Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary table 1. Characterization of chemical constituents of KXS by UPLC/QTOF MS.

No.	Rt/ min	Compound Name	Positive (m/z)		Negativeion (m/z)		Formula	MW(Da)	Origin
			Indicated	ppm	Indicated	ppm			
1	0.83	Asparagine	—	—	131.0739	2.9	$C_4H_7NO_4$	132.0535	d
2	0.83	Bergapten	—	—	215.0344	0	$C_{12}H_8O_4$	216.0423	d
3	0.85	Argininyl-fructosyl-glucose	499.2157	4.0	—	—	$C_{18}H_{34}N_4O_{12}$	498.2173	a
4	0.86	Isopimpinellin	—	—	245.0450	-1.6	$C_{13}H_{10}O_5$	246.0528	d
5	0.90	Mannose	—	—	179.0556	1.1	$C_6H_{12}O_6$	180.0634	a
6	0.93	Valine	118.0863	2.9	—	—	$C_5H_{11}NO_2$	117.0790	d
7	0.93	5-Hydroxymethylfurfural	127.0395	3.4	—	—	$C_6H_6O_3$	126.0317	d
8	0.93	Dimethyl(R)-(+)-malate	163.0402	2.3	161.0398	5	$C_6H_{10}O_5$	162.0528	b
9	0.97	2,3-Dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one	145.0501	1.3	—	—	$C_6H_8O_4$	144.0423	d
10	1.12	Sucrose	—	—	341.1084	-9.1	$C_{12}H_{22}O_{11}$	342.1162	a+c
11	1.53	Nicotinic acid	124.0399	-9.7	—	—	$C_6H_5NO_2$	123.0320	a
12	1.62	Benzoic acid	123.0446	1.8	—	—	$C_7H_6O_2$	122.0368	d
13	1.62	Adenine	136.0623	1.2	—	—	$C_5H_5N_5$	135.0545	b
14	1.62	L-Uridine	—	—	243.0637	3.3	$C_9H_{12}N_2O_6$	244.0695	b
15	1.62	Adenosine	268.1046	1.8	—	—	$C_{10}H_{13}N_5O_4$	267.0968	a
16	1.66	Phenyl acetate	137.0603	2.4	—	—	$C_8H_8O_2$	136.0524	c
17	2.04	Sibiricose A3	—	—	461.1295	2.4	$C_{19}H_{26}O_{13}$	462.1373	c
18	2.04	Gentisin	—	—	257.0450	0.8	$C_{14}H_{10}O_5$	258.0528	c
19	2.09	Kaempferol	287.0556	-8.4	285.0399	-2.1	$C_{15}H_{10}O_6$	286.0477	a
20	2.19	Raffinose	—	—	503.1612	6.4	$C_{18}H_{32}O_{16}$	504.1690	a
21	2.24	Sibiricose A6	—	—	547.1663	3.7	$C_{23}H_{32}O_{15}$	548.1741	c
22	2.26	Sibiricose A5	—	—	517.1557	2.1	$C_{22}H_{30}O_{14}$	518.1636	c
23	2.41	Sibiricose A1	—	—	547.1663	-1.5	$C_{23}H_{32}O_{16}$	548.1741	c
24	2.46	Vitamin B2	377.1461	-9.0	—	—	$C_{17}H_{20}N_4O_6$	376.1383	a
25	2.54	Tatarine C	325.1400	-0.3	—	—	$C_{15}H_{20}N_2O_6$	324.1321	d
26	2.63	Salicylic acid	—	—	137.0239	-1.9	$C_7H_6O_3$	138.0317	a
27	2.73	Lancerin	407.0978	-2.2	405.0822	6.9	$C_{19}H_{18}O_{10}$	406.0900	c+d
28	2.95	PolygalaxanthoneⅢ	569.1507	3.5	567.1349	-5.3	$C_{25}H_{28}O_{15}$	568.1428	c

29	3.17	Sibiricose A2	—	—	561.1878	-2.5	$C_{24}H_{34}O_{15}$	562.1898	c
30	3.21	N-Acetyl-D-glucosamine	221.0899	-2.5	—	—	$C_8H_{15}NO_6$	221.0899	c
31	3.62	1-(3,4-Dimethoxyphenyl)ethan-1-one	181.0865	-2.2	—	—	$C_{10}H_{12}O_3$	180.0786	c
32	4.51	2,4,5-Trimethoxybenzoic acid	213.0737	1.8	—	—	$C_{10}H_{12}O_5$	212.0685	d
33	4.64	Polygalaxanthone Ⅴ	583.1663	0.9	581.1507	2.8	$C_{26}H_{30}O_{15}$	582.1585	c
34	4.88	PolygalaxanthoneⅦ	613.1769	-0.2	611.1612	4.3	$C_{27}H_{32}O_{16}$	612.1690	c
35	5.14	3,4-Dimethoxycinnamic acid	209.0814	-1.3	—	—	$C_{11}H_{12}O_4$	208.0736	c
36	5.57	2,5-Dimethyl-7-hydroxy chromone	191.0708	-3.1	—	—	$C_{11}H_{10}O_3$	190.0630	a
37	5.81	Tenuifoliside B	—	—	693.2031	-0.4	$C_{32}H_{38}O_{17}$	694.2109	c
38	6.24	Campesterol	423.3716	6.1	—	—	$C_{28}H_{48}O$	400.3705	a
39	6.24	20-Glucosylginsenoside Rf	—	—	961.5372	-0.5	$C_{48}H_{82}O_{19}$	962.5450	a
40	6.31	2-Hydroxybenzonic acid	—	—	137.0239	-4.4	$C_7H_6O_3$	138.0317	c
41	6.50	Tenuifoliside A	—	—	681.2031	1.2	$C_{33}H_{40}O_{17}$	708.2266	c
42	6.70	PolygalaxanthoneⅣ	597.1820	2.3	595.1663	2.5	$C_{27}H_{32}O_{15}$	596.1741	c
43	6.85	Asarylaldehyde	197.0814	1.7	—	—	$C_{10}H_{12}O_4$	196.0736	d
44	6.98	Ginsenoside Rh4	621.3287	-0.6	—	—	$C_{36}H_{60}O_8$	620.4288	a
45	7.25	Tenuifoliside C	—	—	767.2399	3	$C_{35}H_{44}O_{19}$	768.2477	c
46	7.77	1,6-Dihydroxy-3,7-dimethoxyxanthone	289.0712	0.0	—	—	$C_{15}H_{12}O_6$	288.0634	c
47	7.78	Dibutyl oxalate	—	—	201.1129	-1	$C_{10}H_{18}O_4$	202.1205	a
48	7.84	3,4,5-Trimethoxy cinnamic acid	—	—	237.0763	7.2	$C_{12}H_{14}O_5$	238.0841	c
49	9.83	Ginsenoside Rf	—	—	799.4906	4.4	$C_{42}H_{72}O_{14}$	800.4922	a
50	9.97	1,6,7-Trihydroxy-2,3-dimethoxyxanthonec	305.0661	-3.6	303.0505	-0.3	$C_{15}H_{12}O_7$	304.0583	c
51	10.12	Notoginsenoside R2	—	—	769.4738	2.9	$C_{41}H_{70}O_{13}$	770.4816	a
52	10.30	1-Hydroxy-3,6,7-trimethoxy xanthone	303.0869	-5.9	—	—	$C_{16}H_{14}O_6$	302.0790	c
53	10.64	Tenuifolin	—	—	679.3694	5.2	$C_{36}H_{56}O_{12}$	680.3772	c
54	10.77	Ginsenoside Rg4/Rg5/Rg6/Rk	767.4946	5.0	—	—	$C_{42}H_{70}O_{12}$	766.4867	a
55	10.79	Ginsenoside Rh3	605.4430	-0.5	—	—	$C_{36}H_{60}O_7$	604.4339	a
56	10.80	Ginsenoside Rb1	—	—	1107.5961	4.4	$C_{54}H_{92}O_{23}$	1108.6029	a
57	11.22	Ginsenoside Rg4/Rg5/Rg6/Rk	767.4946	3.9	—	—	$C_{42}H_{70}O_{12}$	766.4867	a
58	11.31	Ginsenoside Rb3/Rc	—	—	1077.5846	0.5	$C_{53}H_{90}O_{22}$	1078.5924	a
59	11.36	Ginsenoside Ro	—	—	955.4903	-3.3	$C_{48}H_{76}O_{19}$	956.4981	a
60	11.57	Ginsenoside Rg4/Rg5/Rg6/Rk	767.4946	4.0	—	—	$C_{42}H_{70}O_{12}$	766.4867	a

61	11.61	Ginsenoside Rb3/Rc	—	—	1077.5934	3.9	$C_{53}H_{90}O_{22}$	1078.5924	a
62	11.95	Araloside A	—	—	925.4797	-1.1	$C_{47}H_{74}O_{18}$	926.4875	a
63	12.40	Ginsenoside Rg4/Rg5/Rg6/Rk	767.4946	3.9	—	—	$C_{42}H_{70}O_{12}$	766.4867	a
64	12.76	Notoginsenoside R1	—	—	931.5266	0.4	$C_{47}H_{80}O_{18}$	932.5345	a
65	12.78	Senegin VI	—	—	1703.7480	0.8	$C_{80}H_{120}O_{39}$	1704.7407	c
66	12.93	Onjisaponin L	—	—	1847.7854	-1.2	$C_{86}H_{128}O_{43}$	1848.7869	c
67	13.06	Onjisaponin O	—	—	1631.7233	-1.3	$C_{77}H_{116}O_{37}$	1632.7258	c
68	13.35	Senegin III	—	—	1571.7075	3.1	$C_{75}H_{112}O_{35}$	1572.6984	c
69	13.76	Acoronene	235.1698	1.1	—	—	$C_{15}H_{22}O_2$	234.1620	d
70	13.89	Onjisaponin F	—	—	1587.7028	2.4	$C_{75}H_{112}O_{36}$	1588.7041	c
71	14.14	1,6-Dihydroxy-3,5，7-trimethoxyxanthone	319.0818	1.0	317.0661	-5.7	$C_{16}H_{14}O_7$	318.0740	c
72	14.24	Eudesmin	387.1808	0.3	—	—	$C_{22}H_{26}O_6$	386.1729	d
73	14.43	α/γ-Asarone	209.1160	3.8	—	—	$C_{12}H_{16}O_3$	208.1099	d
74	14.49	p-Hydroxy methyl cinnamate	179.0708	-2.8	—	—	$C_{10}H_{10}O_3$	178.0630	c
75	14.97	Poricoic acid H	—	—	499.3424	-0.8	$C_{31}H_{48}O_5$	500.3502	b
76	14.97	α/γ-Asarone	209.1178	2.4	—	—	$C_{12}H_{16}O_3$	208.1099	d
77	15.04	Ginsenoside Roa	—	—	793.4379	4.9	$C_{54}O_{86}O_{24}$	1117.4381	a
78	15.76	Poricoic acid G	487.3424	-7.0	485.3267	-3.5	$C_{30}H_{46}O_5$	486.3345	b
79	16.38	Poricoic acid A	—	—	497.3267	0	$C_{31}H_{46}O_5$	498.3345	b
80	17.23	Ginsenoside Rd	—	—	945.5423	-1.4	$C_{48}H_{82}O_{18}$	946.5501	a
81	17.28	α-Santalol	221.1905	-9.5	—	—	$C_{15}H_{24}O$	220.1827	a
82	17.33	Deoxygomisin A	401.1964	-7.7	—	—	$C_{23}H_{28}O_6$	400.1886	a
83	17.40	25-Hydroxyporicoic acid C	—	—	497.3267	9.2	$C_{31}H_{46}O_5$	498.3345	b
84	17.47	Propyl benzoate	165.0916	9.7	—	—	$C_{10}H_{12}O_2$	164.0837	c
85	17.52	Veraguensin	373.2015	7.5	—	—	$C_{22}H_{28}O_5$	372.1937	d
86	17.55	2-Methoxy-4-vinylphenol	151.0759	2.5	—	—	$C_9H_{10}O_2$	150.0681	c
87	17.59	Gomisin A	417.1875	1.2	—	—	$C_{23}H_{28}O_7$	416.1835	a
88	17.62	3β,16α-Dihydroxylanosta-7,9(11),24-trien-21-oic acid	471.3474	-5.9	469.3318	2.6	$C_{30}H_{46}O_4$	470.3396	b
89	17.66	Poricoic acid B	—	—	483.3111	-1.9	$C_{30}H_{44}O_5$	484.3189	b
90	17.66	Fal-laxsaponin A	—	—	649.3795	-7.7	$C_{35}H_{54}O_{11}$	650.3670	c
91	17.90	6,7-Dehydroporicoic acid H	—	—	497.3267	-2.6	$C_{31}H_{46}O_5$	498.3345	b
92	17.97	16-Deoxyporicoic acid B	469.3318	0.4	467.3161	4.7	$C_{30}H_{44}O_4$	468.3240	b

93	18.00	cis/trans-Methylisoeugenol	179.1072	6.7	—	—	$C_{11}H_{14}O_2$	178.0994	d
94	18.04	Tumulosic acid	—	—	485.3631	2.3	$C_{31}H_{50}O_4$	486.3709	b
95	18.04	Bisasaricin	417.2277	1.0	—	—	$C_{24}H_{32}O_6$	416.2199	d
96	18.05	δ-Cadinene/β-Caryophyllene/Isocaryophyllen	205.1927	-1.1	—	—	$C_{15}H_{24}$	204.1878	d
97	18.09	cis/trans-Methylisoeugenol	179.0726	6.7	—	—	$C_{11}H_{14}O_2$	178.0994	d
98	18.16	25-methoxyporicoic acid	—	—	527.3373	2.5	$C_{32}H_{48}O_6$	528.3451	b
99	18.17	δ-Cadinene/β-Caryophyllene/Isocaryophyllen	205.1930	-2.7	—	—	$C_{15}H_{24}$	204.1878	d
100	18.19	3β-Hydroxy-16α-acetoxy-lanosta-7,9（11),24-trien-21-oic acid	513.3580	-1.9	—	—	$C_{32}H_{48}O_5$	512.3502	b
101	18.31	Daedaleanic acid A	483.3474	-2.1	481.3318	-3.7	$C_{31}H_{46}O_4$	482.3396	b
102	18.49	Dehydroeburiconic acid	467.3525	0.2	—	—	$C_{31}H_{46}O_3$	466.3447	b
103	18.50	Dehydrotu-mulosic acid	—	—	483.3474	-2.3	$C_{31}H_{48}O_4$	484.3553	b
104	18.51	δ-Cadinene/β-Caryophyllene/Isocaryophyllen	205.1952	-5.8	—	—	$C_{15}H_{24}$	204.1878	d
105	18.71	2,6-Di-sec-butyl-4-methylphenol	221.1905	-7.2	—	—	$C_{15}H_{24}O$	220.1827	a
106	19.07	Poricoic acid AE	—	—	525.3580	0.6	$C_{33}H_{50}O_5$	526.3658	b
107	19.99	Pachymic acid	—	—	527.3737	-0.8	$C_{33}H_{52}O_5$	528.3815	b

Note: a: Ginseng Radix; b: Poria; c: Polygalae Radix; d, Acori Tatarinowii Rhizoma

Supplementary table 2. MS and MS/MS data of the identified components from KXS in both positive and negative ion mode.

No.	Rt/ min	Compound Name	Formula	MS/MS data ESI$^-$or ESI$^+$
1	0.83	Asparagine	$C_4H_7NO_4$	131[M-H]$^-$,114[M-H-OH]$^-$,113[M-H-H_2O]$^-$
2	0.83	Bergapten	$C_{12}H_8O_4$	215[M-H]$^-$,179[M-H-3C]$^-$, 161[M-H-C_3H_2O]$^-$,89[M-H-$C_7H_{10}O_2$]$^-$
3	0.85	Argininyl-fructosyl-glucose	$C_{18}H_{34}N_4O_{12}$	499[M+H]$^+$,481[M+H-NH_4]$^+$, 251[M+H-(Glc-H_2O)-$C_3H_8N_3$]$^+$,175[M+H-2(Glc-H_2O)]$^+$
4	0.86	Isopimpinellin	$C_{13}H_{10}O_5$	245[M-H]$^-$,173[M-H-$C_3H_4O_2$]$^-$,131[M-H-$C_5H_6O_3$]$^-$
5	0.90	Mannose	$C_6H_{12}O_6$	179[M-H]$^-$,161[M-H-H_4O]$^-$,96[M-H-CH_8O_4]$^-$
6	0.93	Valine	$C_5H_{11}NO_2$	103[M+H-NH]$^+$,100[M+H-H_2O]$^+$
7	0.93	5-Hydroxymethylfurfural	$C_6H_6O_3$	127[M+H]$^+$,109[M+H-H_2O]$^+$
8	0.93	Dimethyl(R)-(+)-malate	$C_6H_{10}O_5$	148[M+H-CH_3]$^+$,119[M+H-C_2H_4O]$^+$, 161[M-H]$^-$,142[M-H-H_2O]$^-$, 99[M-H-2CH_2OH]$^-$,57[M-H-2CH_2OH-CO-CH_2]$^-$
9	0.97	2,3-Dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one	$C_6H_8O_4$	145[M+H]$^+$,128[M+H-HO]$^+$,111[M+H-H_2O_2]$^+$
10	1.12	Sucrose	$C_{12}H_{22}O_{11}$	341[M-H]$^-$,179[M-H-(Glc-H_2O)]$^-$, 161[M-H-Glc]$^-$,119[M-H-(Glc-H_2O)-CO_3]$^-$, 113[M-H-Glc-CH_4O_2]$^-$
11	1.53	Nicotinic acid	$C_6H_5NO_2$	124[M+H]$^+$,108[M+H-O]$^+$, 106[M+H-H_2O]$^+$,80[M+H-C_2H_6N]$^+$
12	1.62	Benzoic acid	$C_7H_6O_2$	123[M+H]$^+$,108[M+H-O]$^+$
13	1.62	Adenine	$C_5H_5N_5$	136[M+H]$^+$,119[M+H-H_3N]$^+$,109[M+H-CHN]$^+$
14	1.62	L-Uridine	$C_9H_{12}N_2O_6$	243[M-H]$^-$,230[M-H-N]$^-$,216[M-H-C_2H_2]$^-$, 183[M-H-CO_3]$^-$,110[M-H-$C_5H_9O_4$]$^-$
15	1.62	Adenosine	$C_{10}H_{13}N_5O_4$	268[M+H]$^+$,136[M+H-$C_4H_{10}N_3O_2$]$^+$,119[M+H-$C_5H_{13}N_2O_3$]$^+$
16	1.66	Phenyl acetate	$C_8H_8O_2$	137[M+H]$^+$,119[M+H-CH_6]$^+$, 107[M+H-CH_2O]$^+$,91[M+H-C_2H_6O]$^+$
17	2.04	Sibiricose A3	$C_{19}H_{26}O_{13}$	461[M-H]$^-$,281[M-H-Fru]$^-$,

18	2.04	Gentisin	$C_{14}H_{10}O_5$	239[M-H-Fru-C_2H_2O]$^-$,152[M-H-Fru-$C_5H_5O_4$]$^-$, 137[M-H-Fru-（Fru-2H_2O）]$^-$, 257[M-H]$^-$,199[M-H-C_3H_6O]$^-$, 194[M-H-C_4O]$^-$,166[M-H-C_6H_3O]$^-$
19	2.09	Kaempferol	$C_{15}H_{10}O_6$	287[M+H]$^+$,241[M+H-C_2H_6O]$^+$, 208[M+H-C_4O_2]$^+$,193[M+H-C_6H_5-OH]$^+$, 285[M-H]$^-$,223[M-H-$C_2H_6O_2$]$^-$, 154[M-H-$C_8H_3O_2$]$^-$,143[M-H-$C_6H_6O_4$]$^-$
20	2.19	Raffinose	$C_{18}H_{32}O_{16}$	503[M-H]$^-$,323[M-H-Glc]$^-$, 179[M-H-(Glc-H_2O)-(Fru-H_2O)]$^-$,
21	2.24	Sibiricose A6	$C_{23}H_{32}O_{15}$	547[M-H]$^-$,367[M-H-Glc]$^-$,341[M-H-$C_{11}H_{10}O_4$]$^-$, 223[M-H-Glc-(Fru-2H_2O)]$^-$, 205[M-H-Glc-(Fru-H_2O)]$^-$
22	2.26	Sibiricose A5	$C_{22}H_{30}O_{14}$	517[M-H]$^-$,341[M-H-$C_{10}H_8O_3$]$^-$,337[M-H-Glc]$^-$, 193[M-H-Glc-(Fru-2H_2O)]$^-$, 175[M-H-Glc-(Fru-H_2O)]$^-$
23	2.41	Sibiricose A1	$C_{23}H_{32}O_{16}$	547[M-H]$^-$,385[M-H-(Fru-H_2O)]$^-$,367[M-H-Fru]$^-$, 325[M-H-$C_{11}H_{10}O_5$]$^-$,223[M-H-Fru-(Glc-2H_2O)]$^-$, 205[M-H-Fru-(Glc-H_2O)]$^-$
24	2.46	Vitamin B2	$C_{17}H_{20}N_4O_6$	377[M+H]$^+$,359[M+H-H_2O]$^+$, 243[M+H-$C_5H_{10}O_4$]$^+$,172[M+H-$C_7H_{11}NO_6$]$^+$
25	2.54	Tatarine C	$C_{15}H_{20}N_2O_6$	325[M+H]$^+$,307[M+H-H_2O]$^+$, 191[M+H-CH_2-4CH_2O]$^+$,175[M+H-CH_2-4CH_2O-O]$^+$
26	2.63	Salicylic acid	$C_7H_6O_3$	137[M-H]$^-$,108[M-H-2O]$^-$
27	2.73	Lancerin	$C_{19}H_{18}O_{10}$	407[M+H]$^+$,389[M+H-H_2O]$^+$,287[M+H-$C_7H_4O_2$]$^+$, 405[M-H]$^-$,315[M-H-C_6H_2O]$^-$,285[M-H-$C_7H_4O_2$]$^-$, 257[M-H-C_7O_4]$^-$,213[M-H-$C_{10}H_8O_4$]$^-$
28	2.95	Polygalaxanthone Ⅲ	$C_{25}H_{28}O_{15}$	569[M+H]$^+$,551[M+H-H_2O]$^+$,317[M+H-Api-$C_4H_6O_3$]$^+$,

				287[M+H-(Api-H2O)-$C_6H_{14}O_4$]$^+$,
				567[M-H]$^-$,447[M-H-$C_7H_4O_2$]$^-$,417[M-H-Api]$^-$,
				345[M-H-Api-$C_3H_4O_2$]$^-$,315[M-H-Api-$C_4H_6O_3$]$^-$,
				272[M-H-(Api-H_2O)-$C_8H_3O_4$]$^-$,259[M-H-Api-$C_6H_6O_5$]-
				561[M-H]$^-$,237[M-H-Fru-(Glc-2H_2O)]$^-$,
29	3.17	Sibiricose A2	$C_{24}H_{34}O_{15}$	209[M-H-Fru-Glc-CH_2+H_6O]$^-$,
				179[M-H-(Glc-H_2O)-$C_{12}H_{12}O_4$]$^-$
30	3.21	N-Acetyl-D-glucosamine	$C_8H_{15}NO_6$	222[M+H]$^+$,207[M+H-CH_3]$^+$,147[M+H-$C_2H_5NO_2$]$^+$
				181[M+H]$^+$,166[M+H-CH_3]$^+$,
31	3.62	1-(3,4-Dimethoxyphenyl)ethan-1-one	$C_{10}H_{12}O_3$	151[M+H-2CH_3]$^+$,121[M+H-CH_3-C_2H_5O]$^+$
32	4.51	2,4,5-Trimethoxybenzoic acid	$C_{10}H_{12}O_5$	213[M+H]$^+$,198[M+H-CH_3]$^+$,154[M+H-C_3H_7O]$^+$
				583[M+H]$^+$,437[M+H-(Rha-H_2O)]$^+$,
				405[M+H-Rha-O]$^+$,275[M+H-Rha-(Glc-2H_2O)]$^+$,
33	4.64	Polygalaxanthone Ⅴ	$C_{26}H_{30}O_{15}$	581[M-H]$^-$,417[M-H-Rha]$^-$,388[M-H-Rha-CHO]$^-$,
				273[M-H-Rha-(Glc-2H_2O)]$^-$,
				258[M-H-Rha-(Glc-2H_2O)-CH_3]$^-$,
				230[M-H-$C_{14}H_9O_6$-C_3H_9O-OH]$^-$
				613[M+H]$^+$,467[M+H-(Rha-H_2O)]$^+$,
				305[M+H-Rha-(Glc-2H_2O)]$^+$,
				290[M+H-Rha-(Glc-2H_2O)-CH_3]$^+$,
34	4.88	Polygalaxanthone Ⅶ	$C_{27}H_{32}O_{16}$	611[M-H]$^-$,596[M-H-CH_3]$^-$,
				303[M-H-Rha-(Glc-2H_2O)]$^-$,
				287[M-H-Rha-(Glc-2H_2O)-CH_4]$^-$,259[M-H-$C_{16}H_{16}O_9$]$^-$
35	5.14	3,4-Dimethoxycinnamic acid	$C_{11}H_{12}O_4$	209[M+H]$^+$,193[M+H-CH_4]$^+$,
				148[M+H-$C_2H_5O_2$]$^+$,120[M+H-$C_4H_9O_2$]$^+$
36	5.57	2,5-Dimethyl-7-hydroxy chromone	$C_{11}H_{10}O_3$	191[M+H]$^+$,163[M+H-2CH_2]$^+$,148[M+H-C_3H_7]$^+$,
				133[M+H-C_3H_6O]$^+$,105[M+H-$C_4H_6O_2$]$^+$
37	5.81	Tenuifoliside B	$C_{32}H_{38}O_{17}$	693[M-H]$^-$,668[M-H-C_2H]$^-$,
				517[M-H-$C_{10}H_8O_3$]$^-$,499[M-H-$C_{10}H_8O_3$-H_2O]$^-$

38	6.24	Campesterol	$C_{28}H_{48}O$	423[M+Na]$^+$,367[M+H-CH_6O]$^+$, 349[M+H-$C_2H_{12}O$]$^+$,133[M+H-$C_{18}H_{36}O$]$^+$
39	6.24	20-Glucosylginsenoside Rf	$C_{48}H_{82}O_{19}$	961[M-H]$^-$,799[M-H-(Glc-H_2O)]$^-$,781[M-H-Glc]$^-$, 637[M-H-2(Glc-H_2O)]$^-$,475[M-H-3(Glc-H_2O)]$^-$
40	6.31	2-Hhydroxybenzonic acid	$C_7H_6O_3$	137[M-H]$^-$,93[M-H-CO_2]$^-$
41	6.50	Tenuifoliside A	$C_{33}H_{40}O_{17}$	681[M-H-C_2H_2]$^-$,443[M-H-$C_{12}H_{10}O_5$-CH_2OH]$^-$, 281[M-H-$C_{12}H_{10}O_5$-$C_{10}H_7O_3$-OH]$^-$,137[M-H-$C_{27}H_{38}O_{13}$]$^-$
42	6.70	PolygalaxanthoneⅣ	$C_{27}H_{32}O_{15}$	597[M+H]$^+$,451[M+H-(Rha-H_2O)]$^+$, 289[M+H-Rha-(Glc-2H_2O)]$^+$, 595[M-H]$^-$,551[M-H-C_2H_4O]$^-$,515[M-H-C_2H_4O-2H_2O]$^-$, 287[M-H-Rha-(Glc-2H_2O)]$^-$
43	6.85	Asarylaldehyde	$C_{10}H_{12}O_4$	197[M+H]$^+$,182[M+H-CH_3]$^+$, 169[M+H-2CH_2]$^+$,123[M+H-3CH_3-CHO]$^+$
44	6.98	Ginsenoside Rh4	$C_{36}H_{60}O_8$	621[M+H]$^+$,603[M+H-CH_6]$^+$,481[M+H-CH_2OH-$C_8H_{13}O$]$^+$, 264[M+H-(Glc-H_2O)-$C_{20}H_{37}$]$^+$
45	7.25	Tenuifoliside C	$C_{35}H_{44}O_{19}$	767[M-H]$^-$,529[M-H-$C_{12}H_{14}O_5$]$^-$, 205[M-H-$C_{12}H_{14}O_5$-(Glc-H_2O)-(Fru-H_2O)]$^-$, 145[M-H-2$C_{12}H_{14}O_5$-$C_5H_6O_5$]$^-$,
46	7.77	1,6-Dihydroxy-3,7-dimethoxyxanthone	$C_{15}H_{12}O_6$	289[M+H]$^+$,274[M+H-CH_3]$^+$, 243[M+H-2CH_3-O]$^+$, 231[M+H-C_3H_6O]$^+$
47	7.78	Dibutyl oxalate	$C_{10}H_{18}O_4$	201[M-H]$^-$,183[M-H-H_2O]$^-$,139[M-H-C_2H_5-CH_4-OH]$^-$
48	7.84	3,4,5-Trimethoxy cinnamic acid	$C_{12}H_{14}O_5$	237[M-H]$^-$,197[M-H-C_3H_4]$^-$,193[M-H-CO_2]$^-$
49	9.83	Ginsenoside Rf	$C_{42}H_{72}O_{14}$	799[M-H]$^-$,637[M-H-(Glc-H_2O)]$^-$, 475[M-H-2(Glc-H_2O)]$^-$,161[M-H-Glc-$C_{30}H_{50}O_3$]$^-$
50	9.97	1,6,7-Trihydroxy-2,3-dimethoxyxanthone	$C_{15}H_{12}O_7$	305[M+H]$^+$,290[M+H-CH_3]$^+$,275[M+H-2CH_3]$^+$, 247[M+H-2CHO]$^+$,236[M+H-C_3HO_2]$^+$, 303[M-H]$^-$,288[M-H-CH_3]$^-$,273[M-H-2CH_3]$^-$, 259[M-H-2CH_2-O]$^-$,245[M-H-$C_2H_2O_2$]$^-$

51	10.12	Notoginsenoside R2	$C_{41}H_{70}O_{13}$	769[M-H]$^-$,637[M-H-(Xyl-H_2O)]$^-$, 475[M-H-(Xyl-H_2O)-(Glc-H_2O)]$^-$, 161[M-H-(Xyl-H_2O)-$C_{30}H_{52}O_4$]$^-$
52	10.30	1-Hydroxy-3,6,7-trimethoxy xanthone	$C_{16}H_{14}O_6$	303[M+H]$^+$,288[M+H-CH_3]$^+$, 273[M+H-2CH_3]$^+$,245[M+H-3CH_2-O]$^+$
53	10.64	Tenuifolin	$C_{36}H_{56}O_{12}$	679[M-H]$^-$,455[M-H-Glc-CO_2]$^-$, 425[M-H-Glc-CO_2-CHOH]$^-$,179[M-H-$C_{30}H_{44}O_5$]$^-$
54	10.77	Ginsenoside Rg4/Rg5/Rg6/Rk	$C_{42}H_{70}O_{12}$	767[M+H]$^+$,749[M+H-H_2O]$^+$,605[M+H-(Glc-H_2O)]$^+$, 587[M+H-Glc]$^+$,407[M+H-2Glc]$^+$
55	10.79	Ginsenoside Rh3	$C_{36}H_{60}O_7$	605[M+H]$^+$,587[M+H-H_2O]$^+$,515[M+H-C_5H_{12}-H_2O]$^+$, 425[M+H-Glc]$^+$,407[M+H-Glc-H_2O]$^+$
56	10.80	Ginsenoside Rb1	$C_{54}H_{92}O_{23}$	1107[M-H]$^-$,945[M-H-(Glc-H_2O)]$^-$, 783[M-H-2(Glc-H_2O)]$^-$,459[M-H-4(Glc-H_2O)]$^-$
57	11.22	Ginsenoside Rg4/Rg5/Rg6/Rk	$C_{42}H_{70}O_{12}$	767[M+H]$^+$,749[M+H-H_2O]$^+$,605[M+H-(Glc-H_2O)]$^+$, 587[M+H-Glc]$^+$,407[M+H-2Glc]$^+$
58	11.31	Ginsenoside Rb3/Rc	$C_{53}H_{90}O_{22}$	1077[M-H]$^-$,956[M-H-3HO-C_5H_{10}]$^-$, 945[M-H-(Xyl-H_2O)]$^-$, 783[M-H-(Xyl-H_2O)-(Glc-H_2O)]$^-$, 459[M-H-(Xyl-H_2O)-3(Glc-H_2O)]$^-$
59	11.36	Ginsenoside Ro	$C_{48}H_{76}O_{19}$	956[M-H]$^-$,793[M-H-(Glc-H_2O)]$^-$, 731[M-H-Glc-CO_2]$^-$,613[M-H-Glc-(Glc-H_2O)]$^-$
60	11.57	Ginsenoside Rg4/Rg5/Rg6/Rk	$C_{42}H_{70}O_{12}$	767[M+H]$^+$,749[M+H-H_2O]$^+$,605[M+H-(Glc-H_2O)]$^+$, 587[M+H-Glc]$^+$,407[M+H-2Glc]$^+$
61	11.61	Ginsenoside Rb3/Rc	$C_{53}H_{90}O_{22}$	1077[M-H]$^-$,956[M-H-3HO-C_5H_{10}]$^-$, 945[M-H-(Xyl-H_2O)]$^-$, 783[M-H-(Xyl-H_2O)-(Glc-H_2O)]$^-$, 459[M-H-(Xyl-H_2O)-3(Glc-H_2O)]$^-$
62	11.95	Araloside A	$C_{47}H_{74}O_{18}$	925[M-H]$^-$,881[M-H-C_3H_8]$^-$, 845[M-H-2HO-CH_2O_2]$^-$,763[M-H-Xyl]$^-$

63	12.40	Ginsenoside Rg4/Rg5/Rg6/Rk	$C_{42}H_{70}O_{12}$	767$[M+H]^+$,749$[M+H-H_2O]^+$,605$[M+H-(Glc-H_2O)]^+$, 587$[M+H-Glc]^+$,407$[M+H-2Glc]^+$
64	12.76	Notoginsenoside R1	$C_{47}H_{80}O_{18}$	931$[M-H]^-$,859$[M-H-4H_2O]^-$,770$[M-H-(Glc-H_3O)]^-$, 681$[M-H-C_5H_{10}O_4-2CH_3-C_6H_{14}]^-$,425$[M-H-2Glc-C_5H_6O_5]^-$
65	12.78	Senegin VI	$C_{80}H_{120}O_{39}$	1703$[M-H]^-$,1673$[M-H-CH_2O]^-$
66	12.93	Onjisaponin L	$C_{86}H_{128}O_{43}$	1847$[M-H]^-$,1703$[M-H-HMG]^-$
67	13.06	Onjisaponin O	$C_{77}H_{116}O_{37}$	1631$[M-H]^-$,1601$[M-H-CH_2O]^-$
68	13.35	Senegin III	$C_{75}H_{112}O_{35}$	1571$[M-H]^-$,1541$[M-H-CH_2O]^-$
69	13.76	Acoronene	$C_{15}H_{22}O_2$	235$[M+H]^+$,217$[M+H-CH_6]^+$, 189$[M+H-C_3H_{10}]^+$,119$[M+H-C_7H_{16}O]^+$
70	13.89	Onjisaponin F	$C_{75}H_{112}O_{36}$	1587$[M-H]^-$,1557$[M-H-CH_2O]^-$
71	14.14	1,6-Dihydroxy-3,5，7-trimethoxyxanthone	$C_{16}H_{14}O_7$	319$[M+H]^+$,303$[M+H-CH_4]^+$, 275$[M+H-C_3H_8]^+$,258$[M+H-C_3H_9O]^+$, 317$[M-H]^-$,302$[M-H-CH_3]^-$,287$[M-H-2CH_3]^-$, 259$[M-H-3CH_2-O]^-$,215$[M-H-C_5H_9O_2]^-$
72	14.24	Eudesmin	$C_{22}H_{26}O_6$	387$[M+H]^+$,373$[M+H-CH_2]^+$,355$[M+H-2CH_4]^+$, 235$[M+H-CH_3-C_8H_9O_2]^+$,193$[M+H-C_8H_9O_2-C_3H_5O]^+$
73	14.43	α/γ-Asarone	$C_{12}H_{16}O_3$	209$[M+H]^+$,194$[M+H-CH_3]^+$,179$[M+H-2CH_3]^+$, 151$[M+H-3CH_3-CH]^+$,121$[M+H-3CH_3-C_3H_7]^+$
74	14.49	p-Hydroxy methyl cinnamate	$C_{10}H_{10}O_3$	179$[M+H]^+$,163$[M+H-CH_4]^+$, 149$[M+H-CH_2O]^+$,121$[M+H-C2H2O2]^+$
75	14.97	Poricoic acid H	$C_{31}H_{48}O_5$	499$[M-H]^-$,481$[M-H-H_2O]^-$, 419$[M-H-C_6H_8]^-$,389$[M-H-C_7H_{10}-O]^-$
76	14.97	α/γ-Asarone	$C_{12}H_{16}O_3$	209$[M+H]^+$,194$[M+H-CH_3]^+$,179$[M+H-2CH_3]^+$, 151$[M+H-3CH_3-CH]^+$,121$[M+H-3CH_3-C_3H_7]^+$
77	15.04	Ginsenoside Roa	$C_{54}O_{86}O_{24}$	793$[M-H-2Glc]^-$,587$[M-H-Glc-CO_2]^-$, 569$[M-H-Glc-CO_2-H_2O]^-$,523$[M-H-Glc-2CHO_2-H_2O]^-$
78	15.76	Poricoic acid G	$C_{30}H_{46}O_5$	487$[M+H]^+$,407$[M+H-H_2O-CH_2O_2-CH_4]^+$, 201$[M+H-C_{19}H_{26}O_2]^+$,159$[M+H-C_8H_{12}O_2-$

				$C_{11}H_{24}O_2]^+$,
79	16.38	Poricoic acid A	$C_{31}H_{46}O_5$	485$[M-H]^-$,425$[M-H-CH_4-CO_2]^-$, 387$[M-H-C_6H_9-OH]^-$,369$[M-H-C_6H_{12}-CO_2]^-$ 497$[M-H]^-$,479$[M-H-H_2O]^-$, 435$[M-H-H_2O-CO_2]^-$,419$[M-H-CH_4CO_2-H_2O]^-$
80	17.23	Ginsenoside Rd	$C_{48}H_{82}O_{18}$	945$[M-H]^-$,899$[M-H-CH_2O_2]^-$, 631$[M-H-Glc-2CH_2-C_8H_{10}]^-$, 571$[M-H-C_3H_{15}-Glc-(Glc-2H_2O)]^-$,
81	17.28	α-Santalol	$C_{15}H_{24}O$	221$[M+H]^+$,193$[M+H-2CH_2]^+$, 190$[M+H-CH_3O]^+$,165$[M+H-C_3H_4O]^+$
82	17.33	Deoxygomisin A	$C_{23}H_{28}O_6$	401$[M+H]^+$,369$[M+H-2CH_4]^+$, 208$[M+H-C_{10}H_{10}O_3]^+$,193$[M+H-C_{12}H_{16}O_3]^+$
83	17.40	25-Hydroxyporicoic acid C	$C_{31}H_{46}O_5$	497$[M-H]^-$,467$[M-H-2O]^-$, 423$[M-H-C_2H_6-CO_2]^-$
84	17.47	Propyl benzoate	$C_{10}H_{12}O_2$	165$[M+H]^+$,149$[M+H-CH_4]^+$,135$[M+H-2CH_3]^+$, 121$[M+H-C_3H_8]^+$,107$[M+H-C_3H_6O]^+$
85	17.52	Veraguensin	$C_{22}H_{28}O_5$	373$[M+H]^+$,327$[M+H-3CH_3-H]^+$, 295$[M+H-3CH_3-0CH_3-2H]^+$,235$[M+H--2CH_3O-C_6H_4]^+$
86	17.55	2-Methoxy-4-vinylphenol	$C_9H_{10}O_2$	151$[M+H]^+$,135$[M+H-CH_4]^+$, 107$[M+H-C_3H_8]^+$
87	17.59	Gomisin A	$C_{23}H_{28}O_7$	417$[M+H]^+$,224$[M+H-C_{11}H_{13}O_3]^+$, 193$[M+H-C_{12}H_{16}O_4]^+$,165$[M+H-C_{14}H_{20}O_4]^+$
88	17.62	3β,16α-Dihydroxylanosta-7,9(11),24-trien-21-oic acid	$C_{30}H_{46}O_4$	471$[M+H]^+$,453$[M+H-H_2O]^+$, 407$[M+H-CH_2O_2-H_2O]^+$,313$[M+H-C_8H_{12}O_2-H_2O]^+$, 469[M-H]-,407$[M-H-CO_2-H_2O]^-$, 367$[M-H-C_6H_{12}-H_2O]^-$
89	17.66	Poricoic acid B	$C_{30}H_{44}O_5$	483$[M-H]^-$,439$[M-H-CO_2]^-$, 409$[M-H-CO_2-2CH_2]^-$,367$[M-H-2CO_2-2CH_2]^-$
90	17.66	Fal-laxsaponin A	$C_{35}H_{54}O_{11}$	649$[M-H]^-$,603$[M-H-CH_2O_2]^-$,471$[M-H-C_6H_{10}O_6]^-$
91	17.90	6,7-Dehydroporicoic acid H	$C_{31}H_{46}O_5$	497$[M-H]^-$,479$[M-H-H_2O]^-$,

92	17.97	16-Deoxyporicoic acid B	$C_{30}H_{44}O_4$	453[M-H-2CH_3-CH_2]$^-$,423[M-H-C_2H_6-CO_2]$^-$ 469[M+H]$^+$,451[M+H-H_2O]$^+$, 311[M+H-$C_8H_{12}O_2$-H_2O]$^+$,293[M+H-$C_8H_{12}O_2$-CH_8O]$^+$ 467[M-H]$^-$,423[M-H-CO_2]$^-$, 407[M-H-CO_2-CH_4]$^-$,374[M-H-C_7H_9]$^-$
93	18.00	cis/trans-Methylisoeugenol	$C_{11}H_{14}O_2$	179[M+H]$^+$,165[M+H-CH_2]$^+$, 151[M+H-2CH_2]$^+$,121[M+H-2CH_3-2CH-2H]$^+$
94	18.04	Tumulosic acid	$C_{31}H_{50}O_4$	485[M-H]$^-$,441[M-H-CO_2]$^-$,423[M-H-CO_2-H_2O]$^-$
95	18.04	Bisasaricin	$C_{24}H_{32}O_6$	417[M+H]$^+$,403[M+H-CH_2]$^+$,385[M+H-2CH_4]$^+$, 249[M+H-3CH_3O-C_6H_5]$^+$,209[M+H-3CH_3O-C_6H_5-C_3H_4]$^+$
96	18.05	δ-Cadinene/β-Caryophyllene/Isocaryophyllen	$C_{15}H_{24}$	205[M+H]$^+$,161[M+H-2CH_3-CH_2]$^+$, 151[M+H-C_4H_6]$^+$,133[M+H-2CH_3-3CH_2]$^+$
97	18.09	cis/trans-Methylisoeugenol	$C_{11}H_{14}O_2$	179[M+H]$^+$,165[M+H-CH_2]$^+$, 151[M+H-2CH_2]$^+$,121[M+H-2CH_3-2CH-2H]$^+$
98	18.16	25-Methoxyporicoic acid	$C_{32}H_{48}O_6$	527[M-H]$^-$,481[M-H-CH_2O_2]$^-$, 431[M-H-C_6H_8O]$^-$,413[M-H-$C_7H_{14}O$]$^-$
99	18.17	δ-Cadinene/β-Caryophyllene/Isocaryophyllen	$C_{15}H_{24}$	205[M+H]$^+$,161[M+H-2CH_3-CH_2]$^+$, 151[M+H-C_4H_6]$^+$,133[M+H-2CH_3-3CH_2]$^+$
100	18.19	3β-Hydroxy-16α-acetoxy-lanosta-7,9（11),24-trien-21-oic acid	$C_{32}H_{48}O_5$	513[M+H]$^+$,495[M+H-H_2O]$^+$, 453[M+H-$COCH_3$-OH]$^+$, 355[M+H-$C_8H_{12}O_2$-H_2O]$^+$, 295[M+H-$C_8H_{12}O_2$-CH_4O_2-H_2O]$^+$，
101	18.31	Daedaleanic acid A	$C_{31}H_{46}O_4$	483[M+H]$^+$,465[M+H-H_2O]$^+$, 419[M+H-C_3H_{10}-H_2O]$^+$,309[M+H-$C_9H_{16}O_2$-H_2O]$^+$, 481[M-H]$^-$,437[M-H-CO_2]$^-$, 421[M-H-C_3H_8-O]$^-$,403[M-H-C_3H_8-2HO]$^-$
102	18.49	Dehydroeburiconic acid	$C_{31}H_{46}O_3$	467[M+H]$^+$,449[M+H-H_2O]$^+$, 311[M+H-$C_9H_{16}O_2$]$^+$,293[M+H-$C_{10}H_{22}O_2$]$^+$
103	18.50	Dehydrotu-mulosic acid	$C_{31}H_{48}O_4$	483[M-H]$^-$,437[M-H-CH_2O_2]$^-$, 421[M-H-CO_2-H_2O]$^-$,337[M-H-C_6H_{12}-CO_2-

				$H_2O]^-$
104	18.51	δ-Cadinene/β-Caryophyllene/Isocaryophyllen	$C_{15}H_{24}$	$205[M+H]^+$,$161[M+H-2CH_3-CH_2]^+$, $151[M+H-C_4H_6]^+$,$133[M+H-2CH_3-3CH_2]^+$
105	18.71	2,6-Di-sec-butyl-4-methylphenol	$C_{15}H_{24}O$	$221[M+H]^+$,$203[M+H-CH_6]^+$, $193[M+H-CH_3-CH]^+$,$133[M+H-CH_3-CH-4CH_3]^+$
106	19.07	Poricoic acid AE	$C_{33}H_{50}O_5$	$525[M-H]^-$,$479[M-H-C_2H_6O]^-$, $465[M-H-C_2H_4O_2]^-$,$355[M-H-C_9H_{14}O_2-O]^-$
107	19.99	Pachymic acid	$C_{33}H_{52}O_5$	$527[M-H]^-$,$483[M-H-C_2H_4O]^-$, $465[M-H-C_2H_4O-H_2O]^-$,$221[M-H-C_{18}H_{26}O_4]^-$

Note: Glc: β-D-glucose; Xyl: β-D-xylose; Fru: β-D-fructose;Rha:α-L-rhamnose; Api:β-D-Apiose ; HMG: 3s-3-hydroxy-3-methyl-5-pentanoic acid