-sulfonic acid isomer II	PA

63	63	12.41	$C_{29}H_{26}O_{12}$	565.1354 $[M-H]^-$	0.5	519.0923, 367.0858, 339.0489, 321.0394, 293.04555, 277.0501,245.0467, 197.0457, 185.0259, 135.0437	4.83	Ethyl lithospermate	SM
64	64a	12.67	$C_{26}H_{20}O_{10}$	491.0977 $[M-H]^-$	-1.4	311.0549, 293.0445, 276.0409, 265.0497, 249.0548, 197.0447, 179.0348, 159.0442, 135.0462, 128.0357, 109.0320	3.99	Isosalvianolic acid C	SM
	64b	12.7	$C_{29}H_{26}O_{12}$	565.1348 $[M-H]^-$	-0.7	519.0925, 385.1276, 367.0810, 339.0503, 321.0400, 303.0275, 293.0449, 277.0502, 245.0443, 229.0114, 197.0470, 185.0235, 179.0342, 135.0453, 109.0298, 72.9914	4.78	3-Benzofurancarboxylic acid, 2-(3,4-dihydroxyphenyl)-4-[3-[1-[(3,4-dihydroxyphenyl) methyl]-2-ethoxy-2-oxoethoxy]-3-oxo-1-propen-1-yl]-2,3-dihydro-7-hydroxy-	SM
65	65	12.8	$C_{17}H_{14}O_6$	315.0847 $[M+H]^+$ 313.0714 $[M-H]^-$	1.9 -1	300.0623, 283.0595, 167.0337 298.0503, 283.0265, 269.0510, 211.1363, 142.0537	3.98 2.96	Kumatakenin	AM
66	66a	12.8	$C_{37}H_{32}O_{16}$	731.1626 $[M-H]^-$	0.3	551.1200, 533.1085, 353.0661, 335.0557, 339.0511, 321.0398, 309.0757, 295.0605, 197.0430, 179.0343, 135.0450, 109.0311	6.02	9''-Methyl salvianolate B	SM
	66b	12.87	$C_{12}H_{20}O_5S$	275.0947 $[M-H]^-$	0.2	257.0782, 231.1440, 211.1319, 189.9926, 174.9683, 155.1060, 111.0065, 98.0375, 80.9631, 79.9554	2.62	5-Ethyl-2-(1-hydroxyhexyl) furan-3-sulfonic acid	PA
67				1399.6749 $[M+H]^+$, 1421.6571 $[M+Na]^+$	0.1	473.3265, 455.3520, 437.3414	-		
	67a	12.93	$C_{65}H_{106}O_{32}$	1397.6616 $[M-H]^-$, 1443.666 $[M+HCOOH-H]^-$	0.7	1073.5551, 911.5008，893.4883, 749.4526, 603.3902, 585.3756, 471.3449, 179.0553, 161.0442, 101.0232, 89.0232	13.29	Astrogaloside-1397	-
				565.1356 $[M-H]^-$	0.1	519.0923, 385.0935, 367.0826, 339.0513, 321.0406, 293.0431, 277.0436, 245.0445, 185.0286, 179.0331, 161.0217, 135.0434	4.77		
68	68a	13.44	$C_{47}H_{78}O_{19}$	947.5211 $[M+H]^+$	0.2	473.3711, 455.3518, 437.3428, 419.3307, 401.3190	-		AM

				991.5137 [M+HCOOH-H]$^-$	1.8	945.5075, 927.4970, 783.4534, 765.4380, 621.4044, 161.0429, 131.0339, 113.0254, 101.0245, 89.0235, 85.0292	8.57	Astragaloside V/Astragaloside VI/Astragaloside VII	
				567.1515 [M+H]$^+$, 589.1329 [M+Na]$^+$	2.2	369.0977, 323.0559, 315.0872, 295.0610, 277.0507, 269.0819, 249.0554, 221.0602, 187.0396, 137.0234, 109.0292	7.37		
	68b	13.46	$C_{29}H_{26}O_{12}$					Dimethyl lithospermate	SM
				565.1349 [M-H]$^-$	0.7	519.0924, 385.0936, 367.0816, 339.0512, 321.0399, 303.0289, 293.0447, 277.0505, 245.0448, 229.0147, 197.0464, 185.0244, 179.0348, 173.0230, 135.0441, 109.0284, 72.9945	4.96		
69				1075.5623 [M+H]$^+$, 1097.5492 [M+Na]$^+$	0.2	455.3531, 437.3415	-		-
	69a	13.78	$C_{53}H_{86}O_{22}$	1073.5562 [M-H]$^-$, 1119.5613 [M+HCOOH-H]$^-$	0.8	749.4489, 603.3409, 585.3800, 471.3485, 323.0867, 179.0551, 161.0447, 113.0212	10.66	Astrogaloside-1073A	
				947.5228 [M+H]$^+$, 969.503 [M+Na]$^+$	-0.3	473.3613, 455.3520, 437.3414, 419.3308, 401.3196	13.25		
	69b	13.78	$C_{47}H_{78}O_{19}$	945.5063 [M-H]-, 991.5129 [M+HCOOH-H]-	0.9	945.5076, 927.4843, 783.4559, 765.4430, 621.4048, 489.3574, 471.3469, 179.0561, 161.0450, 143.0348, 131.0344, 119.0351, 113.0238, 101.0242, 89.0237, 85.0288	8.53	Astragaloside V/Astragaloside VI/Astragaloside VII	AM
70	70	13.78	$C_{26}H_{20}O_{10}$	491.0981 [M-H]$^-$	-0.5	311.0563, 293.0449, 265.0449, 197.0462, 179.0343, 135.0444, 109.0289	4.21	Salvianolic acid C*	SM
71	71a	14.04	$C_{11}H_{18}O_4S$	245.0836 [M-H]$^-$	-3.9	231.0803, 188.0140, 172.9895, 147.0448, 130.0870, 116.0711, 109.0282, 79.9573	2.51	5-Ethyl-2-pentylfuran-3-sulfonic acid	PA

	71b	14.06	$C_{38}H_{34}O_{16}$	745.1776 $[M-H]^-$	0.3	547.1244, 519.0937, 339.0507, 321.0396, 313.0707, 295.0601, 277.0516, 267.0651, 249.0551, 197.0454, 185.0244, 179.0342, 135.0446, 109.0286	6.16	Dimethyl lithospermate B	SM
72				785.472 $[M+H]^+$,	0.4				
	72a	14.1	$C_{41}H_{68}O_{14}$	807.4481 $[M+Na]^+$		455.3520, 437.3414	10.69	Isoastragaloside IV	AM
				829.4601 $[M+HCOOH-H]^-$	1.2	783.4546, 621.3969, 489.3604	7.56		
	72b	14.1	$C_{19}H_{16}O_5$	325.1072 $[M+H]^+$	0.5	281.1160, 263.1065, 251.1079, 211.0376, 183.0428, 167.0844	4.08	Tanshinonic acid	SM
73	73a	14.37	$C_{12}H_{20}O_5S$	275.0948 $[M-H]^-$	0.2	233.1164, 195.1394, 80.9657, 79.9540	2.73	5-Ethyl-2-(1-hydroxyhexyl) furan-3-sulfonic acid isomer III	PA
				989.5306 $[M+H]^+$,	0.2	455.3478, 437.3414, 419.3308, 401.3181	12.63		
	73b	14.41	$C_{49}H_{80}O_{20}$	1011.5123 $[M+Na]^+$				Agroastragaloside IV	AM
				1033.5244 $[M+HCOOH-H]^-$	1.8	945.5092, 927.4963, 783.4619, 765.4452, 655.3764, 143.0357, 113.0237, 101.0226, 71.0119	9.28		
	73c	14.46	$C_{19}H_{20}O_4$	313.1443 $[M+H]^+$	2.7	285.1422, 269.1537, 253.0852, 249.1266, 239.1076, 199.0752, 171.0807, 157.1013, 143.0882, 129.0227	4.1	17-Hydroxycryptotanshinone	SM
74				785.472 $[M+H]^+$,	0.4				
	74a	14.53	$C_{41}H_{68}O_{14}$	807.4481 $[M+Na]^+$		455.3520, 437.3414	9.99	Astragaloside IV isomer	AM
				829.4602 $[M+HCOOH-H]^-$	1.2	783.4546, 621.3969, 489.3604	7.24		
				989.5317 $[M+H]^+$,	0.5	473.3616, 455.3519, 437.3403, 419.3301, 401.3196	-	*β*-D-Glucopyranoside, (3*β*,20S)-3-[[4-*O*-(2-*O*-acetyl-6-deoxy-3-O-methyl-*β*-D-galactopyranosyl)-2,6-dideoxy-3-*O*-methyl-*α*-D-ribo-hexopyranosyl] oxy] pregn-5-en-20-yl 6-*O*-*β*-D-glucopyranosyl-	
	74b	14.59	$C_{49}H_{80}O_{20}$	1011.5133 $[M+Na]^+$					AM
				1033.5238 $[M+HCOOH-H]^-$	1.2	987.5135, 945.5042, 927.4931, 783.4768, 765.4352, 486.0766, 113.0232	-		

75				947.5199 $[M+H]^-$, 969.5024 $[M+Na]^+$	-0.6	455.3520, 419.3308, 437.3415, 143.1070	-		
	75	14.67	$C_{47}H_{78}O_{19}$	991.5178 $[M+HCOOH-H]^-$	1.6	945.5079, 783.4555，765.4380, 651.4090, 621.3974, 515.3308, 489.3563, 471.3448, 179.0563, 161.0444, 143.0346, 113.0265， 101.0244, 89.0239	9.75	Astragaloside V/Astragaloside VI/Astragaloside VII	AM
76				989.5317 $[M+H]^+$, 1011.5133 $[M+Na]^+$	0.5	473.3616, 455.3519, 437.3403, 419.3301, 401.3196	-		
	76	14.86	$C_{49}H_{80}O_{20}$	1033.5238 $[M+HCOOH-H]^-$	1.2	987.5135, 945.5042, 927.4931, 783.4768, 765.4352, 486.0765, 113.0232	-	Clethroidoside B	AM
77	77a	15.13	$C_{12}H_{14}O_3$	205.0858 $[M-H]^-$	-4.9	177.0930, 161.0976, 148.0159, 132.0578, 120.0211, 92.0284	2.12	6,7-Epoxyligustilide	LC
	77b	15.14	$C_{41}H_{68}O_{14}$	785.4662 $[M+H]^+$, 807.4538 $[M+Na]^+$	-1.1	473.3629, 455.3534, 437.3421, 419.3297	11.66	Astragaloside IV*	AM
				829.4603 $[M+HCOOH-H]^-$	0.1	783.4526, 621.4000, 489.3612, 179.0559, 161.0465, 113.0239, 101.0245	8.18		
78	78	15.22	$C_{12}H_{12}O_2$	189.0919 $[M+H]^+$	0.4	171.0816, 161.0966, 153.0691, 147.0446, 143.0853, 133.0285, 128.0623, 117.0703, 105.0324, 91.0533, 77.0378, 66.8947	2.61	3-Butylidene phthalide	LC
79	79a	15.25	$C_{12}H_{20}O_4S$	259.1008 $[M-H]^-$	-2.1	244.0772, 188.0134, 172.9904, 165.1273, 109.0284, 79.9562	2.69	5-ethyl-2-hexylfuran-3-sulfonic acid	PA
	79b	15.26	$C_{41}H_{68}O_{14}$	785.4605 $[M+H]^+$, 807.4480 $[M+Na]^+$	-1.1	473.3630, 455.3533, 437.3421, 419.3297	9.82	Astragaloside III*	AM
				829.4602 $[M+HCOOH-H]^-$	0.1	783.4540, 621.4002, 489.3577	7.18		
	79c	15.26	$C_{12}H_{14}O_3$	205.0858 $[M-H]^-$	-4.7	187.0738, 161.0972， 119.0521, 83.0480	2.11	(-)-3-Butyl-7-hydroxyphthalide	LC
80	80	15.31	$C_{16}H_{12}O_4$	269.0791 $[M+H]^+$, 291.0643 $[M+Na]^+$	0.3	254.0572, 237.0549, 226.0616, 219.0450, 213.0909, 137.0235, 118.0416	3.89	Formononetin*	AM

				267.063 $[M-H]^-$	-4	252.0418,239.0344, 223.0389, 208.0518, 195.0454, 180.0599, 167.0524, 135.0068, 132.0207, 104.0258, 91.0176	2.56		
81	81	15.35	$C_{12}H_{16}O_3$	207.1018 $[M-H]^-$	-5	189.0916, 163.1116, 150.0318, 121.0665, 109.0667, 85.0664	2.17	Senkyunolide K	LC
82				207.1016 $[M+H]^+$	-1.9	189.0897, 161.0991, 125.9851, 119.0856, 105.0329, 84.9595	-		
	82a	15.75	$C_{12}H_{14}O_3$	205.0858 $[M-H]^-$	-3	191.0696, 179.1087, 161.0966, 132.0588, 106.0423, 91.0182	2.07	(-)-3-Butyl-4-hydroxyphthalide	LC
	82b	15.8	$C_{12}H_{16}O_3$	207.1018 $[M-H]^-$	-5	193.0838, 179.1073, 150.0318, 122.0379, 109.0281	2.09	Senkyunolide G	LC
83	83a	15.86	$C_{17}H_{18}O_5$	303.1229 $[M+H]^+$	0.5	167.0705, 161.0598, 133.0650, 123.0444, 118.0416	3.85	(3R)-7,2'-dihydroxy-3',4'-dimethoxyisoflavan	AM
	83b	15.88	$C_{48}H_{78}O_{18}$	943.5275 $[M+H]^+$, 965.5062 $[M+Na]^+$	-1.2	599.3944, 581.3830, 441.3733, 423.3624, 405.3518	-	Soyasaponin I	AM
				941.5112 $[M-H]^-$, 987.518 $[M+HCOOH-H]^-$	0.3	923.4984, 733.4528, 615.3895, 457.3666, 161.0469, 101.0246	9.32		
	83c	15.91	$C_{47}H_{76}O_{17}$	911.5012 $[M-H]^-$, 957.5070 $[M+HCOOH-H]^-$	0.2	749.4493, 603.3890, 585.3736, 471.3472	8.97	Astragaloside -911	AM
	83d	15.92	$C_{43}H_{70}O_{15}$	827.4775 $[M+H]^+$, 849.4629 $[M+Na]^+$	-1.5	473.3630, 455.3534, 437.3421, 419.3297	12.4		
				871.4694 $[M+HCOOH-H]^-$	0.1	825.4623, 783.4534, 765.4431, 717.4117, 663.3992, 621.3803, 603.3990, 485.3275, 179.0560, 161.0481, 113.0237, 101.0245, 89.0248, 59.0128	8.77	Astragaloside II*	AM
84				645.3947 $[M+Na]^+$	-0.5	-	9.38		
	84a	16.13	$C_{35}H_{58}O_9$	667.4051 $[M+HCOOH-H]^-$	-1.8	487.3	6.59	Astramembrannin II	AM

	84b	16.16	$C_{17}H_{16}O_5$	301.1073 $[M+H]^+$, 323.0898 $[M+Na]^+$	0.3	283.0965, 269.0772, 241.0802, 191.0708, 179.0748, 167.0705, 147.0443, 134.0334, 106.0427	3.92	Farrerol*	AM
				299.0914 $[M-H]^-$	-3.7	284.0685, 269.0460	2.89		
	84c	16.17	$C_{53}H_{86}O_{22}$	1075.5678 $[M+H]^+$, 1097.5481 $[M+Na]^+$	0.3	960.4933, 849.4591, 675.4072, 455.3520, 437.3414	-	Astrogaloside-1073B	AM
				1073.5538 $[M-H]^-$, 1119.5613 $[M+HCOOH-H]^-$	1	911.5130, 749.4482, 603.3894, 585.3790, 471.3471, 113.0271	9.71		
85									
	85a	16.36	$C_{12}H_{12}O_3$	205.0864 $[M+H]^+$	2.3	187.0958, 169.0643, 159.0802, 115.0548, 91.0550, 84.9590	2.85	Senkyunolide E	LC
				203.0703 $[M-H]^-$	-4.6	173.0240, 160.0159, 145.0282, 132.0206, 117.0333, 106.0416, 92.0249	2.06		
	85b	16.41	$C_{43}H_{70}O_{15}$	827.4775 $[M+H]^+$, 849.4629 $[M+Na]^+$	0	473.3630, 455.3534, 437.3422, 419.3298	12.64	Isoastragaloside II*	AM
				871.4695 $[M+HCOOH-H]^-$	0.3	825.4641, 783.4651, 765.4398, 489.3498, 161.0445, 113.0237, 101.0245, 89.0248, 59.0128	8.79		
	86a	16.52	$C_{16}H_{12}O_5$	285.0776 $[M+H]^+$, 307.0594 $[M+Na]^+$	0.2	270.0521, 252.0385, 245.0845, 242.0529, 169.1031, 151.0534	3.5	Wogonin*	AM
				283.061 $[M-H]^-$	-4.7	268.0373, 239.0379, 198.0313, 162.9988	2.59		
	86b	16.53	$C_{18}H_{14}O_4$	295.0972 $[M+H]^+$, 317.0791 $[M+Na]^+$	2.2	277.0850, 249.0907, 221.0971, 185.0584, 165.0726	3.62	3α-Hydroxymethylenetanshinquinone	SM
	86c	16.63	$C_{19}H_{18}O_4$	311.1283 $[M+H]^+$, 333.1094 $[M+Na]^+$	1.7	295.1325, 283.1328, 267.1374, 252.1129, 237.1263, 225.0903, 197.0598, 185.0960	4.7	Hydroxytanshinone IIA	SM
87									
	87	16.76	$C_{43}H_{70}O_{15}$	827.4776 $[M+H]^+$, 849.4631 $[M+Na]^+$	0.7	669.3981, 473.3630, 455.3491, 437.3422, 419.3298	12.66	Trojanoside A	AM
				871.4695 $[M+HCOOH-H]^-$	0.3	825.4641, 783.4530, 765.4433, 603.3899, 489.3608, 161.0459, 113.0237, 101.0245, 89.0248, 59.0128	8.87		

88	88	16.82	$C_{16}H_{22}O_4$	279.1597 $[M+H]^+$, 301.1423 $[M+Na]^+$	4.1	261.1465, 233.1523, 205.1584, 191.1078	3.89	Senkyunolide M/Senkyunolide Q	LC
				277.1445 $[M-H]^-$	-3.8	236.1045, 221.1535, 205.1218, 177.0912, 163.1129, 148.0516	2.81		
89	89a	17.01	$C_{10}H_{22}O_4S$	237.1170 $[M-H]^-$	-2	96.96, 79.9570	2.55	Decyl hydrogen sulfate	HN
	89b	17.04	$C_{19}H_{18}O_4$	311.1285 $[M+H]^+$, 333.1103 $[M+Na]^+$	2.5	293.1179, 275.1075, 251.1059, 219.1180, 169.0650, 141.0699	4.72	Tanshinone IIB	SM
90	90	17.15	$C_{19}H_{18}O_4$	333.1105 $[M+Na]^+$	2.3	293.1177, 275.1063, 263.1067, 227.0721, 215.1044, 199.0750	4.73	1-keto-Isocryptotanshinone	SM
91	91	17.27	$C_{10}H_{22}O_4S$	237.1156 $[M-H]^-$	-4.2	165.0217, 96.9591, 79.9561	2.57	Decyl hydrogen sulfate isomer	HN
92	92a	17.31	$C_{18}H_{32}O_4$	311.2216 $[M-H]^-$	-3	293.2123, 275.2019, 253.1831, 235.1707, 223.1703, 174.9544, 87.0448	3.1	(9E)-9-Octadecenedioic acid	HN/PA
	92b	17.33	$C_{45}H_{72}O_{16}$	869.4911 $[M+H]^+$, 891.4743 $[M+Na]^+$	-0.2	873.4537, 831.4497, 689.4242, 671.4175, 653.4064, 473.3631, 455.3535, 437.3422, 419.3298	12.64	Astragaloside I*	AM
				913.483 $[M+HCOOH-H]^-$	1.5	825.4655, 766.4537, 487.3426	9.28		
93	93	17.56	$C_{11}H_{10}O_3$	193.1225 $[M+H]^+$	0.9	175.1113, 147.1171, 137.0601, 119.0851	2.78	Senkyunolide A	LC
94	94a	17.63	$C_{18}H_{14}O_3$	279.1003 $[M+H]^+$	-3.2	261.0912, 251.1033, 233.0951, 205.1011, 169.0643	3.46	Methylenetanshinquinone	SM
	94b	17.65	$C_{18}H_{16}O_4$	297.1121 $[M+H]^+$, 319.0949 $[M+Na]^+$	2.6	205.1021, 189.0704, 165.0703	3.75	Tanshinol B	SM
95	95	17.73	$C_{45}H_{72}O_{16}$	869.4912 $[M+H]^+$, 891.4744 $[M+Na]^+$	0	689.4269, 671.4175, 653.4086, 473.3542, 455.2007, 437.3422, 419.3298	13.06	Isoastragaloside I	AM
				913.4798 $[M+HCOOH-H]^-$	1.7	869.4809, 827.4778, 809.4560	9.41		
96	96	17.83	$C_{20}H_{20}O_5$	341.1373 $[M+H]^+$, 363.1205 $[M+Na]^+$	0.7	323.1278, 309.1154, 295.1314, 281.1160, 263.1065, 253.0887, 235.1114, 220.0875, 207.1169, 192.0921	4.4	Trijuganone C	SM
97	97a	18.02	$C_{11}H_{24}O_4S$	251.1313 $[M-H]^-$	0.6	165.0244, 96.9602, 79.9570	2.65	Undecyl sulfuric acid isomer I	HN

	97b	18.06	$C_{30}H_{50}O_5$	513.3556 $[M+Na]^+$	1.1	473.3620, 455.3517, 437.3411, 419.3307	7	Cyclosieversigenin*	AM
	97c	18.1	$C_{19}H_{22}O_4$	313.1439 $[M-H]^-$	-2.2	285.1503, 269.1549, 241.1591, 226.0996, 213.1284, 198.1057, 185.0961, 171.0831	3.27	Tanshinone V	SM
	97d	18.12	$C_{28}H_{48}NO_7P$	542.3246 $[M+H]^+$	0.4	524.3135, 376.9124, 184.0731, 104.1069, 86.0962	7.36	(2R)-3-Hydroxy-2-[(5Z,8Z,11Z,14Z,17Z)-5,8,11,14,17-icosapentaenoyloxy] propyl 2-(trimethylammonio) ethyl phosphate	HN
				586.3151 $[M+HCOOH-H]^-$	0.1	526.2928, 301.2165, 257.2295, 224.0670, 168.0429	5.70		
98				542.3246 $[M+H]^+$	0.4	524.3135, 258.1097, 184.0731, 166.0583, 124.9999, 104.1073, 86.0962, 60.0791	7.23		
	98a	18.33	$C_{28}H_{48}NO_7P$					LysoPC 20:5	HN
				586.3153 $[M+HCOOH-H]^-$	0.4	526.2934, 301.2164, 257.2242, 242.0802, 224.0673, 203.1779, 168.0429, 152.9941, 78.9581	5.71		
	98b	18.33	$C_{26}H_{48}NO_7P$	518.3247 $[M+H]^+$	0	184.0731, 104.1069, 86.0955	7.03	Lysophosphatidylcholine (18:3)	HN
				562.3142 $[M+HCOOH-H]^-$	0.5	502.2906, 277.2165, 224.0674, 152.9948	5.54		
99				869.4914 $[M+H]^+$, 891.4746 $[M+Na]^+$	0.3	689.4249, 671.4148, 653.4043, 635.3910, 473.3614, 455.3517, 437.3412, 419.3305, 401.3214	13.51		
	99	18.38	$C_{45}H_{72}O_{16}$					Astragaloside I isomer	AM
				867.4747 $[M-H]^-$, 913.483 $[M+HCOOH-H]^-$	1.7	825.4658, 469.0039, 179.0563, 161.0447, 119.0353, 101.0241, 89.0240, 71.0134, 59.0135	9.48		
100	100	18.45	$C_{11}H_{24}O_4S$	251.1313 $[M-H]^-$	1.3	96.9592, 79.9562	2.68	Undecyl sulfuric acid	HN
101	101	18.58	$C_{11}H_{24}O_4S$	251.1313 $[M-H]^-$	1.3	165.0244, 96.9594, 79.9562	2.7	Undecyl sulfuric acid isomer II	HN
102	102a	18.63a	$C_{18}H_{14}O_3$	279.102 $[M+H]^+$, 301.0837 $[M+Na]^+$	1.1	261.0903, 251.1033, 233.0951, 205.1011, 169.0643, 141.0701	3.3	Dihydrotanshinone I	SM
	102b	18.72	$C_{18}H_{16}O_3$	281.1173 $[M+H]^+$	0.4	263.1067, 252.0772, 235.1113, 220.0854, 207.1167, 192.0935	3.51	Neotanshinone B	SM
103	103a	18.95	$C_{18}H_{14}O_3$	279.0952 $[M+H]^+$, 301.0833 $[M+Na]^+$	-1.6	187.1	3.42	1,2-Dihydrotanshinone I*	SM

	103b	18.95	$C_{24}H_{50}NO_6P$	480.3445 $[M+H]^+$	-0.7	462.3284,299.2610,184.0733,166.0362,124.9999, 104.1068, 86.0961, 71.0710, 60.0796	7.15	(R, E)-3-(hexadec-9-en-1-yloxy)-2-hydroxypropyl (2-(trimethylammonio) ethyl) phosphate	HN
				524.3362 $[M+HCOOH-H]^-$	0.1	464.3144,393.2404,375.2300,326.2785,241.2165, 224.0687, 168.0423, 78.9582	5.35		
	103c	18.96	$C_{28}H_{50}NO_7P$	544.3383 $[M+H]^+$	-0.9	353.2743, 184.0731, 125.0007, 86.0952	7.54	3-Hydroxy-2-[(5Z,8Z,11Z,14Z)-5,8,11,14-icosatetraenoyloxy] propyl 2-(trimethylammonio) ethyl phosphate	HN
				588.3343 $[M+HCOOH-H]^-$	-1.7	528.3124, 303.2324, 259.2443, 242.0791	5.78		
	103d	18.96	$C_{26}H_{50}NO_7P$	520.3392 $[M+H]^+$	-1.1	502.3280, 365.3524, 184.0743, 166.0647, 124.9999, 104.1067, 86.0965	7.37	2-linoleoyl-sn-glycero-3-phosphocholine	HN
				564.3297 $[M+HCOOH-H]^-$	-1.5	504.3088, 279.2320, 242.0800, 224.0680, 168.0417, 152.9942, 78.9582	5.58		
104	104	19.05	$C_{20}H_{26}O_2$	299.2011 $[M+H]^+$	0.1	187.0759, 159.0808	4.22	5,6-Dehydrosugiol	SM
				297.1854 $[M-H]^-$	1.9	282.1616, 267.1354	3.14		
105	105a	19.11	$C_{23}H_{50}NO_6P$	468.3449 $[M+H]^+$	0.3	285.27881, 240.0995, 184.0732, 181.0260, 166.0628, 124.9998, 104.1070, 86.09661, 71.073	7.25	3-hydroxy-2-(pentadecyloxy)propyl (2-(trimethylammonio)ethyl) phosphate	HN
				512.3349 $[M+HCOOH-H]^-$	0.1	452.3159, 407.2548, 381.2396, 363.2292, 224.0694, 168.0421, 78.9578	5.31		
	105b	19.12	$C_{19}H_{22}O_4$	315.1597 $[M+H]^+$, 339.1419 $[M+Na]^+$	2.1	297.1480, 279.1378, 251.1423, 215.1052, 183.0829	4.22	Neocryptotanshinone	SM
				313.1439 $[M-H]^-$	-2.1	295.1328, 283.1331, 267.1383, 255.1387	3.11		
106	106a	19.31	$C_{20}H_{18}O_5$	339.1000 $[M+H]^+$	-0.5	311.1237, 279.1022, 261.0917, 233.0951, 205.1018, 190.0786	4.25	Methyl tanshinonate	SM
	106b	19.32	$C_{23}H_{50}NO_6P$	468.3450 $[M+H]^+$	0	450.3340, 391.2608, 365.2468，285.2792,240.0999, 184.0732, 181.0269, 166.0627, 155.0131, 124.9997, 104.1069, 86.0966, 71.0732， 60.0802	7.25	(2R)-2-Hydroxy-3-(pentadecyloxy) propyl 2-(trimethylammonio) ethyl phosphate	HN

				512.3356 [M+HCOOH-H]$^-$	1.5	452.3143, 438.29734, 381.2396, 363.2292, 224.0684, 168.0420, 78.9582	5.32		
107	107	19.35	$C_{19}H_{18}O_3$	295.135 [M+H]$^+$, 317.1150 [M+Na]$^+$	1.4	280.1099, 262.0976, 242.1261, 234.1029, 219.0799, 191.0850, 178.0774, 165.0694, 152.0614, 141.0699, 128.0614, 115.0537, 91.0537	3.82	Isotanshinone IIA	SM
108	108a	19.49	$C_{47}H_{74}O_{17}$	911.501 [M+H]$^+$, 933.4825 [M+Na]$^+$	0.7	731.4326, 713.4281, 695.4151, 677.4075, 455.3480, 437.3443, 419.3341, 401.3195	-	Acetyl astragaloside I	AM
				955.4921 [M+HCCOH-H]$^-$	1.4	909.46632, 515.3358	10.03		
	108b	19.50	$C_{26}H_{52}NO_6P$	506.3598 [M+H]$^+$	-2.3	491.3385, 184.0727, 166.0637, 124.9999, 104.1071, 86.0942	7.29	Lysophosphatidylcholine (18:1)	HN
				550.3501 [M+HCOOH-H]$^-$	0.4	490.3300, 419.2556, 401.2418, 293.1228, 267.2322, 236.1038, 224.0698, 168.0422, 152.9971, 78.9581	5.54		
109	109	19.68	$C_{19}H_{24}O_3$	301.1801 [M+H]$^+$	0.9	271.1697, 256.1460, 241.1225, 227.1072, 215.1053, 203.1061, 187.0749, 177.0909, 165.0694, 152.0614, 141.0700, 128.0617, 115.0541, 91.0537	4.04	Miltipolone	SM
110	110	19.96	$C_{26}H_{52}NO_7P$	522.3556 [M+H]$^+$	0.2	504.3511, 337.2738, 184.0730, 124.9999, 86.0965	7.70	2-Oleoyl-sn-glycero-3-phosphorylcholine	HN
				566.3475 [M+HCOOH-H]$^-$	-0.2	506.3257, 281.3487, 242.0780, 224.0690, 152.9973	5.70		
111	111	20.05	$C_{24}H_{52}NO_6P$	482.3612 [M+H]$^+$	-0.4	464.3495,278.2830,184.0731,166.0626, 146.9820,124.9997,104.1068, 86.0967,60.0802	7.50	Phosphatidylcholinelyso alkyl 16:0	HN
				526.3535 [M+HCOOH-H]$^-$	3.3	466.3289,281.2485,242.0773,224.0668,168.0419, 152.9945, 146.9636	5.45		
112	112	20.17	$C_{18}H_{12}O_3$	277.0859 [M+H]$^+$, 299.0683 [M+Na]$^+$	1.3	249.0913, 221.0599, 207.0803, 193.1012, 178.0775, 141.0708	3.27	Tanshinone I*	SM
113	113	20.18	$C_{25}H_{52}NO_6P$	494.3603 [M+H]$^+$	-0.4	476.3402, 311.2588, 285.0133, 184.0729, 166.0620, 124.9999, 104.1069, 98.9835, 86.0960, 60.0794	7.56		HN

				538.3517 [M+HCOOH-H]$^-$	-0.8	478.3304, 407.2572, 389.2456, 377.2445, 224.0675, 168.0424, 152.9936, 136.9989, 96.9693, 78.9581	-	(2R)-3-[(1Z)-1-Heptadecen-1-yloxy]-2-hydroxypropyl 2-(trimethylammonio) ethyl phosphate	
114									
	114a	20.21	$C_{19}H_{20}O_3$	297.1491 [M+H]$^+$, 319.1295 [M+Na]$^+$	1.2	282.1253, 279.1379, 271.1690, 267.10211, 241.1218, 221.0951, 207.0800, 193.1005, 178.0778, 165.0701, 153.0694, 141.0702, 128.0617, 115.0541, 91.0538	2.98	Isocryptotanshinone	SM
	114b	20.21	$C_{18}H_{12}O_4$	293.08 [M+H]$^+$	-0.2	265.0875, 209.0957, 194.0730, 191.0862, 165.0702	-	Monohydroxytanshinone I	SM
115									
	115a	20.25	$C_{26}H_{52}NO_7P$	522.3546 [M+H]$^+$	0.2	504.3451, 184.0737, 124.9980, 104.1062, 86.0954	7.62	Oleoyl-lysophosphatidylcholine	HN
				566.3459 [M+HCOOH-H]$^-$	-0.2	506.3243, 281.3488, 224.0714	5.74		
	115b	20.25	$C_{24}H_{52}NO_6P$	482.3612 [M+H]$^+$	-0.4	464.3483, 359.1905, 245.14445, 184.0731, 166.0629, 124.9999, 104.1069, 86.09685, 60.0795	7.48	Lysophosphatidylcholine *O*-16:0/0:0	HN
				526.3676 [M+HCOOH-H]$^-$	0.1	466.3302, 395.2563, 377.2459, 168.0423,78.9581	5.47		
116									
	116	20.26	$C_{20}H_{28}O_2$	301.2 [M+H]$^+$	0.7	259.1700, 213.1282	4.33	Sugiol	SM
				299.2 [M-H]$^-$	-3.5	285.1547, 269.1530, 227.1079, 213.0148, 197.9926,	3.15		
117									
	117	20.53	$C_{28}H_{54}NO_7P$	548.3705 [M+H]$^+$	-1.1	530.3638, 264.2670, 184.0731, 166.0583,124.9999, 104.1073, 86.0962, 60.0791	7.79	2-Eicosadienoyl-sn-glycero-3-phosphocholine	HN
				592.3614 [M+HCOOH-H]$^-$	-0.3	532.3408, 307.2635, 242.0746, 224.0670, 152.9970, 116.9278, 78.9576	-		
118									
	118a	20.63	$C_{19}H_{20}O_4$	313.1444 [M+H]$^+$	2	295.1329, 267.1061, 254.0938, 251.1430, 241.1223, 169.1012	4.11	1,2,6,7,8,9-Hexahydro-1,6,6-trimethyl-3,11-dioxanaphtho[2,1-e]azulene-10,12-dione	SM
	118b	20.65	$C_{24}H_{30}O_4$	405.2042 [M+Na]$^+$	1.4	253.1062, 191.1073, 175.1117, 147.1182, 105.0695, 91.0532	5.41	Senkyunolide P	LC
119									
	119	20.79	$C_{28}H_{54}NO_7P$	548.3711 [M+H]$^+$	0	530.3638, 264.2670, 184.0731, 166.0583,124.9999, 104.1073, 86.0962, 60.0791	7.76	Lysophosphatidylcholine (20:2)	HN

				592.3615 [M+HCOOH-H]$^-$	-0.4	532.3408, 307.2635, 242.0746, 224.0670, 152.9970, 116.9278, 78.9576	5.61		
120	120	21.13	$C_{17}H_{12}O_3$	265.0866 [M+H]$^+$	2.7	237.0910, 209.0961, 181.0648	3.29	Tanshinlactone	SM
				309.0765 [M+HCOOH-H]$^-$	-2.8	235.0792, 223.0741, 221.0972	-		
121	121	21.49	$C_{24}H_{28}O_4$	381.2068 [M+H]$^+$, 403.1884 [M+Na]$^+$	1.2	385.1661, 365.1109, 347.2213, 321.2133, 261.0388, 213.0872	5.06	Levistolide A*	LC
122				524.3709 [M+H]$^+$	-0.8	506.3579, 483.1754, 341.3075, 258.1137, 184.0733, 166.0583, 124.9999, 104.1073, 86.0962, 60.0791	7.9		
	122	21.65	$C_{26}H_{54}NO_7P$					1-Stearoyl-lysophosphatidylcholine	HN
				568.3620 [M+HCOOH-H]$^-$	0	508.3394, 283.2628, 242.0770, 224.0668, 152.9950, 116.9284, 78.9585	5.86		
123	123	21.76	$C_{19}H_{18}O_3$	295.1326 [M+H]$^+$	-1	280.1099, 277.1218, 262.0997, 249.1285, 234.1023, 219.0804	3.87	Tanshinone IIA*	SM
124	124	22.17	$C_{19}H_{22}O_2$	283.1695 [M+H]$^+$, 305.1512 [M+Na]$^+$	0.1	265.1585, 240.1142, 223.1115, 207.0809, 195.1161, 178.0775, 165.0698, 152.0618, 115.0536, 91.0535, 67.0537	4.79	Miltirone	SM
125	125	22.2	$C_{18}H_{20}O_2$	269.1538 [M+H]$^+$	0.9	254.1301, 239.1069, 225.0915, 208.1244, 193.1014, 178.0776, 165.0700, 152.0619, 128.0615, 115.0538, 91.0535, 69.0363	3.66	Salviolone	SM
126				510.4 [M+H]$^+$	-0.4	492.3812, 468.3211, 368.3230，327.2879, 184.0731, 166.0608, 124.9999, 104.1068, 98.9844，86.0956, 60.0799	7.97		
	126	22.29	$C_{26}H_{56}NO_6P$					Lyso-PAF C-18	HN
				554.3829 [M+HCOOH-H]$^-$	-0.3	494.3615, 473.2866, 449.2999, 423.2872, 405.2771, 224.067, 168.0422,78.9580	5.79		
127	127	22.32	$C_{28}H_{56}NO_7P$	550.3863 [M+H]$^+$	-0.7	532.3757, 473.3063, 367.3164, 258.1073, 184.0734, 166.0630, 124.9999, 104.1067, 86.0956	8.21	1-*O*-(13'Z-Eicosaenoyl)-sn-glycero-3-phosphocholine	HN

				594.3767 [M+HCOOH-H]$^-$	-1.6	534.3554, 309.2794, 281.2478, 242.0813, 224.0689, 168.0420, 152.9964, 78.9580	6.07		
128	128	22.88	$C_{20}H_{30}O_2$	301.2189 [M-H]$^-$	4.5	283.2067, 257.2278, 229.1953, 203.1815,	3.32	Eicosapentanoic acid	PA
129	129	23.03	$C_{18}H_{30}O_2$	277.2176 [M-H]$^-$	1.08	264.0779, 251.1067, 199.8477	-	8,12,15-Octadecatrienoic acid, (8E,12Z,15Z)	PA/SM
130	130	23.38	$C_{19}H_{20}O_3$	297.1595 [M+H]$^+$	3.4	282.124, 279.1376, 254.0926	4.07	Cryptotanshinone*	SM
131	131	23.6	$C_{16}H_{30}O_2$	253.2177 [M-H]$^-$	1.6	239.1700, 116.9287	2.84	2-Pentadecenoic acid	PA
132	132	23.61	$C_{30}H_{48}O_3$	455.3516 [M-H]$^-$	3.3	412.2453, 394.2400, 227.2068, 206.8958, 116.9276	-	*β*-Ursolic acid	SM
133	133	23.83	$C_{19}H_{18}O_3$	295.1326 [M+H]$^+$	-1	277.1218, 249.1270, 235.0743, 207.0791, 179.0863, 141.0715	3.78	1,2-Didehydrocryptotanshinone	SM
134	134	23.89	$C_{20}H_{32}O_2$	303.233 [M-H]$^-$	0	285.2180, 259.2444, 238.8341, 199.8497	3.31	Arachidonic acid	PA
135	135	24.06	$C_{18}H_{32}O_2$	279.233 [M-H]$^-$	0	261.2697, 251.1058, 239.1436, 196.0272	3.1	Linoleic acid	PA

Note: Rt: retention time; SM: *Salvia miltiorrhiza* Bge.; AM: *Astragalus membranaceus* (Fisch.) Bge.var.*mongholicus* (Bge.) Hsiao; LC: *Ligusticum chuanxiong* Hort.; HN: *Hirudo nipponica* Whitman ; PA: *Pheretima aspergillum* (E.Perrier).

*compared with a reference standard.