

Table S1. Summary of the chemical constituents detected for San-Miao-Wan using the multiple-data processing approach and UPLC-MS in positive ionization mode.

No	RT (min)	m/z [M+H] ⁺	Error (ppm)	Molecular formula	MS/MS fragment ion (m/z)	Identification	Source
1	0.81	337.1655	5.3	C19H20N4O2	308.1273 [M+H-C2H5] ⁺ 295.1195 [M+H-C3H6] ⁺ 277.1089 [M+H-C3H8O] ⁺ 200.0334 [M+H-C10H17] ⁺ 133.0653 [M+H-C10H12N4O] ⁺ 106.0419 [M+H-C12H15N4O] ⁺ 74.0156 [M+H-C13H19N4O2] ⁺	2-(2-Amino-5-morpholin-4-yl-phenyl)-4-methyl-2H-phthalazin-1-one	RA
2	0.85	118.0771	-4.6	C5H11NO2	102.0555 [M+H-CH4] ⁺ 87.0446 [M+H-CH5N] ⁺ 74.0242 [M+H-C3H8] ⁺ 58.0657 [M+H-C2H4O2] ⁺	Valine	RA
3	0.9	325.1049	2.5	C14H16N2O7	279.0159 [M+H-C3H10] ⁺ 277.0097 [M+H-C3H12] ⁺ 247.0719 [M+H-C2H6O3] ⁺ 225.0511 [M+H-C5H8O2] ⁺ 217.0249 [M+H-C4H12O3] ⁺	Dimethyl 2-(morpholin-4-yl)-5-nitroterephthalate	牛膝
4	0.91	145.0451	-4.7	C6H8O4	133.0501 [M+H-C] ⁺ + 128.0473 [M+H-HO] ⁺ + 115.0395 [M+H-CH2O] ⁺ + 99.0446 [M+H-CH2O2] ⁺ + 73.0290 [M+H-C3H4O2] ⁺ + 55.0184 [M+H-C3H6O3] ⁺ +	Meldrum's Acid	RA
5	1.61	325.1082	-1.8	C20H12N4O	271.0871 [M+H-C2H2N2] ⁺ 154.0387 [M+H-C9H7N4] ⁺ 130.0531 [M+H-C12H7N2O] ⁺	11-Methyl-7H,10H-benzo[de]imidazo[4',5':5,6]benzimidazo[2,1-a]isoquinolin-7-one	牛膝
6	1.95	180.1307	-6.5	C11H18NO	150.0919 [M+H-C2H7] ⁺ 133.0528 [M+H-C3H12] ⁺ 122.0732 [M+H-C3H9N] ⁺ 119.0497 [M+H-C3H12N] ⁺ 70.0657 [M+H-C7H11O] ⁺	candicine	CRC
7	2.1	192.0979	-4.3	C10H9NO3	163.0390 [M+H-CH3N] ⁺ 160.0399 [M+H-CH4O] ⁺ 151.0395 [M+H-C2H3N] ⁺ 60.0443 [M+H-C8H4O2] ⁺	Noroxyhydrastinine	CRC
8	2.95	314.1611	5.1	C19H23NO3	281.1052 [M+H-C2H9] ⁺ 189.0790 [M+H-C8H13O] ⁺ 161.0477 [M+H-C10H17O] ⁺ 150.0681 [M+H-C10H14NO] ⁺ 146.0368 [M+H-C10H18NO] ⁺ 121.0290 [M+H-C12H19NO] ⁺ 107.0497 [M+H-C12H17NO2] ⁺	Evoeuropine	CRC
9	2.98	298.1326	3.7	C14H19NO6	250.1093 [M+H-CH4O2] ⁺ , 223.0481 [M+H-C4H11O] ⁺ , 209.0688 [M+H-C4H9O2] ⁺ 177.0426 [M+H-C5H13O3] ⁺ , 161.0477 [M+H-C5H13O4] ⁺ , 89.0265 [M+H-C8H17O6] ⁺	3,4,5-pyridinetricarboxylic acid, 1,4-dihydro-2,6-dimethyl-, 3,5-diethyl ester	RA
10	3.09	448.1909	0.7	C30H25NO3	357.1365 [M+H-C7H7] ⁺ 343.1572 [M+H-C7H5O] ⁺ 147.0446 [M+H-C21H19NO] ⁺ 131.0497 [M+H-C21H19NO2] ⁺ 130.0055 [M+H-C22H24NO] ⁺	8-[(dibenzylamino)methyl]-7-hydroxy-3-phenyl-4H-chromen-4-one	CRC
11	3.16	192.0969	-4.1	C11H13NO2	175.0633 [M+H-CH5] ⁺ + 151.0759 [M+H-C2H3N] ⁺ + 122.0368 [M+H-C4H8N] ⁺ + 109.0290 [M+H-C5H9N] ⁺ + 87.9949 [M+H-C5H14NO] ⁺ +	Dehydroheliamine	CRC
12	3.16	342.1562	2.9	C12H19N7O5	315.1645 [M+H-CHN] ⁺ 314.1616 [M+H-CH2N] ⁺ 298.1287 [M+H-C2H6N] ⁺ 249.0916 [M+H-C3H10NO2] ⁺ 192.1025 [M+H-C9H10O2] ⁺ 177.0552 [M+H-C10H14NO] ⁺ 145.0290 [M+H-C11H19NO2] ⁺	Tetrahydrojatrorrhizine	CRC
13	3.4	344.1803	-3.4	C15H25N3O6	343.1704 [M+H-H] ⁺ 222.1004 [M+H-C4H12NO3] ⁺ 209.0562 [M+H-C6H17NO2] ⁺ 192.0773 [M+H-C6H16O4] ⁺ 163.0144 [M+H-C8H23NO3] ⁺ 95.0007 [M+H-C11H25N2O4] ⁺	Methyl N-{[(2-methyl-2-propanyl)oxy]carbonyl}glycylprolyl glycinate	CRC
14	3.45	342.1439	-3.6	C15H23N3O6	325.1400 [M+H-H2N] ⁺ 313.1274 [M+H-C2H5] ⁺ 311.1481 [M+H-CH3O] ⁺ 298.1039 [M+H-C3H8] ⁺ 293.1012 [M+H-C2H9O] ⁺ 290.1505 [M+H-H4O3] ⁺ 287.1481 [M+H-C3H3O] ⁺	2-{3,3-Bis[(2-hydroxyethyl)amino]-2-nitroprop-2-en-1-ylidene}-5,5-dimethylcyclohexane-1,3-dione	CRC
15	3.52	274.1326	-3.3	C11H19N3O5	257.1376 [M+H-HO] ⁺ 217.1063 [M+H-C3H5O] ⁺ 189.0875 [M+H-C4H7NO] ⁺ 179.0695 [M+H-C3H11O3] ⁺	5-[(1R,2S)-1,2-Dihydroxy-2-methyl-3-(4-morpholinyl)prop	CRC

					127.0395 [M+H-C5H13N3O2]+ 95.0735 [M+H-C5H11N2O5]+	yl]-2,4- imidazolidinedione	
16	3.67	177.0478	4.2	C6H4N6O	149.0338 [M+H-CH2N] + 149.0212 [M+H-C2H3] + 133.0514 [M+H-N2O] + 145.0263 [M+H-CH3O] + 117.0327 [M+H-H2N3O] +	5,7- Diamino[1,2,5]ox adiazolo[3,4- b]pyridine-6- carbonitrile	CRC
17	4.24	314.1661	5.7	C15H23NO6	219.0532 [M+H-C4H15O2]+ 177.0552 [M+H-C5H15NO3]+ 162.0681 [M+H-C5H14NO4]+ 149.0239 [M+H-C7H19NO3]+ 147.0082 [M+H-C7H21NO3]+ 116.9926 [M+H-C8H23NO4]+	Methyl 4-{3- [bis(2- hydroxyethyl)ami no]-2- hydroxypropoxy} benzoate	RA
18	4.94	356.1712	3.8	C13H21N7O5	261.0736 [M+H-C3H13NO2]+ 260.1022 [M+H-C2H10NO3]+ 242.0916 [M+H-C2H12NO4]+ 177.0525 [M+H-C7H17NO4]+	2-Amino-N-(3- amino-2- hydroxypropyl)ad enosine	CRC
19	5.31	304.1467	4.3	C19H17N3O	286.0889 [M+H-CH6]+ 260.0773 [M+H-C3H8]+	7, 8- dihydroxyrutaecar pine	CRC
20	6.08	356.1749	-4.8	C21H25NO4	324.1236 [M+H-C2H8]+ 147.0446 [M+H-C12H19NO2]+ 130.0055 [M+H-C13H24NO2]+	tetrahydropalmati ne	CRC
21	6.58	396.7954	-1.8	C22H28N4O3	356.1848 [M+H-C3H5]+ 249.1239 [M+H-C9H12N2]+ 161.0477 [M+H-C13H22N3O]+ 100.0762 [M+H-C17H19N3O2]+ 69.9929 [M+H-C20H29N3O]+	Dictamnine	CRC
22	7.49	338.1274	-3.1	C20H20NO4	209.0477 [M+H-C7H14O2]+ 167.0007 [M+H-C10H20O2]+ 88.0187 [M+H-C14H19O4]+	Jatrorrhizine	CRC
23	7.73	370.1969	-3.2	C17H27N3O6	343.1743 [M+H-C2H3]+ 328.1872 [M+H-C2H2O]+ 261.1113 [M+H-C4H13O3]+ 177.0426 [M+H-C8H21N2O3]+ 114.0919 [M+H-C11H16N2O5]+ 81.0578 [M+H-C12H21N2O6]+	2-{2-[4-(4,5- Dimethoxy-2- nitrobenzyl)-1- piperazinyl]ethox y}ethanol	CRC
24	8.08	218.2074	-2.6	C12H27NO2	200.1776 [M+H-H3N]+ 170.0970 [M+H-H15O2]+ 149.0265 [M+H-CH24O2]+ 137.0477 [M+H-C5H20]+ 100.0762 [M+H-C7H17O]+	ammonium laurate	RA
25	8.83	352.126	-4.8	C21H22NO4	338.1392 [M+H-CH3]+ 324.1236 [M+H-C2H5]+ 169.0528 [M+H-C10H16O3]+ 161.0603 [M+H-C11H14NO2]+ 147.0446 [M+H-C12H16NO2]+ 121.0290 [M+H-C14H18NO2]+ 93.0340 [M+H-C15H18NO3]+	Palmatine	CRC
26	9.04	336.0914	0.9	C20H18NO4	145.0290 [M+H-C11H14NO2]+ 133.0290 [M+H-C12H14NO2]+ 88.0313 [M+H-C13H15NO4]+	Berberine	CRC
27	12.63	471.1917	-2.1	C26H30O8	435.1808 [M+H-H4O2]+ 425.1964 [M+H-CH2O2]+ 347.1859 [M+H-C6H4O3]+ 205.0501 [M+H-C15H22O4]+	Obaculactone	CRC
28	13.56	274.2635	0.7	C13H31N5O	230.2232 [M+H-CH4N2]+ 172.1576 [M+H-C4H12N3]+ 158.1293 [M+H-C6H16N2]+ 130.1106 [M+H-C7H18N3]+	N-[3-({4-[(3- aminopropyl)amin o]butyl} amino)pr opyl]-β- alaninamide	RA
29	13.88	231.1331	-2.1	C15H18O2	190.0994 [M+H-C3H5]+ 187.1123 [M+H-C2H4O]+ 175.0759 [M+H-C4H8]+ 161.0966 [M+H-C4H6O]+ 119.0861 [M+H-C6H8O2]+ 105.0704 [M+H-C7H10O2]+ 69.0704 [M+H-C10H10O2]+	Atractylenolide-1	RA
30	13.97	455.1999	-5.3	C26H30O7	439.1757 [M+H-CH4]+ 419.1859 [M+H-H4O2]+ 395.1859 [M+H-C2H4O2]+ 359.1859 [M+H-C5H4O2]+ 333.2066 [M+H-C6H2O3]+ 249.1491 [M+H-C11H10O4]+ 163.0759 [M+H-C16H20O5]+	Obacunone	CRC
31	15.18	302.2998	5.2	C15H35N5O	158.1217 [M+H-C8H20N2]+ 130.1106 [M+H-C9H22N3]+ 130.1232 [M+H-C8H20N4]+ 85.0402 [M+H-C12H31N3]+ 85.0528 [M+H-C11H29N4]+ 81.0340 [M+H-C10H31N5]+ 57.0578 [M+H-C12H29N4O]+	-	RA
32	16.44	231.1282	-1.7	C10H18N2O4	201.0875 [M+H-C2H6]+ 185.1290 [M+H-CH2O2]+ 170.0817 [M+H-C2H7NO]+ 167.0821 [M+H-C2H8O2]+ 105.0664 [M+H-C7H10O2]+ 57.0704 [M+H-C6H10N2O4]+	4-Boc-piperazine- 2-carboxylic acid	RA
33	16.46	165.0633	5.1	C6H12O5	149.0429 [M+H-CH4]+ 131.0359 [M+H-CH6O]+ 121.0459 [M+H-C2H4O]+ 81.0044 [M+H-C2H12O3]+	Rhamnose	RA
34	16.51	325.1225	0.3	C12H18N6O5	263.1256 [M+H-CH4O3]+	-	RA

35	16.51	341.1057	5.3	C20H12N4O2	211.0943 [M+H-C5H8O3]+	4-[2-(9H-Fluoren-9-ylidene)hydrazino]-3-nitrobenzonitrile 4-hydroxy-5-(pentyloxy)pentan-4-ehydrazide	RA
					166.0603 [M+H-C7H13O4]+		
					180.0813 [M+H-C7H3N3O2]+		
					149.0589 [M+H-C13H6NO]+		
36	17.03	219.1677	0	C10H22N2O3	100.0187 [M+H-C13H11N3O2]+		CRC
					205.1650 [M+H-CH2]+		
					202.1364 [M+H-CH5]+		
					175.1005 [M+H-C3H8]+		
					161.1178 [M+H-C2H6N2]+		
					147.0770 [M+H-C5H12]+		
					81.0578 [M+H-C5H16NO3]+		

Note: CRC, Cortex Phellodendri Chinensis; RA, Rhizoma Atractylodis; RAB, Radix Achyranthis Bidentatae

Table S2. Chemical constituents detected for SMW using UPLC-MS in negative ionization mode.

No	RT (min)	mass[M-H]-	Error (ppm)	Molecular formula	MS/MS fragment ion (m/z)	Identification	Source
1.	0.82	145.0611	-2.8	C5H10N2O3	132.0661 [M-H-N]- 131.0821 [M-H-O]- 128.0586 [M-H-HO]- 128.0348 [M-H-H3N]- 113.0239 [M-H-H4N2]- 74.0242 [M-H-C3H5NO]- 71.0133 [M-H-C2H6N2O]-	Glutamine	RAB
2.	0.83	131.0443	-5.7	C4H8N2O3	118.0504 [M-H-N]- 115.0269 [M-H-H2N]- 104.0348 [M-H-CHN]- 88.0399 [M-H-CHNO]- 70.0293 [M-H-CH3NO2]- 59.0133 [M-H-C2H4N2O]-	-	RA
3.	0.83	293.0997	0.0	C10H18N2O8	292.0907 [M-H-H2]- 290.0750 [M-H-H4]- 281.0985 [M-H-CH]- 281.0046 [M-H-H13]- 280.1032 [M-H-N]-	N-L- β -Asparty1- β -D- glucopyranosylamine	RA
4.	0.84	317.0559	-0.3	C13H10N4O6	280.0444 [M-H-C3H]- 275.0542 [M-H-CNO]- 257.0311 [M-H-C2H4O2]- 243.0154 [M-H-C3H6O2]- 239.0569 [M-H-CH2O4]- 227.0178 [M-H-C6H4N]- 225.0022 [M-H-C6H6N]- 223.0229 [M-H-C5H4NO]-	3,5-Dinitro-4-[(3- pyridinylmethyl)amino]benzoi c acid	RA
5.	0.85	207.0506	-2.4	C14H8O2	207.0446 [M-H-H]- 202.0055 [M-H-H6]-	9,10-phenanthraquinone	RA
6.	0.86	195.0489	-4.6	C3H4N10O	181.0732 [M-H-O]- 113.0338 [M-H-CN5]- 85.0388 [M-H-C2N5O]-	1,3-Di-2H-tetrazol-5-ylurea	RA
7.	0.88	439.08	-0.5	C22H12N6O5	422.0764 [M-H-HO]- 391.0791 [M-H-C4]- 379.0917 [M-H-C4N]- 319.0467 [M-H-C6H4N2O]- 277.0362 [M-H-C8H6N2O2]- 243.0154 [M-H-C12H8N2O]-	N'-[(11Z)-11H-Indeno[1,2- b]quinoxalin-11-ylidene]-3,5- dinitrobenzohydrazide	RA
8.	0.89	191.0524	-3.5	C7H12O6	191.0556 [M-H-H]- 173.0450 [M-H-H2O]- 93.0340 [M-H-CH6O5]- 85.0290 [M-H-C3H6O4]- 59.0133 [M-H-C5H8O4]-	Kinic acid	RA
9.	0.92	179.0549	-5.0	C6H12O6	162.0528[M-H-HO]- 150.0528 [M-H-CHO]- 146.0579 [M-H-HO2]- 144.0423 [M-H-H3O2]- 132.0423 [M-H-CH3O2]- 129.0188 [M-H-CH6O2]- 126.0317 [M-H-H5O3]- 121.0501 [M-H-C2H2O2]- 116.0473 [M-H-CH3O3]- 114.0317 [M-H-CH5O3]-	Fructose	RA
10.	0.93	341.1008	2.6	C15H14N6O4	293.0423 [M-H-C2H8O]- 207.0518 [M-H-C7H6N2O]- 173.0589 [M-H-C6H6N3O3]- 145.0402 [M-H-C7H8N4O3]- 128.0222 [M-H-C11H9N4O]- 113.0225 [M-H-C12H10N3O2]- 85.0276 [M-H-C13H10N3O3]-	5-[(1,5-Dimethyl-3-oxo-2- phenyl-2,3-dihydro-1H- pyrazol-4- yl)hydrazono]pyrimidine- 2,4,6(1H,3H,5H)-trione	CRC
11.	0.93	503.1598	-5.2	C18H32O16	473.1507 [M-H-CH2O]- 456.1843 [M-H-O3]- 445.1557 [M-H-C2H2O2]- 383.1190 [M-H-C4H8O4]- 371.1190 [M-H-C5H8O4]-	Melezitose	RA
12.	0.93	665.2152	0.8	C24H42O21	665.2140 [M-H-H]- 657.1514 [M-H-H9]- 651.1045 [M-H-H15]- 646.0654 [M-H-H20]- 642.1280 [M-H-CH12]- 641.1565 [M-H-H9O]- 638.1906 [M-H-C2H4]- 636.2113 [M-H-CHO]- 119.0344 [M-H-O]-	a-D-Glucopyranosyl-(1->4)-a- D-glucopyranosyl-(1->4)-a-D- glucopyranosyl-(1->4)-a-D- glucopyranose	RA
13.	0.96	133.0139	0	C4H6O5	115.0031 [M-H-H2O]- 104.0473 [M-H-O2]- 99.0082 [M-H-H2O2]-	MALIC ACID	RA
14.	1.61	200.0555	-3.5	C4H7N7O3	196.0219 [M-H-H5]- 167.0079 [M-H-H6N2]- 164.0321 [M-H-H5O2]- 151.0130 [M-H-H5N2O]- 135.0181 [M-H-H5N2O2]- 130.0729 [M-H-CN2O2]- 125.0100 [M-H-CH5N3O]-	3-(Nitroamino)-1,2,4a,5,7,7a- hexahydro-6H-imidazo[4,5- e][1,2,4]triazin-6-one	RAB
15.	2.37	529.1562	-0.4	C23H30O14	481.0982 [M-H-C2H8O]- 393.0822 [M-H-C5H12O4]- 359.0978 [M-H-C8H10O4]- 197.0450 [M-H-C14H20O9]- 151.0395 [M-H-C15H22O11]-	Pikuroside	CRC

16.	2.4	319.1591	-3.8	C12H24N4O6	251.1144 [M-H-CH8O3]- 197.0562 [M-H-C4H14N2O2]- 179.0695 [M-H-C4H14NO4]- 85.0402 [M-H-C9H18N2O5]-	2,2',2''-Nitrilotris[N-(2-hydroxyethyl)acetamide]	RA
17.	2.41	493.2296	-2.2	C22H38O12	479.2129 [M-H-CH2]- 463.2179 [M-H-CH2O]- 385.1135 [M-H-C5H16O2]- 285.1702 [M-H-C7H12O7]- 191.0556 [M-H-C15H26O6]- 161.0450 [M-H-C16H28O7]- 89.0239 [M-H-C19H32O9]-	(1R,4S,6R)-1,3,3-Trimethyl-2-oxabicyclo[2.2.2]oct-6-yl 6-O-β -D-glucopyranosyl- β -D-glucopyranoside	RA
18.	2.59	431.1533	1.9	C15H24N6O9	389.1547 [M-H-CNO]- 353.0859 [M-H-CH8N3O]- 293.0886 [M-H-C3H10N2O4]- 193.0487 [M-H-C7H16N3O6]- 179.0695 [M-H-C7H14N3O7]- 134.0453 [M-H-C11H15N5O5]- 91.0058 [M-H-C10H22N5O8]-	-	CRC
19.	2.92	134.0371	-1.0	C6H5N3O	134.0354 [M-H-H]- 109.0276 [M-H-C2H2]- 108.0449 [M-H-N2]- 96.0198 [M-H-C3H3]- 75.0235 [M-H-HN3O]-	N-Hydroxybenzotriazole	CRC
20.	2.92	193.0488	-2.3	C10H10O4	179.0344 [M-H-CH2]- 166.0630 [M-H-CO]- 149.0603 [M-H-CO2]- 135.0446 [M-H-C2H2O2]- 117.0340 [M-H-C2H4O3]- 59.0133 [M-H-C8H6O2]-	Ferulic acid	CRC
21.	2.93	367.1003	-1.1	C12H20N2O11	296.1220 [M-H-C2O3]- 271.0930 [M-H-CH4O5]- 235.0692 [M-H-C4H6NO4]- 206.1267 [M-H-C4HO7]- 134.0453 [M-H-C8H11NO7]-	3,11-Bis(carboxymethyl)-4,7,10-trioxa-3,11-diazatridecane-1,13-dioic acid	CRC
22.	3.29	590.2238	1.9	C25H33N7O10	519.1866 [M-H-H7O4]- 495.1866 [M-H-C2H7O4]- 371.0839 [M-H-C12H17N3O]- 207.0406 [M-H-C16H25N5O6]- 195.0280 [M-H-C18H27N4O6]- 136.0035 [M-H-C19H30N6O7]-	-	CRC
23.	3.66	173.0436	-5.8	C7H10O5	157.0501 [M-H-O]- 137.0239 [M-H-H4O2]- 111.0810 [M-H-O4]- 111.0446 [M-H-CH2O3]- 94.0419 [M-H-CH3O4]- 71.0497 [M-H-C3H2O4]- 67.0184 [M-H-C3H6O4]-	Shikimic acid	CRC
24.	3.66	367.093	-4.4	C17H20O9	325.0923 [M-H-C2H2O]- 195.0657 [M-H-C7H8O5]- 135.0446 [M-H-C9H12O7]- 134.0368 [M-H-C9H13O7]-	3-O-feruloylquinic acid	CRC
25.	6.87	187.0946	-4.1	C9H16O4	169.0865 [M-H-H2O]- 141.0916 [M-H-CH2O2]- 126.1045 [M-H-CHO3]- 125.0966 [M-H-CH2O3]- 97.0653 [M-H-C3H6O3]- 57.0340 [M-H-C6H10O3]-	Nonanedioic acid	RAB
26.	8.19	243.124	-1.2	C14H16N2O2	243.1134 [M-H-H]- 225.0790 [M-H-H5N]- 207.0195 [M-H-C2H13]- 207.0320 [M-H-CH11N]- 199.0058 [M-H-H15NO]- 171.0109 [M-H-CH15NO2]-	Etomidate	RA
27.	11.49	503.1927	-0.6	C26H32O10	387.1808 [M-H-C4H4O4]- 367.1393 [M-H-C8H8O2]- 327.2324 [M-H-C4HO8]- 305.1389 [M-H-C9H10O5]- 281.1389 [M-H-C11H10O5]- 96.9773 [M-H-C26H31O4]-	6,7,9,10,12,13,20,21,23,24,26,27-Dodecahydrodibenzo[b,n][1,4,7,10,13,16,19,22]octaoxacyclopentacosine-2,17-dicarbaldehyde	CRC
28.	11.58	329.2276	-3.3	C18H34O5	250.9981 [M-H-C4H31]- 224.9977 [M-H-C2H33O3]- 171.0657 [M-H-C10H23O]-	Sanleng acid	CRC
29.	11.9	953.4375	-2.2	C40H66N12O15	909.4556 [M-H-CH2NO]- 487.2431 [M-H-C16H32N7O9]- 487.2391 [M-H-C21H32N5O7]- 283.0917 [M-H-C30H52N7O10]- 265.0937 [M-H-C29H52N8O11]-	-	RAB
30.	12.08	955.4557	1.6	C47H72O20	874.3623 [M-H-C3H13O2]- 375.1655 [M-H-C30H44O11]- 327.1596 [M-H-C27H48O16]- 311.1131 [M-H-C32H52O13]-	(2aR,4aS,6aR,10R,11R,12aR,12bS,14bR)-11-Hydroxy-2a,12a-dimethyl-6-oxo-2a,4,4a,6a,7,9,10,11,12,12a,12b,13,14,14b-tetradecahydro-6H-2,3,5-trioxapentaleno[1',6':5,6,7]cyclonona[1,2-a]naphthalen-10-yl β -D-glucopyranosyl-(1->4)-2,6-dideoxy-3-O-methyl- α -L-ribo-hexopyranosyl-(1->4)-2,6-dideoxy- β -D-ribo-hexopyranosyl-(1->4)-2,6-dideoxy-3-O-methyl- β -L-ribo-hexopyranoside	RAB
31.	12.1	485.1811	-2.3	C26H30O9	407.1706 [M-H-C5H3O]- 313.1076 [M-H-C8H12O4]- 211.0970 [M-H-C15H14O5]- 209.0814 [M-H-C15H16O5]- 167.0344 [M-H-C18H22O5]- 61.9793 [M-H-C22H31O8]-	3,11-Bis(4-hydroxy-3-methoxyphenyl)-2,4,10,12-tetraoxadispiro[5.1.5.3]hexadecan-7-one	CRC
32.	12.61	469.1759	-2.1	C26H30O8	427.2121 [M-H-CO2]- 411.1444 [M-H-C3H6O]-	Nbaculactone	CRC

33.	12.62	515.1826	-2.1	C26H30O8	330.2195 [M-H-C5O5]- 283.1334 [M-H-C8H10O5]- 196.9875 [M-H-C15H29O4]- 61.9793 [M-H-C22H31O7]- 427.2121 [M-H-CO2]- 411.1444 [M-H-C3H6O]- 330.2195 [M-H-C5O5]- 283.1334 [M-H-C8H10O5]- 196.9875 [M-H-C15H29O4]- 61.9793 [M-H-C22H31O7]-	Obaculactone+ Formic acid	CRC
34.	12.86	471.2001	0.8	C22H28N6O6	375.1668 [M-H-C4H4N2O]- 323.0780 [M-H-C6H16N2O2]- 307.1519 [M-H-C9H8O3]- 265.1049 [M-H-C12H14O3]- 291.1233 [M-H-C10H10O2]- 171.0082 [M-H-C16H26O4]-	benzoic acid, 3,5-dimethoxy-, 2-[4-(2,3,6,7-tetrahydro-1,3- dimethyl-2,6-dioxo-1H-purin- 8-yl)-1-piperazinyl]ethyl ester obacunone	CRC CRC
35.	13.95	453.1906	-5.3	C26H30O7	680.2833 [M-H-CH5O]- 667.3482 [M-H-O3]- 645.2911 [M-H-C4H4O]- 649.3013 [M-H-CH4O3]- 623.0826 [M-H-C5H31]- 621.2700 [M-H-C3H8O3]- 613.3013 [M-H-C4H4O3]- 608.2622 [M-H-C4H9O3]- 605.2387 [M-H-C4H12O3]-	(2R,3R,3aR,4R,6S,7S,8S,10E, 12S,13aR)-2,7,8-Triacetoxy- 3,13a-dihydroxy-2,9,9,12- tetramethyl-4-[(2- methylbutanoyl)oxy]-5- methylene-13-oxo- 2,3,3a,4,5,6,7,8,9,12,13,13a- dodecahydro-1H- cyclopenta[12]annule n-6-yl benzoate	RA
36.	15.25	713.3152	-3.1	C38H50O13			
37.	15.25	723.3391	2.6	C46H48N2O6	678.3458 [M-H-CHO2]- 575.2672 [M-H-C9H10NO]- 325.1467 [M-H-C23H28NO5]-	(8Z,8'Z)-1,1',6,6'- Tetrahydroxy-5,5'-diisopropyl- 3,3'-dimethyl-8,8'-bis{[(1- phenylethyl)amino]methylene }-2,2'-binaphthalene- 7,7'(8H,8'H)-dione	RA
38.	15.51	593.2799	0.8	C27H46O14	505.3084 [M-H-C2O4]- 339.1291 [M-H-C14H22O4]- 307.1393 [M-H-C14H22O6]- 253.0923 [M-H-C18H28O6]-	3-O-[(1S)-1-Carboxy-2- cyclohexylethyl]- β -D- galactopyranosyl-(1->3)-[6- deoxy- α -L-galactopyranosyl- (1->4)]-1,5-anhydro-2,6- dideoxy-D-arabino-hexitol Galnon	RA RA
39.	15.51	677.333	-0.9	C40H46N4O6	593.2764 [M-H-C5H8O]- 509.2315 [M-H-C9H14NO2]- 491.2083 [M-H-C10H18O3]- 391.1618 [M-H-C22H22]- 309.2052 [M-H-C24H18NO3]- 265.1426 [M-H-C27H26NO3]- 253.1063 [M-H-C29H30NO2]- 101.0477 [M-H-C36H38N3O4]-		RA
40.	16.74	293.2122	0.3	C18H30O3	289.1804 [M-H-H5]- 285.1491 [M-H-H9]- 272.1776 [M-H-H6O]- 267.1960 [M-H-C2H2]- 249.1491 [M-H-C3H8]- 389.1713 [M-H-C3H8]- 378.1791 [M-H-C4H7]- 355.1869 [M-H-C6H6]- 337.2127 [M-H-C5H4O2]- 311.1607 [M-H-C8H10O]- 297.2430 [M-H-C5HN2O3]-	2-{2-[4-(1,1,3,3- TETRAMETHYLBUTYL)PH ENOXY]ETHOXY}ETHAN OL	RA
41.	16.77	433.2355	0.2	C23H34N2O6	485.2638 [M-H-C14H18N3O3]- 433.1598 [M-H-C20H30N3O]- 353.1461 [M-H-C24H32N4O2]- 294.1580 [M-H-C24H31N6O4]- 265.1301 [M-H-C27H36N4O5]-	N,N'-1,3-Propanediylbis(4,7,7- trimethyl-3-oxo-2- oxabicyclo[2.2.1]heptane-1- carboxamide)	RA
42.	17.75	761.3991	-0.7	C39H54N8O8	353.0899 [M-H-C25H44NO6]- 309.1239 [M-H-C26H42O9]- 293.1389 [M-H-C28H38N2O7]- 265.1314 [M-H-C30H40NO8]-	N-(pyrazin-2-ylcarbonyl)-D- valyl-D-valyl-(4R)-4-[(3,4- dihydroisoquinolin-2(1H)- ylcarbonyl)oxy]-N-[1,2-dioxo- 1-(propan-2-ylamino)hexan-3- yl]-L-prolinamide (9E,19E)-2,15,17,27,29- Pentahydroxy-11-methoxy- 3,7,12,14,16,18,22- heptamethyl-26-[(4-methyl-1- piperidiny)methyl]-6,23- dioxo-8,30-dioxa-24- azatetracyclo[23.3.1.14,7.05,2 8]triaconta-1(29),2,4,9,19, 21,25,27-octaen-13-yl acetate	RA RA
43.	18.6	807.4001	-0.2	C44H60N2O12			

Note: CRC, Cortex Phellodendri Chinensis; RA, Rhizoma Atractylodis; RAB, Radix Achyranthis Bidentatae