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Supporting Information

Ultra-high performance liquid chromatography/ion mobility time-of-flight mass spectrometry-based untargeted metabolomics combined with quantitative assay unveiled the metabolic difference among the root, leaf, and flower bud of *Panax notoginseng*

Content

Table S6 Method validation results for the UHPLC/UV approach enabling the quantitative assay of five ginsenosides.

Table S7 Results for the quantitative assays of five ginsenosides among 45 batches of *P. notoginseng* samples.

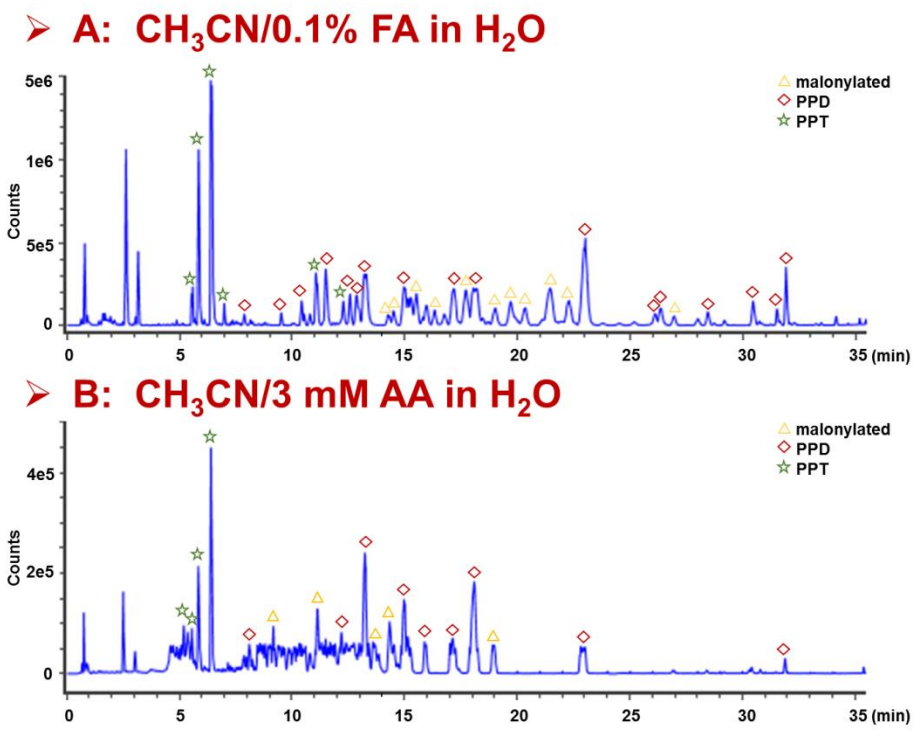

Fig. S1 Comparison of the base peak chromatograms of a QC sample (prepared by pooling the equal volume of the test solutions of R-1, L-1, and F-1) obtained by UHPLC/QTOF-MS with 0.1% formic acid (FA) or 3 mM ammonium acetate (AA) as the additive in the water phase.

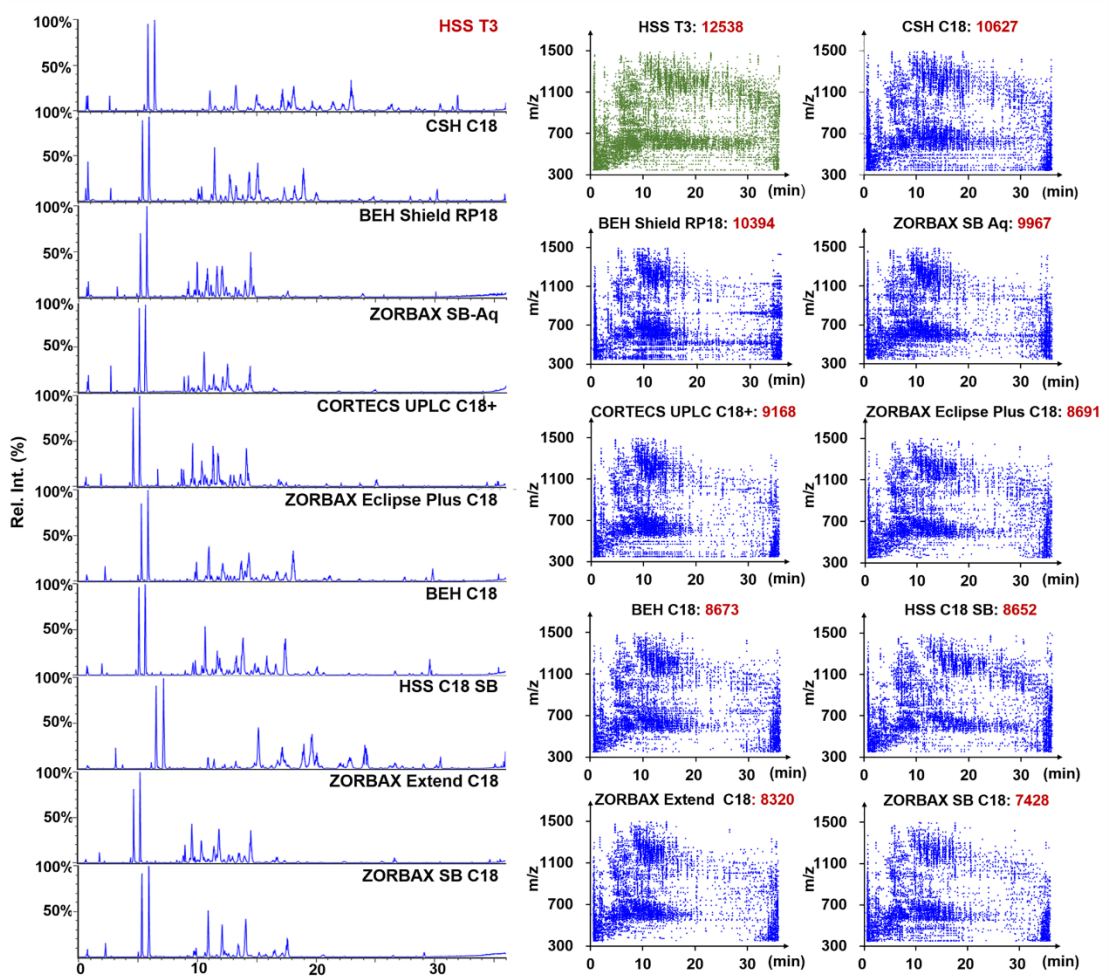

Fig. S2 Selection of the chromatographic column for separating the multicomponents from three parts of *P. notoginseng* by the UHPLC/IM-QTOF-MS. The left displays the base peak intensity chromatograms of the QC sample obtained on ten candidate sub-2 μm particles packed columns; and the right is the corresponding scattering plots (t_R VS *m/z*) for the peaks resolved by MS after UHPLC separation, with the total resolvable peaks annotated.

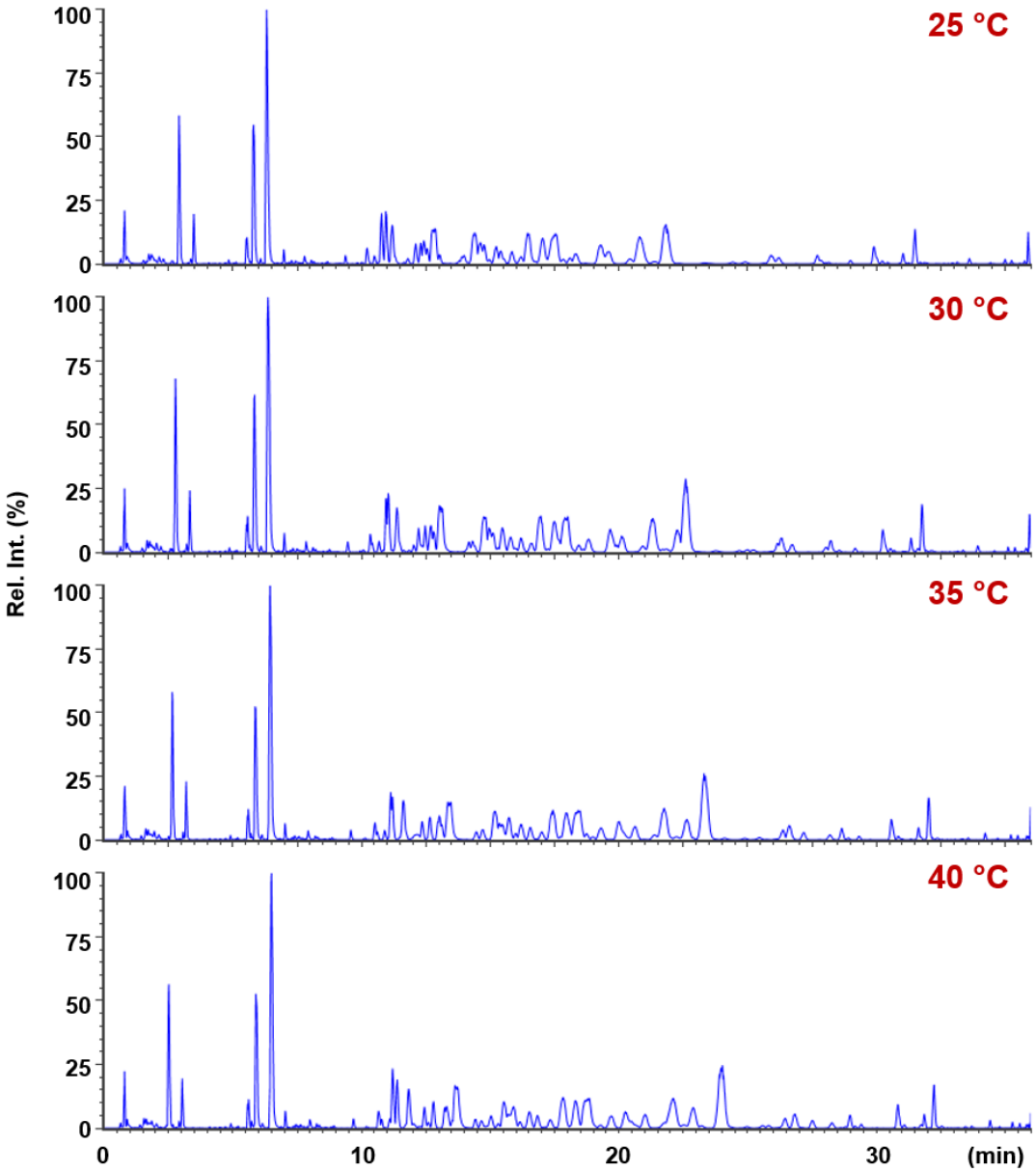

Fig. S3 Column temperature optimization to enhance the revolution of the multicomponents from three parts of *Panax notoginseng* by using the HSS T3 column.

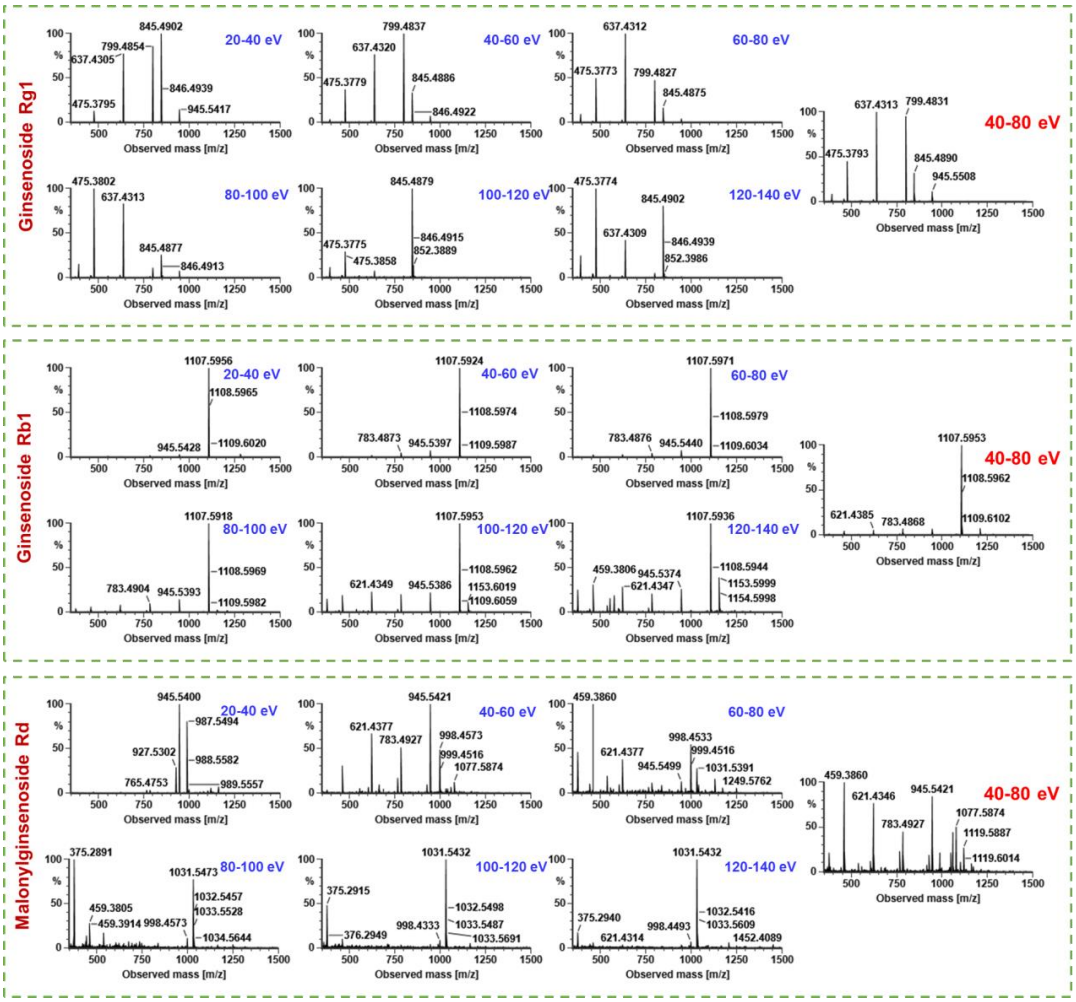

Fig. S4 Optimization of ramp collision energy (RCE) in the negative-mode HDMS^{E} profiling of ginsenosides from different parts of *P. notoginseng*.

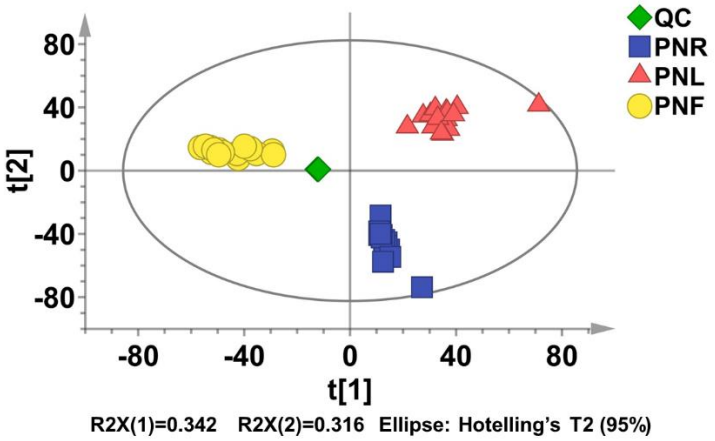

Fig. S5 PCA score plot of 45 batches of *P. notoginseng* samples including three different parts (**PNR**: root; **PNL**: leaf; **PNF**: flower bud).

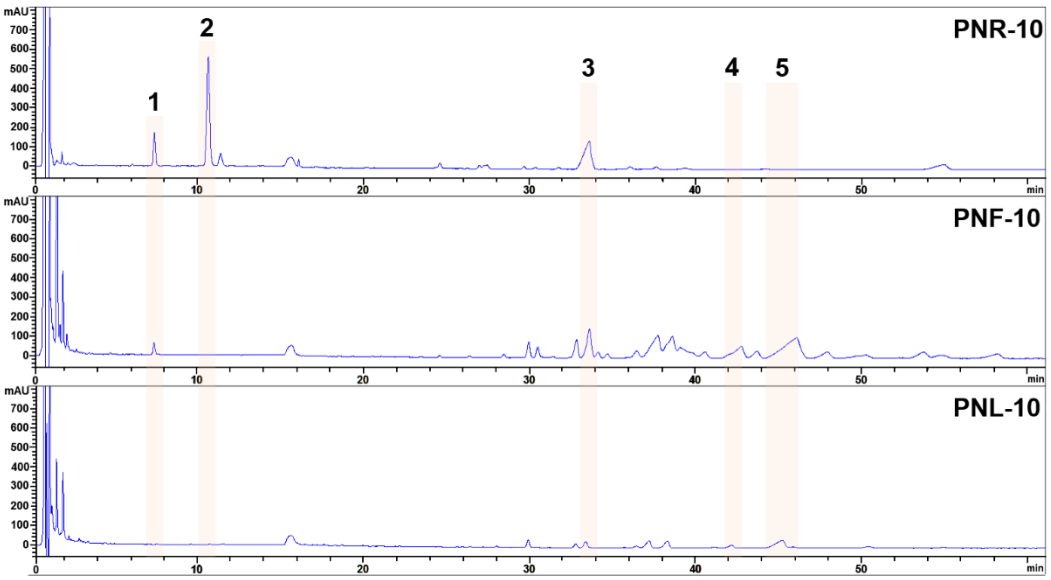

Fig. S6 The UHPLC-UV chromatograms (203 nm) of the representative root (PNR-10), flower (PNF-10), and leaf (PNL-10) samples for *P. notoginseng*. (Peak **1**: notoginsenoside R1; Peak **2**: ginsenoside Rg1; Peak **3**: ginsenoside Rb1; Peak **4**: ginsenoside Rb2; Peak **5**: ginsenoside Rb3).

Table S1 Information of 69 ginsenoside reference compounds used in this work.

No.	Compound	Formula	Exact Mass	Subclass
1	ginsenoside F1	$C_{36}H_{62}O_9$	638.4394	
2	ginsenoside Rh1	$C_{36}H_{62}O_9$	638.4394	
3	20(*R*)-ginsenoside Rh1	$C_{36}H_{62}O_9$	638.4394	
4	ginsenoside F3	$C_{41}H_{70}O_{13}$	770.4816	
5	20(*S*)-sanchinoside A3	$C_{41}H_{70}O_{13}$	770.4816	
6	ginsenoside F5	$C_{14}H_{70}O_{13}$	770.4816	
7	pseudoginsenoside Rt3	$C_{41}H_{70}O_{13}$	770.4816	
8	notoginsenoside R2	$C_{41}H_{70}O_{13}$	770.4816	
9	20(*R*)-notoginsenoside R2	$C_{41}H_{70}O_{13}$	770.4816	
10	ginsenoside Rg2	$C_{42}H_{72}O_{13}$	784.4973	
11	ginsenoside Rf	$C_{42}H_{72}O_{14}$	800.4922	**PPT**
12	ginsenoside Rg1	$C_{42}H_{72}O_{14}$	800.4922	
13	notoginsenoside Rt	$C_{44}H_{74}O_{15}$	842.5028	
14	notoginsenoside R1	$C_{47}H_{80}O_{18}$	932.5345	
15	notoginsenoside Fp1	$C_{47}H_{80}O_{18}$	932.5345	
16	ginsenoside Re	$C_{48}H_{82}O_{18}$	946.5501	
17	vinaginsenoside R4	$C_{48}H_{82}O_{19}$	962.5450	
18	20-*O*-glucosyl-ginsenoside Rf	$C_{48}H_{82}O_{19}$	962.5450	
19	notoginsenoside N	$C_{48}H_{82}O_{19}$	962.5450	
20	ginsenoside Re2	$C_{48}H_{82}O_{19}$	962.5450	
21	ginsenoside Re3	$C_{48}H_{82}O_{19}$	962.5450	
22	malonyl-floralginsenoside Re1	$C_{51}H_{84}O_{21}$	1032.5505	
23	ginsenoside Rh2	$C_{36}H_{62}O_8$	622.4445	
24	20(*R*)-ginsenoside Rh2	$C_{36}H_{62}O_8$	622.4445	
25	compound K	$C_{36}H_{62}O_8$	622.4445	
26	ginsenoside F2	$C_{42}H_{72}O_{13}$	784.4973	
27	ginsenoside Rg3	$C_{42}H_{72}O_{13}$	784.4973	
28	20(*R*)-ginsenoside Rg3	$C_{42}H_{72}O_{13}$	784.4973	
29	ginsenoside Rs3	$C_{44}H_{74}O_{14}$	826.5079	
30	notoginsenoside Ft1	$C_{47}H_{80}O_{17}$	916.5396	
31	notoginsenoside Fe	$C_{47}H_{80}O_{17}$	916.5396	
32	notoginsenoside Fd	$C_{47}H_{80}O_{17}$	916.5396	**PPD**
33	notoginsenoside K	$C_{48}H_{82}O_{18}$	946.5501	
34	ginsenoside Rd	$C_{48}H_{82}O_{18}$	946.5501	
35	malonyl-floralginsenoside Rd5	$C_{51}H_{84}O_{21}$	1032.5505	
36	malonyl-ginsenoside Rd	$C_{51}H_{84}O_{21}$	1032.5505	
37	ginsenoside Rb2	$C_{53}H_{90}O_{22}$	1078.5924	
38	ginsenoside Rb3	$C_{53}H_{90}O_{22}$	1078.5924	
39	ginsenoside Rc	$C_{53}H_{90}O_{22}$	1078.5924	
40	ginsenoside Rb1	$C_{54}H_{92}O_{23}$	1108.6029	
41	malonyl-ginsenoside Rc	$C_{56}H_{92}O_{25}$	1164.5928	

42	malonyl-ginsenoside Rb2	$C_{56}H_{92}O_{25}$	1164.5928	
43	malonyl-ginsenoside Rb1	$C_{57}H_{94}O_{26}$	1194.6033	
44	ginsenoside Ra1	$C_{58}H_{98}O_{26}$	1210.6346	
45	ginsenoside Ra2	$C_{58}H_{98}O_{26}$	1210.6346	
46	ginsenoside Ra3	$C_{59}H_{100}O_{27}$	1240.6452	
47	notoginsenoside R4	$C_{59}H_{100}O_{27}$	1240.6452	
48	notoginsenoside Fa	$C_{59}H_{100}O_{28}$	1240.6452	
49	notoginsenoside S	$C_{63}H_{106}O_{30}$	1342.6769	
50	notoginsenoside T	$C_{64}H_{108}O_{31}$	1372.6875	
51	oleanic acid	$C_{30}H_{48}O_3$	456.3603	
52	chikusetsusaponin IVa	$C_{42}H_{66}O_{14}$	794.4453	
53	chikusetsusaponin IV	$C_{47}H_{74}O_{18}$	926.4875	**OA**
54	pseudoginsenoside Rt1	$C_{47}H_{74}O_{18}$	926.4875	
55	ginsenoside Ro	$C_{48}H_{76}O_{19}$	956.4981	
56	24(*R*)-pseudoginsenoside Rt5	$C_{36}H_{62}O_{10}$	654.4343	**OT**
57	24(*R*)-pseudoginsenoside F11	$C_{42}H_{72}O_{14}$	800.4922	
58	ginsenoside Rk3	$C_{36}H_{60}O_8$	620.4288	
59	ginsenoside Rh4	$C_{36}H_{60}O_8$	620.4288	
60	ginsenoside Rh7	$C_{36}H_{60}O_9$	636.4237	
61	ginsenoside Rh8	$C_{36}H_{60}O_9$	636.4237	
62	notoginsenoside T5	$C_{41}H_{68}O_{12}$	752.4711	
63	ginsenoside Rg5	$C_{42}H_{70}O_{12}$	766.4868	**Other**
64	ginsenoside Rg6	$C_{46}H_{70}O_{12}$	766.4867	
65	ginsenoside F4	$C_{42}H_{70}O_{12}$	766.4867	
66	ginsenoside Rk1	$C_{42}H_{70}O_{12}$	766.4868	
67	5,6-didehydroginsenoside Rd	$C_{48}H_{80}O_{18}$	944.5345	
68	vinaginsenoside R8	$C_{48}H_{82}O_{19}$	962.5450	
69	5,6-didehydroginsenoside Rb1	$C_{54}H_{90}O_{23}$	1106.5873	

Table S2 Information of 45 batches of the root, leaf, and flower bud samples of *Panax notoginseng* analyzed in the current work.

No.	Label	Different Parts	Producing regions	Collection time
1	F-1	Flower bud	WenShan City, YunNan Province	2018.04
2	F-2	Flower bud	WenShan City, YunNan Province	2018.04
3	F-3	Flower bud	WenShan City, YunNan Province	2018.04
4	F-4	Flower bud	WenShan City, YunNan Province	2018.04
5	F-5	Flower bud	WenShan City, YunNan Province	2018.09
6	F-6	Flower bud	WenShan City, YunNan Province	2018.09
7	F-7	Flower bud	WenShan City, YunNan Province	2018.09
8	F-8	Flower bud	WenShan City, YunNan Province	2018.09
9	F-9	Flower bud	WenShan City, YunNan Province	2018.09
10	F-10	Flower bud	WenShan City, YunNan Province	2018.09
11	F-11	Flower bud	WenShan City, YunNan Province	2018.09
12	F-12	Flower bud	WenShan City, YunNan Province	2018.09
13	F-13	Flower bud	WenShan City, YunNan Province	2018.09
14	F-14	Flower bud	WenShan City, YunNan Province	2018.09
15	F-15	Flower bud	KunMing City, YunNan Province	2018.09
16	L-1	Leaf	WenShan City, YunNan Province	2018.04
17	L-2	Leaf	WenShan City, YunNan Province	2018.04
18	L-3	Leaf	WenShan City, YunNan Province	2018.04
19	L-4	Leaf	WenShan City, YunNan Province	2018.09
20	L-5	Leaf	WenShan City, YunNan Province	2018.09
21	L-6	Leaf	WenShan City, YunNan Province	2018.09
22	L-7	Leaf	WenShan City, YunNan Province	2018.09
23	L-8	Leaf	WenShan City, YunNan Province	2018.09
24	L-9	Leaf	WenShan City, YunNan Province	2018.09
25	L-10	Leaf	WenShan City, YunNan Province	2018.09
26	L-11	Leaf	WenShan City, YunNan Province	2018.09
27	L-12	Leaf	WenShan City, YunNan Province	2018.09
28	L-13	Leaf	WenShan City, YunNan Province	2018.09
29	L-14	Leaf	WenShan City, YunNan Province	2018.09
30	L-15	Leaf	WenShan City, YunNan Province	2018.09
31	R-1	Root (20 tou)	WenShan City, YunNan Province	2018.04
32	R-2	Root (20 tou)	WenShan City, YunNan Province	2018.04
33	R-3	Root (40 tou)	WenShan City, YunNan Province	2018.04
34	R-4	Root (40 tou)	WenShan City, YunNan Province	2018.04
35	R-5	Root (60 tou)	WenShan City, YunNan Province	2018.04
36	R-6	Root (60 tou)	WenShan City, YunNan Province	2018.04
37	R-7	Root (80 tou)	WenShan City, YunNan Province	2018.04
38	R-8	Root (80 tou)	WenShan City, YunNan Province	2018.04
39	R-9	Root (100 tou)	WenShan City, YunNan Province	2018.04

40	R-10	Root (100 tou)	WenShan City, YunNan Province	2018.04
41	R-11	Root (120 tou)	WenShan City, YunNan Province	2018.04
42	R-12	Root (120 tou)	WenShan City, YunNan Province	2018.04
43	R-13	Rhizome	WenShan City, YunNan Province	2018.04
44	R-14	Rhizome	WenShan City, YunNan Province	2018.04
45	R-15	Rhizome	WenShan City, YunNan Province	2018.04

Table S3 Information of the Chinese patent medicines (CPMs) analyzed in this work.

No.	CPM	Batch Number
1-1	Naodesheng Tablet	20200505
1-2	Naodesheng Tablet	170901
1-3	Naodesheng Tablet	190903
2-1	Shenyang Hongyao Capsule	20200410
2-2	Shenyang Hongyao Capsule	20200615
2-3	Shenyang Hongyao Capsule	170901
3-1	Xinkeshu Tablet	0170839
3-2	Xinkeshu Tablet	0130519
3-3	Xinkeshu Tablet	0100594
4-1	Jingtong Particle	19101094
4-2	Jingtong Particle	17101073
4-3	Jingtong Particle	19101028
5-1	Danqi Tablet	20120094
5-2	Danqi Tablet	17120902
5-3	Danqi Tablet	20120093
6-1	Shuxiong Tablet	201709001
6-2	Shuxiong Tablet	201501001
6-3	Shuxiong Tablet	201504001
7-1	Sanqi xueshangning Capsule	200901
7-2	Sanqi xueshangning Capsule	161201
7-3	Sanqi xueshangning Capsule	130704
8-1	Sanqi Shangyao Tablet	7007002
8-2	Sanqi Shangyao Tablet	20140410
8-3	Sanqi Shangyao Tablet	20140908
9-1	Compound Xueshuantong Capsule	140408
9-2	Compound Xueshuantong Capsule	140102
9-3	Compound Xueshuantong Capsule	200713
10-1	Compound Danshen Dripping Pill	190117
10-2	Compound Danshen Dripping Pill	180916
10-3	Compound Danshen Dripping Pill	170521
11-1	Gucining Capsule	17081101
11-2	Gucining Capsule	190505060
11-3	Gucining Capsule	200301058
12-1	Xiaoshuan Tongluo Capsule	191024
12-2	Xiaoshuan Tongluo Capsule	20200503
12-3	Xiaoshuan Tongluo Capsule	20160503033
13-1	Compound Danshen Tablet	20120865
13-2	Compound Danshen Tablet	20120860
13-3	Compound Danshen Tablet	16121424
14-1	Dingkun Pill	3271812015
14-2	Dingkun Pill	146161032

No.	CPM	Batch Number
14-3	Dingkun Pill	3271912081
15-1	Wenxin Granule	2004071
15-2	Wenxin Granule	2008021
15-3	Wenxin Granule	1909023

Table S4 Information of 328 components identified from the root (**R**), leaf (**L**), and flower bud (**FB**) of *P. notoginseng*.

No.	Observed t_R (min)	Observed m/z	Formula	Mass error (ppm)	Observed CCS (Å²)	Adducts	ESI-MS²	Identification	R	L	FB
1	3.64	1093.5821	$C_{53}H_{90}O_{23}$	1.9	334.64	-H	1093.5791,931.5335,637.4313,475.3788,391.2850	PPT-3Glc-Xyl	√		
2	3.75	961.5401[a]	$C_{48}H_{82}O_{19}$	2.5	318.26	-H	961.5401,799.4845,637.4321,475.3791,391.2849	Notoginsenoside N	√		
3	3.77	1153.6305	$C_{54}H_{92}O_{23}$	2.1	341.02	+HCOO, -H	1107.5946,945.5407,799.4845,637.4321,475.3791,391.2849	PPT-3Glc-Rha	√		
4	4.03	1139.5887	$C_{53}H_{90}O_{23}$	2.8	342.77	+HCOO	1093.5796,961.5369,799.4843,637.4317,475.3790,391.2852	PPT-3Glc-Xyl	√		
5	4.09	1007.5455[a]	$C_{48}H_{82}O_{19}$	2.2	328.71	+HCOO, -H	961.5369,799.4843,637.4317,475.3790,391.2852	20-O-glucosyl-Ginsenoside Rf	√		
6	4.10	931.5275[a]	$C_{47}H_{80}O_{18}$	0.3	314.15	-H, +HCOO	779.4269,637.4349,475.3789	Notoginsenoside Fp1			√
7	4.16	831.4766	$C_{41}H_{70}O_{14}$	2.3	285.50	+HCOO, -H	785.4689,779.4276,653.4289,491.3745	OT-Xyl-Glc	√		
8	4.19	699.4346[b]	$C_{36}H_{62}O_{10}$	3.0	260.27	+HCOO	653.4289,491.3745	OT-Xyl	√		
9	4.26	977.5331[a]	$C_{47}H_{80}O_{18}$	0.4	326.35	+HCOO, -H	931.5253,823.4534,637.4322,535.2551,475.3783,391.2850	Notoginsenoside R1	√		√
10	4.42	1169.5943[b]	$C_{54}H_{92}O_{24}$	-1.5	356.14	+HCOO	1123.5840,961.5364,799.4844,475.3787	PPT-4Glc	√		
11	4.44	991.5503	$C_{48}H_{82}O_{18}$	2.0	331.55	+HCOO	945.5411,783.4863,619.4211,475.3787,375.1098	PPT-2Glc-Rha	√		
12	4.61	1025.5557	$C_{48}H_{84}O_{20}$	1.9	339.97	+HCOO	979.5465,817.4906,655.4427,475.5788	(PPT+H_2O)-3Glc	√	√	
13	4.68	991.5493[a]	$C_{48}H_{82}O_{18}$	1.0	330.17	+HCOO, -H	945.5393,783.4816,637.4308,475.3786,391.2850	Ginsenoside Re	√	√	√
14	4.73	845.4920[a]	$C_{42}H_{72}O_{14}$	1.9	301.07	+HCOO, -H	845.4888,799.4841,637.4311,475.3787,391.2846	Ginsenoside Rg1	√		√
15	4.77	683.4407	$C_{36}H_{62}O_9$	4.6	309.71	+HCOO	637.4314,475.3789,391.2849	PPT-Glc	√		
16	4.85	1301.6396[b]	$C_{59}H_{100}O_{28}$	1.0	384.31	+HCOO	1255.6308,1123.5884,781.4732,619.4203	($C_{30}H_{50}O_3$+H_2O)-4Glc-Xyl		√	
17	4.87	991.5504	$C_{48}H_{82}O_{18}$	2.1	330.77	+HCOO	945.5414,783.4878,621.4050,459.3486	PPD-3Glc	√		
18	4.94	1111.5922	$C_{53}H_{92}O_{24}$	1.4	264.65	-H	1111.5891,979.5385,817.4946,799.4847,655.4420,493.3893	(OT+2H)-3Glc-Xyl		√	
19	5.15	1025.5563[b]	$C_{48}H_{84}O_{20}$	2.4	338.36	+HCOO, -H	979.5495,817.4928,655.4436,493.3899	(OT+2H)-3Glc	√		
20	5.25	799.4866	$C_{42}H_{72}O_{14}$	2.1	292.69	-H	799.4834,637.4310,475.3787,391.2852	PPT-2Glc	√		
21	5.25	1255.6348[b]	$C_{59}H_{100}O_{28}$	1.6	372.15	-H	1255.6318,1123.5894,961.5357,799.4833,637.4313,475.3787	PPT-4Glc-Xyl		√	
22	5.28	887.4999[a]	$C_{44}H_{74}O_{15}$	-1.2	309.75	+HCOO	841.4960,799.4833,637.4313,475.3787	Notoginsenoside Rt	√	√	
23	5.53	1123.5915	$C_{53}H_{90}O_{22}$	0.8	361.07	+HCOO	1123.5894,783.4842,475.3787,391.2849	PPT-2Glc-Rha-Xyl	√		

24	5.63	1225.6230[b]	$C_{58}H_{98}O_{27}$	0.6	382.64	-H, +HCOO	1225.6201,1093.5805,961.5388,799.4847,781.4737,637.4315,475.3790	PPT-3Glc-2Xyl			√
25	5.64	845.4920	$C_{43}H_{74}O_{16}$	1.9	348.09	+HCOO	799.4855	$C_{30}H_{52}O_4$-2Glc	√		
26	5.64	1255.6345[b]	$C_{59}H_{100}O_{28}$	1.3	370.04	-H	1093.5793,961.5339,799.4834,637.4315,475.3786	PPT-4Glc-Xyl		√	
27	5.70	961.5033	$C_{47}H_{78}O_{20}$	2.0	312.65	-H	961.5317,799.4834,637.4315,475.3786	PPT-3Glc		√	
28	5.73	1031.5456[a]	$C_{51}H_{84}O_{21}$	2.3	325.34	-H	987.5481,945.5425,783.4894,620.4255,475.3792	Malonyl-floralginsenoside Re1	√		
29	5.90	1225.6239[b]	$C_{58}H_{98}O_{27}$	1.3	356.07	-H, +HCOO	1225.6227,1093.5850,961.5354,799.4829,781.4734,637.4310,475.3790,391.2879	PPT-3Glc-2Xyl			√
30	5.93	841.4972	$C_{44}H_{74}O_{15}$	2.0	469.08	-H	841.4945,799.4840,637.4314,475.3789,391.2850	PPT-2Glc-Ace	√		
31	6.06	1169.5979	$C_{54}H_{92}O_{24}$	1.6	354.51	+HCOO	1123.5909,1093.5783,961.5397,799.4840,637.4309,475.3786,375.2905	PPT-4Glc	√	√	√
32	6.10	1271.6294[b]	$C_{58}H_{98}O_{27}$	1.3	373.42	+HCOO, -H	1225.6187,1093.5783,961.5397,799.4840,781.4732,637.4309,475.3786,375.2905	PPT-3Glc-2Xyl		√	√
33	6.11	1005.5300	$C_{48}H_{80}O_{19}$	2.4	337.07	+HCOO, -H	959.5216,797.4698,637.4320,475.3787	PPT-3Glc	√		
34	6.12	815.4818[a]	$C_{41}H_{70}O_{13}$	2.4	294.21	+HCOO	769.4788,637.4320,475.3787	Pseudoginsenoside Rt3	√		
35	6.18	961.5038	$C_{46}H_{76}O_{18}$	2.5	312.49	+HCOO	783.4807,637.4312,475.3794	PPT-Glc-Rha-Xyl		√	
36	6.27	1225.6227[b]	$C_{58}H_{98}O_{27}$	0.4	364.92	-H, +HCOO	1225.6271,1093.5776,961.5383,799.4799,781.4731,765.4434,637.4314,475.3795	PPT-3Glc-2Xyl			√
37	6.32	1139.5872	$C_{53}H_{90}O_{23}$	1.5	366.08	+HCOO	1093.5776,961.5383,799.4790,781.4731,637.4314,475.3795	PPT-3Glc-Xyl		√	√
38	6.47	1007.5445	$C_{48}H_{82}O_{19}$	1.3	334.61	+HCOO	961.5352,799.4836,637.4325,475.3788,391.2850	PPT-3Glc	√		
39	6.53	845.4907	$C_{42}H_{72}O_{14}$	0.3	298.56	+HCOO	799.4832,637.4320,475.3788,391.2851	PPT-2Glc	√		
40	6.58	1169.5983	$C_{54}H_{92}O_{24}$	1.9	359.68	+HCOO	1123.5923,1093.5797,961.5379,799.4822,637.4320,475.3789	PPT-4Glc			√
41	6.59	1271.6295[b]	$C_{58}H_{98}O_{27}$	1.4	380.25	+HCOO	1225.6238,1093.5807,961.5357,799.4849,637.4307,475.3794	PPT-3Glc-2Xyl		√	√
42	6.75	961.5387	$C_{47}H_{80}O_{17}$	1.0	325.22	+HCOO	915.5310,783.4884,637.4310,475.3784,391.2846	PPT-Glc-Xyl-Rha	√		
43	6.85	1225.6237	$C_{58}H_{98}O_{27}$	1.2	374.28	-H, +HCOO	1225.6208,1093.5794,961.5393,905.4746,799.4840,781.4733,637.4316,475.3785	PPT-3Glc-2Xyl		√	√
44	6.94	815.4816[a]	$C_{42}H_{72}O_{15}$	2.1	298.59	+HCOO	769.4760,637.4315,475.3788	20(S)-sanchinoside A3	√		
45	7.00	1169.5983	$C_{54}H_{92}O_{24}$	1.9	358.39	+HCOO	1123.5899,799.4859,637.4315,475.3788	PPT-4Glc	√		
46	7.08	995.5454[b]	$C_{48}H_{84}O_{21}$	2.2	326.44	-H	961.5378,799.4837,637.4313,475.3791	PPT-2Glc-Mal-Ace-But		√	
47	7.12	1093.5818	$C_{53}H_{90}O_{23}$	1.6	351.61	-H	1093.5804,961.5418,799.4850,781.4731,637.4313,475.3788	PPT-3Glc-Xyl		√	√
48	7.17	1179.5832[b]	$C_{56}H_{92}O_{26}$	2.4	349.84	-H	1093.5788,799.4837,781.4738,637.4313,475.3791	PPT-3Glc-Mal-Xyl		√	
49	7.31	1139.5890	$C_{53}H_{90}O_{23}$	3.1	352.59	+HCOO	1093.5799,961.5366,799.4847,637.4325,475.3794	PPT-3Glc-Xyl		√	

50	7.33	1151.5874[b]	$C_{54}H_{90}O_{23}$	1.6	352.85	+HCOO, -H	1105.5803,943.5231,619.4212,457.3686	5,6-didehydro-PPD-4Glc	√		
51	7.35	1225.5869[b]	$C_{57}H_{94}O_{28}$	0.8	345.73	-H	1093.5797,797.4705,637.4306,475.3791	PPT-3Glc-2Xyl			√
52	7.39	975.5181[b]	$C_{48}H_{80}O_{20}$	1.1	322.82	-H	799.4865,637.4318,587.3959,475.3786,391.2852	PPT-2Glc-GlurA	√		
53	7.42	1093.5817	$C_{53}H_{90}O_{23}$	1.6	357.09	-H	961.5405,799.4865,637.4318,475.3786,391.2852	PPT-3Glc-Xyl	√		
54	7.69	1139.5877	$C_{53}H_{90}O_{23}$	1.9	362.00	-H, +HCOO	1093.5806,961.5349,799.4852,781.4735,637.4313,475.3794	PPT-3Glc-Xyl		√	
55	7.83	1179.5834[b]	$C_{56}H_{92}O_{26}$	2.5	347.59	-H	1093.5795,799.4854,781.4729,637.4320,475.3792	PPT-3Glc-Mal-Xyl		√	
56	8.03	1139.5877	$C_{53}H_{90}O_{23}$	2.0	361.91	+HCOO	1093.5797,961.5384,799.4838,781.4740,637.4321,475.3797	PPT-3Glc-Xyl		√	
57	8.04	1179.5844[b]	$C_{56}H_{92}O_{26}$	3.4	341.17	-H	1093.5797,961.5384,799.4838,781.4740,637.4312,475.3797	PPT-3Glc-Mal-Xyl		√	
58	8.07	961.5392[a]	$C_{48}H_{82}O_{19}$	1.5	329.00	-H	961.5367,799.4838,637.4312,475.3788,391.2852	Vinaginsenoside R4	√		√
59	8.16	1179.5826[b]	$C_{56}H_{92}O_{26}$	1.9	344.49	-H	1093.5793,1075.5653,799.4870,637.4310,475.3792	PPT-3Glc-Xyl-Mal			√
60	8.30	1269.6166[b]	$C_{58}H_{96}O_{27}$	3.5	373.10	+HCOO	1223.6065,1091.5656,961.5357,797.4712,635.4174,473.3651	(PPT-2H)-3Glc-2Xyl		√	
61	8.56	1179.5832[b]	$C_{56}H_{92}O_{26}$	2.4	347.08	-H	1093.5803,799.4857,781.4726,637.4323,475.3790	PPT-3Glc-Mal-Xyl		√	
62	8.65	887.5023	$C_{44}H_{74}O_{15}$	1.5	312.35	+HCOO	799.4823,638.4346,4310,475.3791	PPT-2Glc-Ace	√		
63	8.68	1007.5454	$C_{48}H_{82}O_{19}$	2.2	334.25	+HCOO	961.5333,799.4823,637.4320,475.3790,391.2847	PPT-3Glc	√	√	
64	8.71	1169.5989	$C_{54}H_{92}O_{24}$	2.4	354.15	+HCOO	1123.5892,961.5333,945.5424,799.4823,783.4910,637.4320,475.3790,391.2847	PPT-4Glc	√		
65	8.75	1401.6945[b]	$C_{65}H_{110}O_{32}$	2.7	390.39	-H	1401.6920,1239.6368,1107.5949,945.5424,783.4910,637.4320,475.3790	PPT-Rha-4Glc-Xyl	√		
66	8.77	667.4452	$C_{36}H_{62}O_{8}$	3.8	267.70	+HCOO	621.4356,459.3846	PPD-Glc	√		
67	8.80	829.4974	$C_{42}H_{72}O_{13}$	2.3	300.42	+HCOO	783.4910,621.4356,459.3846	PPD-2Glc	√		
68	9.00	1371.6832[a]	$C_{64}H_{108}O_{31}$	2.2	391.07	-H, +HCOO	1371.6794,1239.6367,1107.5942,1077.5848,945.5417,783.4895,621.4364,459.3837	Notoginsenoside T	√	√	√
69	9.06	1049.5533	$C_{50}H_{84}O_{20}$	-0.5	342.73	+HCOO	1003.5417,961.5347,799.4748,637.4345,475.3785	PPT-3Glc-Ace	√		
70	9.36	799.4861[a]	$C_{42}H_{72}O_{14}$	1.4	306.81	-H	799.4838,637.4315,475.3786,391.2850	Ginsenoside Rf	√		
71	9.45	1269.6490	$C_{60}H_{102}O_{28}$	0.4	286.10	-H	1269.6468,1107.5949,945.5416,783.4892,621.4366,459.3858,	PPD-5Glc	√		
72	9.55	699.4345[b]	$C_{36}H_{62}O_{10}$	2.9	275.47	+HCOO	653.4275,491.3758	OT-Glc	√		
73	9.59	845.4926[a]	$C_{42}H_{72}O_{14}$	2.6	302.88	+HCOO, -H	799.4848,653.4275,491.3758	24(R)-Pseudoginsenoside F11	√		
74	9.67	959.5249	$C_{48}H_{80}O_{19}$	3.0	401.57	-H	959.5215,797.4694,635.4170,473.3643	(PPT-2H)-3Glc	√		
75	9.74	1371.6826[b]	$C_{64}H_{108}O_{31}$	1.8	385.07	-H	1371.6816,1209.6295,1077.5862,945.5432,783.4887,621.4362,459.3848	PPD-4Glc-2Xyl		√	√

76	9.80	1285.6461[a]	$C_{59}H_{100}O_{27}$	2.1	372.15	+HCOO, -H	1239.6371,1107.5947,1077.5862,945.5432,783.4886,621.4362,459.3848	Notoginsenoside R4	√		√
77	9.81	1223.6452[b]	$C_{59}H_{100}O_{26}$	1.8	372.76	-H, +HCOO	1107.5936,1091.5997,929.5456,783.4905,621.4357,475.3786,391.2851	PPT-2Glc-2Rha-Xyl		√	
78	9.82	1269.6486	$C_{60}H_{102}O_{28}$	0.1	374.78	-H	1107.5936,945.5421,929.5456,783.4905,621.4357,475.3786,391.2851	PPT-4Glc-Rha		√	
79	9.88	845.4924	$C_{42}H_{72}O_{14}$	2.4	369.15	+HCOO, -H	799.4864,637.4328,475.3796,391.2857	PPT-2Glc	√		
80	9.96	977.5356	$C_{47}H_{80}O_{18}$	3.0	247.23	+HCOO	931.5338,799.4834,637.438	$C_{30}H_{52}O_4$-2Glc-Xyl		√	
81	10.14	1371.6825[b]	$C_{64}H_{108}O_{31}$	1.7	387.62	-H	1371.6850,1209.6270,1077.5857,945.5422,783.4889,621.4363,459.3846,375.2907	PPD-4Glc-2Xyl		√	
82	10.14	1341.6726[b]	$C_{63}H_{106}O_{30}$	2.2	377.36	-H, +HCOO	1341.6712,1209.6270,1077.5857,945.5422,783.4889,621.4363,459.3846,375.2907	PPD-3Glc-3Xyl		√	√
83	10.28	769.4767	$C_{41}H_{70}O_{13}$	3.1	300.95	-H, +HCOO	769.4745,637.4320,475.3793,391.2852	PPT-Glc-Xyl	√		
84	10.28	1269.6504[b]	$C_{60}H_{102}O_{28}$	1.5	103.10	-H, +HCOO	1269.6475,1107.5944,945.5425,783.4895,621.4372,459.3837,375.2899	PPD-5Glc		√	√
85	10.31	1371.6827	$C_{64}H_{108}O_{31}$	1.8	387.89	-H, +HCOO	1371.6793,1269.6466,1239.6384,1107.5945,945.5414,785.4975,603.4272, 460.3889,375.2885	PPD-4Glc-2Xyl			√
86	10.33	815.4820[a]	$C_{41}H_{70}O_{13}$	2.6	229.96	+HCOO	769.4745,637.4320,475.3793,391.2852	Notoginsenoside R2	√		
87	10.39	947.5239	$C_{46}H_{78}O_{17}$	1.9	325.58	+HCOO, -H	901.5156,769.4731,637.4350,475.3789,391.2854	PPT-Glc-2Xyl		√	√
88	10.48	1269.6518	$C_{60}H_{102}O_{28}$	2.6	368.98	-H, +HCOO	1269.6488, 1107.5957,945.5445,783.4899,621.4372,460.3521	PPD-5Glc	√		
89	10.63	977.5356	$C_{47}H_{80}O_{18}$	3.0	328.10	+HCOO	931.5280,799.4865,637.4330,475.3796,391.2852	PPT-Xyl-2Glc	√		
90	10.65	1325.6403	$C_{62}H_{102}O_{30}$	1.5	363.59	-H	1239.6357,945.5411,783.4890,621.4362,459.3836,375.2903	PPD-4Glc-Xyl-Mal			√
91	10.67	1371.6812[b]	$C_{64}H_{108}O_{31}$	0.7	388.29	-H, +HCOO	1371.6783,1239.6357,1107.5936,945.5410,783.4886,621.4362,459.3886	PPD-4Glc-2Xyl			√
92	10.68	1371.6842[b]	$C_{64}H_{108}O_{31}$	2.9	388.58	-H, +HCOO	1371.6806,1239.6378,1077,5853,945.5422,783.4903,637.4333,475.3796	PPT-Rha-2Glc-2Xyl	√		
93	10.77	1239.6387[a]	$C_{59}H_{100}O_{27}$	0.6	370.55	-H, +HCOO	1239.6356,1077.5936,945.5412,783.4884,621.4360,459.3837,375.2900	Notoginsenoside Fa	√	√	√
94	10.78	1263.1403[b]	$C_{33}H_{52}O_{51}$	0.0	288.63	-H	1107.5938,945.5417,783.4890,621.4366,459.3838	PPD-4Glc-But-Ace		√	
95	10.85	1341.6705	$C_{63}H_{106}O_{30}$	0.7	384.67	-H, +HCOO	1341.6674,1209.6251,1077.5834,945.5412,783.4884,621.4360,459.3837,375.2906	PPD-3Glc-3Xyl		√	√
96	11.16	1387.6787[b]	$C_{63}H_{106}O_{30}$	2.6	392.86	+HCOO	1341.6707,1209.6272,1077.5836,915.5321,753.4785,621.4366	$C_{30}H_{52}O_3$-3Glc-3Xyl		√	
97	11.19	1151.5883[a]	$C_{54}H_{90}O_{23}$	2.4	351.82	+HCOO, -H	1105.5791,943.5274,781.4739,619.4199,457.3693	5,6-didehydroginsenoside Rb1	√		
98	11.26	815.4809[a]	$C_{41}H_{70}O_{13}$	1.3	307.02	+HCOO	637.4329,475.3782	Ginsenoside F5		√	
99	11.35	1239.6401	$C_{59}H_{100}O_{27}$	1.8	368.97	-H, +HCOO	1239.6378,1077.5936,945.5412,783.4884,621.4360,459.3837,375.2900	PPD-4Glc-Xyl		√	√
100	11.37	1371.6823[b]	$C_{64}H_{108}O_{31}$	1.5	386.71	-H	1371.6794,1239.6378,1209.6266,1077.5849,945.5424,783.4897,621.4373,	PPD-4Glc-2Xyl		√	√

							459.3843,375.2905				
101	11.39	1209.6301	$C_{58}H_{98}O_{26}$	2.3	358.74	-H, +HCOO	1209.6266,1077.5849,945.5424,783.4897,621.4373,459.3843,375.2905	PPD-3Glc-2Xyl			√
102	11.43	829.4991	$C_{42}H_{72}O_{13}$	4.4	383.46	+HCOO	783.4897,621.4373,459.3843,375.2905	PPD-2Glc			√
103	11.44	829.4972 [a]	$C_{42}H_{72}O_{13}$	2.1	306.08	+HCOO, -H	783.4895,637.4317,475.3790,391.2848	Ginsenoside Rg2	√	√	
104	11.44	977.5352	$C_{47}H_{80}O_{18}$	2.6	320.13	+HCOO, -H	931.5273,637.4381,475.3793	PPT-2Glc-Xyl		√	
105	11.53	811.4854	$C_{43}H_{72}O_{14}$	0.6	312.21	-H, +HCOO	811.4846,769.4739,637.4317,475.3790	PPT-Glc-Xyl-Ace	√		
106	11.66	1427.6740[b]	$C_{66}H_{108}O_{33}$	2.8	407.48	-H	1281.6480,1107.5954,945.5428,783.4897,621.4369,459.3841	PPD-4Glc-Xyl-Ace-Rha			√
107	11.67	1281.6519	$C_{61}H_{102}O_{28}$	2.7	381.77	-H, +HCOO	1281.6480,1239.6380,1107.5954,945.5428,783.4897,621.4369,459.3841,375.2903	PPD-4Glc-Xyl-Ace	√		√
108	11.69	1325.6407 [b]	$C_{62}H_{102}O_{30}$	1.8	369.94	-H	1239.6378,1107.5959,945.5420,783.4902,621.4374,459.3842,375.2909	PPD-4Glc-Xyl-Mal		√	√
109	11.96	1193.5987 [b]	$C_{57}H_{94}O_{26}$	2.2	358.87	-H	1105.5789,943.5276,781.4749,619.4213,457.3693	(5,6-didehydro-PPD+2H)-4Glc-Mal	√		
110	11.97	1209.6306	$C_{58}H_{98}O_{26}$	2.7	227.31	-H, +HCOO	1209.6272,1077.5847,945.5429,783.4896,621.4371,459.3843,375.2910	PPD-3Glc-2Xyl		√	√
111	11.99	1151.5886	$C_{54}H_{90}O_{23}$	2.7	353.44	+HCOO, -H	1105.5789,943.5276,781.4749,619.4213,457.3693	5,6-didehydro-PPD-4Glc	√		
112	12.07	1341.6726 [b]	$C_{63}H_{106}O_{30}$	2.2	514.93	-H	1341.6694,1209.6264,1077.5846,915.5320,783.4897,621.4371,603.4279, 459.3841,375.2897	PPD-3Glc-3Xyl		√	√
113	12.14	1427.6748[b]	$C_{66}H_{108}O_{33}$	3.4	396.16	-H	1077.5846,945.5421,783.4897,621.4371,459.3841	PPD-3Glc-3Xyl-Mal			√
114	12.19	1239.6399[a]	$C_{59}H_{100}O_{27}$	1.6	366.31	-H, +HCOO	1239.6374,1077.5859,945.5423,783.4904,621.4374,459.3842	Ginsenoside Ra3	√		
115	12.24	1325.6411 [b]	$C_{62}H_{102}O_{30}$	2.1	291.95	-H	1239.6382,1107.5945,945.5418,783.4894,621.4364,459.3841,375.2904	PPD-4Glc-Xyl-Mal	√	√	√
116	12.24	1281.6529 [b]	$C_{61}H_{102}O_{28}$	3.4	514.45	-H, +HCOO	1281.6485,1239.6376,1221.6263,1089.5851,945.5422,783.4897,621.4370, 459.3839,375.2907	PPD-4Glc-Xyl-Ace			√
117	12.31	1153.6030[a]	$C_{54}H_{92}O_{23}$	1.6	356.44	+HCOO, -H	1107.5945,945.5418,783.4894,621.4365,459.3841,375.2907	Ginsenoside Rb1	√	√	√
118	12.45	1153.6040	$C_{54}H_{92}O_{23}$	2.5	258.20	+HCOO	1107.5952,946.5458,783.4906,621.4372,459.3841	PPD-4Glc	√		
119	12.45	1209.6292	$C_{58}H_{98}O_{26}$	1.5	359.54	-H, +HCOO	1209.6262,1077.5851,945.5420,783.4897,621.4367,459.3840,375.2904	PPD-3Glc-2Xyl		√	√
120	12.51	1221.5919	$C_{57}H_{92}O_{25}$	0.8	364.96	+HCOO	1107.5952,945.5424,784.4937,621.4372,459.3841	PPD-4Glc-But	√		
121	12.60	1107.5965	$C_{54}H_{92}O_{23}$	0.8	219.38	-H, +HCOO	1107.5947,945.5421,783.4900,621.4370,459.3841,375.2906	PPD-4Glc	√		
122	12.72	1107.5983[b]	$C_{53}H_{90}O_{21}$	2.4	343.72	+HCOO	1061.5879,915.5328,753.4788,621.4369,459.3839	PPD-2Glc-Xyl-Rha		√	
123	12.72	1255.6357 [b]	$C_{58}H_{98}O_{26}$	2.3	380.34	+HCOO	1209.6268,1047.5747,915.5328,753.4788,621.4369,459.3839	PPD-3Glc-2Xyl		√	

124	12.82	871.5072	$C_{44}H_{74}O_{14}$	1.3	310.56	+HCOO, -H	825.4996,783.4895,637.4311,475.3786,391.2852	PPT-Glc-Rha-Ace	√		
125	12.84	1297.6386[b]	$C_{60}H_{100}O_{27}$	-3.7	370.30	+HCOO	1251.6357,1209.6271,1077.5847,945.5413,783.4895,621.4367,459.3841	PPD-3Glc-2Xyl-Ace			√
126	12.84	1295.6296[b]	$C_{61}H_{100}O_{29}$	1.4	367.99	-H	1251.6357,1209.6271,1077.5847,945.5413,783.4895,621.4367,459.3841	PPD-3Glc-2Xyl-Mal			√
127	12.86	1177.6037[b]	$C_{57}H_{94}O_{25}$	2.2	344.54	-H	1091.5947,929.5402,825.4996,783.4895,637.4311,475.3786,391.2852	PPT-2Glc-3Rha-Mal	√		
128	12.87	977.5343	$C_{47}H_{80}O_{18}$	1.7	247.98	+HCOO	931.5256,915.5307,637.4320,475.3791	PPT-2Glc-Xyl		√	
129	13.00	1325.6400	$C_{62}H_{102}O_{30}$	1.3	512.38	-H	1281.6486,1239.6360,1221.6257,1077.5836,945.5417,765.4790	$C_{30}H_{52}O_3$-4Glc-Xyl-Mal	√		
130	13.09	1285.6446	$C_{59}H_{100}O_{27}$	0.9	443.06	+HCOO	1239.6360,1077.5836,945.5413,783.4889,621.4359,459.3838,375.2901	PPD-4Glc-Xyl		√	
131	13.17	1295.6286[b]	$C_{61}H_{100}O_{29}$	0.7	375.20	-H	1251.6350,1149.6033,1107.5935,1089.5828,945.5413,765.4781, 621.4359,459.3838	PPD-4Glc-Rha-Ace		√	
132	13.18	1251.6406[b]	$C_{60}H_{100}O_{27}$	2.2	370.58	-H, +HCOO	1251.6357,1209.6063,1191.6160,1077.5847,945.5425,783.4897, 621.4367,459.3841,375.2906	PPD-3Glc-2Xyl-Ace			√
133	13.19	1295.6296[b]	$C_{61}H_{100}O_{29}$	1.4	373.54	-H	1251.6357,1209.6263,1077.5847,945.5425,783.4897,621.4367,459.3841	PPD-3Glc-2Xyl-Mal			√
134	13.21	1193.5976[a]	$C_{57}H_{94}O_{26}$	1.3	351.90	-H	1149.6047,1107.5937,945.5414,783.4895,621.4360, 459.3836,375.2902	Malonyl-Ginsenoside Rb1	√		√
135	13.22	1149.6081 [b]	$C_{58}H_{94}O_{24}$	1.6	246.67	-H	1149.6047,1107.5937,1089.5835,945.5414,783.4895,621.4360,459.3836	PPD-4Glc-Ace	√	√	
136	13.28	725.4494	$C_{38}H_{64}O_{10}$	1.7	345.82	+HCOO, -H	679.4420,637.4315,475.3786,391.2851	PPT-Glc-Ace	√		
137	13.41	1209.6285	$C_{58}H_{98}O_{26}$	0.9	369.92	-H, +HCOO	1209.6254,1077.5835,945.5413,783.4888,621.4366,459.3833,375.2906	PPD-3Glc-2Xyl		√	√
138	13.41	1427.6753[b]	$C_{66}H_{108}O_{33}$	3.7	395.93	-H	1209.6256,1077.5841,945.5412,783.4890,621.4363,459.3838	PPD-3Glc-3Xyl-Mal			√
139	13.42	955.4924[a]	$C_{48}H_{76}O_{19}$	1.7	250.62	-H	955.4902,793.4379,659.4169,631.3812,569.3846,455.3527	Ginsenoside Ro	√		
140	13.50	1193.5974 [b]	$C_{57}H_{94}O_{26}$	1.1	356.55	-H	1149.6047,1107.5938,945.5413,783.4892,621.4362,459.3838	PPD-Mal-4Glc			√
141	13.53	1087.5354 [b]	$C_{53}H_{84}O_{23}$	2.1	216.99	-H	1087.5333,925.4763,749.4495,731.4373,587.3957,569.3846,455.3528	OA-2Glc-GlurA-Xyl	√		
142	13.80	1297.6389[b]	$C_{60}H_{100}O_{27}$	-3.5	370.30	+HCOO, -H	1251.6362,1191.6155,1059.5749,945.5417,783.4890,621.4364,459.3840,375.2906	PPD-3Glc-2Xyl-Ace			√
143	13.81	1295.6306[b]	$C_{61}H_{100}O_{29}$	2.2	369.61	-H	1251.6362,1059.5749,945.5417,783.4890,621.4364,459.3840	PPD-3Glc-2Xyl-Mal		√	√
144	13.90	1077.5864[a]	$C_{53}H_{90}O_{22}$	1.2	260.33	-H, +HCOO	1077.5838,945.5417,783.4890,621.4364,459.3840,375.2906	Ginsenoside Rc		√	√
145	13.98	1145.6115	$C_{57}H_{94}O_{23}$	0.2	272.57	-H	1077.5836,915.534,783.4888,621.4364,459.3839,375.2907	PPD-3Glc-Xyl-But			√
146	14.00	1149.6082	$C_{58}H_{94}O_{24}$	1.7	435.04	-H	1149.6046,1107.5944,1089.5807,945.5421,783.4898,621.4367,459.3838,375.2910	PPD-4Glc-Ace	√		
147	14.01	1193.5975 [b]	$C_{57}H_{94}O_{26}$	1.2	343.63	-H	1149.6046,1107.5944,1089.5807,945.5421,783.4898,621.4367,459.3838	PPD-4Glc-Mal	√		

148	14.02	885.4870[b]	$C_{45}H_{74}O_{17}$	1.9	254.68	-H	621.4367,459.3838	PPD-Glc-2Xyl	√		
149	14.04	1209.6285	$C_{58}H_{98}O_{26}$	1.0	280.62	-H, +HCOO	1209.6258,1077.5836,945.5414,783.4894,621.4365,459.3839,375.2911	PPD-3Glc-2Xyl		√	√
150	14.05	1047.5549	$C_{55}H_{84}O_{19}$	1.4	255.70	-H	915.5318,783.4894,621.4365,459.3839	PPD-2Glc-2Xyl		√	
151	14.11	1295.6304[b]	$C_{61}H_{100}O_{29}$	2.0	368.50	-H	1251.6367,1149.6048,1107.5947,1078.5879,945.5422,783.4894,621.4368,459.3842	PPD-4Glc-Ace-Rha			√
152	14.12	1193.5979	$C_{57}H_{94}O_{26}$	1.6	251.08	-H	1149.6048,1107.5947,945.5422,783.4894,621.4368,459.3842,375.2907	PPD-Mal-4Glc			√
153	14.16	1123.5931[b]	$C_{53}H_{90}O_{22}$	2.2	479.83	+HCOO	945.5423,783.4894,621.4368,459.3842	PPD-3Glc-Xyl			√
154	14.18	1255.6369	$C_{58}H_{98}O_{26}$	3.2	418.90	+HCOO	945.5424,783.4896,621.4370,459.3842	PPD-3Glc-2Xyl			√
155	14.25	1193.5977[b]	$C_{57}H_{94}O_{26}$	1.4	352.55	-H	1149.6045,1107.5946,1089.5840,945.5422,783.4893,621.4367,459.3842	PPD-4Glc-Mal	√		√
156	14.25	1411.1830[b]	$C_{39}H_{60}O_{56}$	3.9	288.96	-H	1149.6045,1107.5946,1089.5840,945.5422,783.4893,621.4367,459.3842	PPD-2Mal-4Glc-Xyl	√		
157	14.26	1149.6096	$C_{56}H_{94}O_{24}$	2.9	289.19	-H	1149.6053,1107.5955,1089.5843,945.5424,783.4900,621.4370,459.3840,375.2909	PPD-Ace-4Glc	√		√
158	14.56	987.5189[b]	$C_{49}H_{80}O_{20}$	1.9	309.53	-H	945.5416,783.4895,621.4363,459.3838,375.2903	PPD-3Glc-Ace		√	
159	14.59	1341.6713[a]	$C_{63}H_{106}O_{30}$	1.2	381.57	-H, +HCOO	1341.6688,1209.6257,1077.5839,945.5416,783.4895,621.4363,459.3838,375.2903	Notoginsenoside S		√	√
160	14.68	955.4932	$C_{48}H_{76}O_{19}$	2.5	288.37	-H	955.4910,793.4386,569.3850,455.3532	OA-2Glc-GlurA	√		
161	14.94	1193.5991[b]	$C_{57}H_{94}O_{26}$	2.6	362.69	-H	1149.6015,1107.5948,459.3463	PPD-Mal-4Glc	√		
162	14.99	1119.5981[b]	$C_{55}H_{92}O_{23}$	2.2	520.84	-H	1119.5935,1077.5838,1059.5731,945.5421,783.4891,621.4363,459.3835	PPD-3Glc-Xyl-Ace		√	√
163	15.01	1163.5868[a]	$C_{56}H_{92}O_{25}$	1.1	349.03	-H	1119.5935,1077.5838,1059.5731,945.5421,783.4891,621.4363,459.3835,375.2901	Malonyl-Ginsenoside Rc		√	
164	15.08	1255.6359	$C_{58}H_{98}O_{26}$	2.4	385.89	+HCOO	1209.6260,945.5421,783.4891,621.4363,459.3835	PPD-3Glc-2Xyl		√	
165	15.15	1195.6137[b]	$C_{56}H_{94}O_{24}$	1.7	373.36	+HCOO	1149.6055,1108.5993,945.5424,783.4895,621.4374,459.3841	PPD-4Glc-Ace	√		
166	15.18	1251.6408[b]	$C_{60}H_{100}O_{27}$	2.3	382.53	-H, +HCOO	1251.6372,1209.6277,1191.6171,1077.5843,945.5419,783.4900,621.4369,459.3841	PPD-3Glc-2Xyl-Ace			√
167	15.18	1295.6305[b]	$C_{61}H_{100}O_{29}$	2.1	373.40	-H	1251.6372,1209.6277,1077.5843,945.5419,783.4900,621.4369,459.3841	PPD-3Glc-2Xyl-Mal			√
168	15.25	1279.5989[b]	$C_{60}H_{96}O_{29}$	1.2	362.05	-H	1193.6233,1149.6056,1107.5946,1089.5849,945.5425,783.4892,621.4369, 459.3842,375.2906	PPD-4Glc-Dimal	√		√
169	15.28	1235.6098[b]	$C_{59}H_{96}O_{27}$	2.6	235.08	-H	1191.6169,1149.6056,1107.5946,1089.5849,946.5459,783.4892,621.4369, 459.3842	PPD-4Glc-Mal-Ace	√		√
170	15.39	1223.6453	$C_{59}H_{100}O_{26}$	1.9	372.99	-H, +HCOO	1077.5836,945.5422,783.4896,621.4366,459.3841	PPD-3Glc-Xyl-Rha		√	
171	15.42	1119.5984[b]	$C_{55}H_{92}O_{23}$	2.4	218.20	-H	1119.5945,1077.5846,1059.5742,945.5426,783.4902,621.4369,459.3843,375.2908	PPD-3Glc-Xyl-Ace			√

172	15.42	1163.5867[b]	$C_{56}H_{92}O_{25}$	1.0	347.20	-H	1119.5945,1077.5846,1059.5742,945.5426,783.4902,621.4369,459.3843	PPD-3Glc-Xyl-Mal		√	√
173	15.43	1297.6388[b]	$C_{60}H_{100}O_{27}$	-3.5	372.94	+HCOO, -H	1251.6364,1209.6277,1077.5836,945.5422,783.4896,621.4366,459.3841	PPD-3Glc-2Xyl-Ace		√	
174	15.43	1295.6296[b]	$C_{61}H_{100}O_{29}$	1.4	369.97	-H	1077.5936,945.5422,783.4896,621.4366,459.3841	PPD-3Glc-Mal-2Xyl		√	
175	15.50	1235.6101[b]	$C_{59}H_{96}O_{27}$	2.8	359.54	-H	1149.6057,1107.5954,945.5426,783.4900,621.4369,459.3843,375.2909	PPD-4Glc-Mal-Ace			√
176	15.51	793.4404	$C_{42}H_{66}O_{14}$	3.1	286.17	-H	793.4390,631.3861,569.33861,455.3532	OA-Glc-GlurA	√		
177	15.64	1251.6415[b]	$C_{60}H_{100}O_{27}$	2.8	377.34	-H, +HCOO	1251.6372,1209.6273,1191.6167,1078.5886,945.5430,783.4898,621.4369,603.4277	$C_{30}H_{52}O_3$-3Glc-2Xyl-Ace			√
178	15.65	1295.6310[b]	$C_{61}H_{100}O_{29}$	2.5	279.82	-H	1251.6372,1209.6273,1078.5886,945.5430,783.4898,603.4277	$C_{30}H_{52}O_3$-3Glc-2Xyl-Mal			√
179	15.77	1193.5982	$C_{57}H_{94}O_{26}$	-1.3	365.71	-H	1149.6050,1107.5943,1089.5842,945.5427,783.4899,621.4366,459.3840,375.2910	PPD-Mal-4Glc	√		
180	15.78	1077.5862[a]	$C_{53}H_{90}O_{22}$	1.1	262.21	-H, +HCOO	1077.5837,945.5418,783.4894,621.4366,459.3839,375.2902	Ginsenoside Rb2	√	√	√
181	16.12	1251.6421[b]	$C_{60}H_{100}O_{27}$	3.4	382.93	-H, +HCOO	1251.6374,1119.5958,1059.5748,945.5430,765.4787,621.4371,459.3844,375.2903	PPD-3Glc-2Xyl-Ace			√
182	16.12	1119.5996[b]	$C_{55}H_{92}O_{23}$	3.5	291.74	-H	1119.5958,1059.5748,945.5430,765.4787,621.4371,459.3844	PPD-3Glc-Xyl-Ace		√	√
183	16.12	1295.6318[b]	$C_{61}H_{100}O_{29}$	3.1	377.73	-H	1251.6374,1119.5958,1059.5748,945.5430,764.4823,621.4371,459.3844	PPD-3Glc-2Xyl-Mal			√
184	16.16	1163.5875	$C_{56}H_{92}O_{25}$	1.7	267.74	-H	1119.5946,1059.5742,945.5421,783.4902,603.4273,459.3838	PPD-3Glc-Xyl-Mal		√	
185	16.26	1163.5883[b]	$C_{56}H_{92}O_{25}$	2.4	224.02	-H	1059.5746,945.5428,765.4797,621.4366,459.3843	PPD-3Glc-Xyl-Mal			√
186	16.30	1123.5930	$C_{53}H_{90}O_{22}$	2.2	347.61	+HCOO	1107.5958,945.5444,783.4920,621.4368,459.3846	PPD-3Glc-Xyl	√		
187	16.40	683.4394[a]	$C_{36}H_{62}O_9$	2.7	227.87	+HCOO	637.4337,621.4370,475.3794,459.3842,391.2853	Ginsenoside F1	√		
188	16.45	1295.6329[b]	$C_{61}H_{100}O_{29}$	4.0	381.62	-H	1251.6371,1209.6263,1059.5736,945.5424,783.4893,459.3839	PPD-3Glc-2Xyl-Mal			√
189	16.46	1123.5922	$C_{53}H_{90}O_{22}$	1.4	240.37	+HCOO	1077.5835,945.5412,783.4893,621.4364,459.3838	PPD-3Glc-Xyl	√	√	
190	16.48	1101.5903[b]	$C_{54}H_{88}O_{20}$	4.7	380.48	+HCOO	945.5412,783.4893,621.4364,459.3838	PPD-3Glc-But-Ace		√	
191	16.59	1077.5857[a]	$C_{53}H_{90}O_{22}$	0.6	394.29	-H, +HCOO	1077.5837,945.5419,783.4890,621.4364,459.3840,375.2907	Ginsenoside Rb3		√	
192	16.65	1193.5992[b]	$C_{57}H_{94}O_{26}$	2.6	360.84	-H	1149.6078,1107.5959,1089.5857,946.5479,783.4904,622.4411,459.3853	PPD-Mal-4Glc	√		
193	16.66	1123.5936	$C_{53}H_{90}O_{22}$	2.7	295.43	+HCOO	1077.5851,945.5426,783.4905,621.4368,459.3846	PPD-3Glc-Xyl			√
194	16.78	1123.5918	$C_{53}H_{90}O_{22}$	1.1	286.24	+HCOO	1077.5837,945.5420,783.4892,765.4792,621.4363,459.3836,375.2907	PPD-3Glc-Xyl		√	√
195	16.79	1251.6357[b]	$C_{60}H_{100}O_{27}$	-1.8	387.09	-H, +HCOO	1251.6425,1209.6256,1077.5837,945.5420,783.4892,621.4363,459.3835,375.2907	PPD-3Glc-2Xyl-Ace		√	√
196	16.87	1295.6315[b]	$C_{61}H_{100}O_{29}$	2.9	375.35	-H	1251.6383,1209.6275,1077.5852,945.5427,783.4902,621.4370,459.3844	PPD-3Glc-2Xyl-Mal		√	√
197	16.91	1123.5939	$C_{53}H_{90}O_{22}$	2.9	359.23	+HCOO	1077.5852,945.5427,783.4902,621.4370,375.2905	$C_{30}H_{52}O_3$-3Glc-Xyl			√

198	16.94	925.4814[a]	$C_{47}H_{74}O_{18}$	1.3	394.50	-H	925.4787,793.4375,631.3851,569.3842,455.3531	Chikusetsusaponin IV	√		
199	17.07	1163.5874[a]	$C_{56}H_{92}O_{25}$	1.6	364.03	-H	1119.5939,1077.5842,1059.5737,945.5427,783.4901,621.4373,459.3843,375.2908	Malonyl-Ginsenoside Rb2		√	
200	17.29	1209.6294	$C_{58}H_{98}O_{26}$	1.7	276.13	-H, +HCOO	1209.6267,1077.5845,945.5420,783.4897,621.4367,459.3840,375.2906	PPD-3Glc-2Xyl			√
201	17.33	1165.6051[b]	$C_{55}H_{92}O_{23}$	3.4	375.50	+HCOO	1077.5845,945.5421,783.4897,621.4367,459.3840	PPD-3Glc-Xyl-Ace			√
202	17.48	1077.5872	$C_{53}H_{90}O_{22}$	2.0	351.02	-H, +HCOO	1077.5839,945.5413,783.4890,621.4363,459.3838,375.2902	PPD-3Glc-Xyl	√	√	√
203	17.64	943.5295[a]	$C_{48}H_{80}O_{18}$	2.4	323.85	-H, +HCOO	943.5266,781.4741,619.4271,457.3687,373.2752	5,6-didehydro-Rd	√		
204	17.66	1153.6034	$C_{54}H_{92}O_{23}$	2.0	370.47	+HCOO	1107.5957,943.5266,781.4741,619.4220,457.3687,373.2752	5,6-didehydro PPD-4Glc	√		
205	17.70	1249.5892[b]	$C_{59}H_{94}O_{28}$	2.7	358.96	-H	1161.6066,1101.5851,927.5313,765.4798,621.4370,459.3842	PPD-3Glc-Xyl-Dimal			√
206	17.80	1059.5749	$C_{52}H_{86}O_{19}$	0.3	343.89	+HCOO	1059.5741,945.5422,783.4897,621.4368,459.3841,375.2906	PPD-3Glc-But		√	
207	17.85	1163.5877[b]	$C_{56}H_{92}O_{25}$	1.9	265.77	-H	1119.5945,1077.5845,1059.5741,945.5422,783.4897,621.4369,459.3841,375.2905	PPD-3Glc-Xyl-Mal		√	√
208	17.86	1119.5983[b]	$C_{55}H_{92}O_{23}$	2.3	217.61	-H	1119.5945,1077.5845,1059.5741,945.5422,783.4897,621.4369,459.3841,375.2905	PPD-3Glc-Xyl-Ace		√	
209	18.07	1163.5882	$C_{56}H_{92}O_{25}$	2.4	350.31	-H	1119.5955,1077.5847,1059.5748,945.5420,783.4902,621.4372,459.3844,375.2909	PPD-3Glc-Xyl-Mal			√
210	18.07	1119.5992[b]	$C_{55}H_{92}O_{23}$	3.2	219.45	-H	1119.5955,1077.5847,1059.5748,945.5420,783.4902,621.4372,459.3844	PPD-3Glc-Xyl-Ace			√
211	18.29	1163.5882[b]	$C_{56}H_{92}O_{25}$	2.3	203.41	-H	1119.5955,1077.5849,945.5430,783.4905,621.4371,459.3842	PPD-3Glc-Xyl-Mal			√
212	18.42	1163.5883	$C_{56}H_{92}O_{25}$	2.4	348.34	-H	1119.5957,1077.5854,1059.5749,945.5429,783.4904,621.4372,459.3844,375.2904	PPD-3Glc-Xyl-Mal			√
213	18.42	1119.5993[b]	$C_{55}H_{92}O_{23}$	3.2	215.84	-H	1119.5957,1077.5854,1059.5749,945.5429,783.4904,621.4372,459.3844	PPD-3Glc-Xyl-Ace			√
214	18.87	1195.6139[b]	$C_{56}H_{94}O_{24}$	1.8	362.14	+HCOO, -H	1107.5950,1089.5851,945.5429,783.4894,621.4371,459.3849	PPD-4Glc-Ace	√		
215	18.87	1165.6025[b]	$C_{55}H_{92}O_{23}$	1.1	378.08	+HCOO, -H	1119.5943,1077.5844,1059.5737,945.5419,783.4900,621.4369,459.3841,375.2902	PPD-3Glc-Xyl-Ace			√
216	18.88	1163.5864[b]	$C_{56}H_{92}O_{25}$	0.8	260.52	-H	1119.5943,1077.5844,1059.5737,945.5419,783.4900,621.4369,459.3841	PPD-3Glc-Xyl-Mal			√
217	18.96	1093.5833[b]	$C_{52}H_{88}O_{21}$	3.0	382.65	+HCOO	1047.5760,915.5353,621.4364,459.3835	PPD-2Glc-2Xyl		√	
218	19.00	1205.5982[b]	$C_{58}H_{94}O_{26}$	1.8	357.72	-H	1163.6129,1120.5979,1101.5846,945.5425,765.4787,621.4371,459.3838	PPD-3Glc-Xyl-Mal-Ace			√
219	19.01	1249.5877[b]	$C_{59}H_{94}O_{28}$	1.5	359.70	-H	1249.5856,1163.6129,1041.5627,945.5425,783.4900,621.4371,459.3838	PPD-3Glc-Xyl-Dimal			√
220	19.19	1119.5990[b]	$C_{55}H_{92}O_{23}$	3.0	365.47	-H	1119.5956,1077.5852,945.5434,783.4895,621.4368,459.3842,375.2904	PPD-3Glc-Xyl-Ace			√
221	19.22	793.4399[a]	$C_{42}H_{66}O_{14}$	2.5	365.00	-H	793.4376,631.3851,569.3850,455.3532	Chikusetsusaponin IVa	√		
222	19.23	1163.5876[b]	$C_{56}H_{92}O_{25}$	1.8	344.71	-H	1119.5946,1077.5843,1059.5747,945.5417,783.4899,621.4370,459.3842,375.2905	PPD-3Glc-Xyl-Mal		√	√
223	19.40	1163.5877	$C_{56}H_{92}O_{25}$	1.9	264.69	-H	1119.5955,1059.5741,945.5429,783.4900,621.4371,459.3842,375.2908	PPD-3Glc-Xyl-Ace			√

224	19.41	1221.6302[b]	$C_{58}H_{96}O_{24}$	2.3	378.90	+HCOO, -H	1107.5946,945.5445,783.4915,621.4377,459.3846	PPD-4Glc-But	√		
225	19.41	1119.5991[b]	$C_{55}H_{92}O_{23}$	3.1	217.15	-H	1119.5955,1059.5741,945.5428,783.4900,621.4371,459.3842,375.2908	PPD-3Glc-Xyl-Ace			√
226	19.66	1165.6019[b]	$C_{55}H_{92}O_{23}$	0.6	374.21	+HCOO, -H	1119.5946,1077.5849,1059.5745,945.5424,783.4903,621.4368,459.3843	PPD-3Glc-Xyl-Ace			√
227	19.67	1163.5872[b]	$C_{56}H_{92}O_{25}$	1.5	352.17	-H	1119.5946,1077.5849,1059.5742,945.5424,783.4903,621.4368,459.3843	PPD-3Glc-Xyl-Mal			√
228	19.84	1149.6087[b]	$C_{58}H_{94}O_{24}$	2.2	360.44	-H	1107.5955,1089.5849,945.5419,783.4900,765.4795,621.4371,459.3858,391.2846	PPD-4Glc-Ace	√		
229	19.90	1225.6245[b]	$C_{57}H_{96}O_{25}$	1.8	369.84	+HCOO	1179.6176,1047.5759,915.5336,753.4796,621.4370,459.3846,375.2906	PPD-2Glc-3Xyl		√	
230	19.91	1179.6196[b]	$C_{56}H_{92}O_{26}$	2.4	364.93	-H	1179.6176,1047.5759,915.5356,621.4370,459.3846	PPD-2Glc-3Xyl		√	
231	19.97	725.4499	$C_{38}H_{64}O_{10}$	2.4	337.73	+HCOO	679.4421,475.3791,391.2853	PPT-Glc-Ace	√		
232	20.03	1119.5986[b]	$C_{55}H_{92}O_{23}$	2.6	361.76	-H	1077.5857,945.5407,783.4900,765.4796,603.4259,475.3800	PPT-2Glc-Ace-Xyl-Rha		√	
233	20.03	1163.5877[b]	$C_{56}H_{92}O_{25}$	1.9	347.57	-H	1077.5857,945.5407,783.4900,603.4259,475.3800	PPT-2Glc-Mal-Xyl-Rha		√	
234	20.04	1295.6305[b]	$C_{61}H_{100}O_{29}$	2.1	367.96	-H	1251.6374,1209.6269,1077.5844,945.5423,784.4935,621.4363,459.3839,375.2899	PPD-3Glc-2Xyl-Mal			√
235	20.05	1119.5988[b]	$C_{55}H_{92}O_{23}$	2.8	518.05	-H	1077.5844,945.5423,783.4896,621.4364,459.3839	PPD-3Glc-Xyl-Ace			√
236	20.18	1163.5881[b]	$C_{56}H_{92}O_{25}$	2.2	282.67	-H	1119.5947,1077.5844,1059.5741,945.5423,783.4897,621.4368,459.3841,375.2902	PPD-3Glc-Xyl-Mal			√
237	20.19	1119.5988	$C_{55}H_{92}O_{23}$	2.8	360.81	-H	1119.5947,1077.5844,1059.5741,945.5423,783.4897,621.4368,459.3841,375.2902	PPD-3Glc-Xyl-Ace			√
238	20.19	1251.6390[b]	$C_{60}H_{100}O_{27}$	0.9	392.49	-H	1251.6369,1209.6269,1119.5947,1077.5844,1059.5741,945.5423,783.4897,621.4368, 459.3841,375.2902	PPD-3Glc-Xyl-Ace			√
239	20.27	1295.6313[b]	$C_{61}H_{100}O_{29}$	2.7	366.33	-H	1251.6370,1209.6270,1077.5845,945.5421,783.4899,621.4371,459.3841	PPD-3Glc-2Xyl-Mal			√
240	20.31	1163.5880[b]	$C_{56}H_{92}O_{25}$	2.2	497.17	-H	1077.5845,945.5422,783.4899,621.4371,459.3842	PPD-3Glc-Xyl-Mal			√
241	20.65	1205.6002[b]	$C_{58}H_{94}O_{26}$	3.4	364.70	-H	1163.6060,1077.5844,765.4798,603.4259,459.3843	PPD-3Glc-Xyl-Mal-Ace			√
242	20.65	1249.5889[b]	$C_{59}H_{94}O_{28}$	2.4	355.83	-H	1077.5844,1059.5738,765.4798,603.4259,459.3843	PPD-3Glc-Xyl-Dimal			√
243	20.70	1165.6026	$C_{55}H_{92}O_{23}$	1.3	425.59	+HCOO	1077.5844,765.4798,603.4259,459.3843	PPD-3Glc-Xyl-Ace			√
244	20.72	1163.5891[b]	$C_{56}H_{92}O_{25}$	3.1	371.93	-H	1119.5945,1077.5853,947.5484,783.4896,621.4367,459.3840	PPD-3Glc-Xyl-Mal		√	
245	20.76	945.5454[a]	$C_{48}H_{82}O_{18}$	2.7	54.61	-H	947.5490,783.4901,765.4790,621.4370,459.3844	Ginsenoside Rd	√	√	√
246	20.89	1119.5994[b]	$C_{55}H_{92}O_{23}$	3.3	372.52	-H	1119.5949,1077.5849,945.5424,783.4899,621.4373,459.3842	PPD-3Glc-Xyl-Ace			√
247	20.95	991.8427[b]	$C_{48}H_{82}O_{18}$	-0.3	337.86	+HCOO	945.5426,783.4900,621.4371,459.3843,375.2905	PPD-3Glc	√		
248	20.95	1249.5885[b]	$C_{59}H_{94}O_{28}$	2.1	358.69	-H	1163.6121,1119.5949,1077.5849,783.4899,621.4373,459.3841,375.2901	PPD-3Glc-Xyl-Dimal			√

249	20.96	1205.5998[b]	$C_{58}H_{94}O_{26}$	3.1	350.74	-H	1163.6121,1119.5949,1077.5849,783.4899,621.4373,459.3841,375.2901	PPD-3Glc-Xyl-Mal-Ace			√
250	21.11	725.4498[b]	$C_{38}H_{64}O_{10}$	2.3	285.52	+HCOO	679.4421,475.3791,391.2853	PPT-Glc-Ace	√		
251	21.24	1249.5879[b]	$C_{59}H_{94}O_{28}$	1.6	360.73	-H	1119.5949,1077.5839,1059.5740,783.4893,622.4408,459.3839	PPD-3Glc-Xyl-Dimal			√
252	21.40	1163.5868[b]	$C_{56}H_{92}O_{25}$	1.1	369.97	-H	1119.5940,1077.5834,1059.5729,945.5403,783.4893,621.4360,459.3838,375.2904	PPD-3Glc-Xyl-Mal		√	
253	21.48	1119.5972[b]	$C_{55}H_{92}O_{23}$	1.4	270.92	-H	1077.5833,945.5403,783.4930,621.4362,459.3838	PPD-3Glc-Xyl-Ace		√	
254	21.58	1205.5992[b]	$C_{58}H_{94}O_{26}$	2.6	352.96	-H	1163.6134,1119.5955,1077.5848,945.5425,783.4898,621.4371,459.3842	PPD-3Glc-Xyl-Mal-Ace			√
255	21.59	1249.5878[b]	$C_{59}H_{94}O_{28}$	1.5	365.61	-H	1249.5925,1163.6134,1119.5955,1059.5741,945.5425,783.4898,621.4371,459.3842	PPD-3Glc-Xyl-Dimal			√
256	21.79	1251.6364[b]	$C_{60}H_{100}O_{27}$	-1.2	379.58	-H	1209.6022,1077.5837,945.5412,783.4888,621.4362,459.3835,375.2903	PPD-3Glc-2Xyl-Ace		√	
257	21.84	987.5557	$C_{50}H_{84}O_{19}$	2.3	333.87	-H, +HCOO	987.5520,945.5421,783.4900,621.4369,459.3840,375.2903	PPD-3Glc-Ace	√		
258	21.85	1031.5445[a]	$C_{51}H_{84}O_{21}$	1.2	342.00	-H	945.5412,783.4888,621.4362,459.3835,375.2901	Malonyl-Ginsenoside Rd	√	√	
259	21.91	1249.5879[b]	$C_{59}H_{94}O_{28}$	1.6	281.54	-H	1077.5842,1059.5734,945.5422,783.4901,621.4367,459.3841	PPD-3Glc-Xyl-Dimal			√
260	21.93	1205.5991[b]	$C_{58}H_{94}O_{26}$	2.5	239.91	-H	1077.5842,945.5425,783.4901,621.4367,459.3841	PPD-3Glc-Xyl-Mal-Ace			√
261	21.98	1119.5966[b]	$C_{55}H_{92}O_{23}$	0.9	365.43	-H	1119.5939,1077.5845,1059.5738,915.5313,783.4887,621.4364,460.3871	$C_{30}H_{52}O_3$-3Glc-Xyl-Ace		√	√
262	21.98	1163.5869[b]	$C_{56}H_{92}O_{25}$	1.2	344.71	-H	1119.5939,1077.5845,1059.5738,915.5313,783.4887,621.4364,460.3871	$C_{30}H_{52}O_3$-3Glc-Xyl-Mal		√	
263	22.03	1251.6385[b]	$C_{59}H_{96}O_{28}$	0.5	386.55	-H, +HCOO	1251.6368,1209.6022,1077.5846,915.5318,783.4887,621.4363,375.2905	$C_{30}H_{52}O_3$-3Glc-2Xyl-Ace		√	√
264	22.06	1249.5884[b]	$C_{59}H_{94}O_{28}$	2.0	363.63	-H	1249.5638,1163.6125,1119.5947,1077.5846,783.4900,621.4366,459.3840	PPD-3Glc-Xyl-Dimal			√
265	22.07	1205.5991[b]	$C_{58}H_{94}O_{26}$	2.5	349.87	-H	1163.6125,1119.5947,1077.5846,783.4900,621.4366,459.3840	PPD-3Glc-Xyl-Mal-Ace			√
266	22.31	1031.5453	$C_{51}H_{84}O_{21}$	2.0	325.52	-H	987.5527,945.5424,783.4898,621.4368,459.3842,375.2905	PPD-3Glc-Mal		√	√
267	22.31	987.5566	$C_{50}H_{84}O_{19}$	3.3	518.73	-H	987.5529,945.5423,927.5316,783.4903,621.4370,459.3841,375.2899	PPD-3Glc-Ace	√		√
268	22.64	987.5562	$C_{50}H_{84}O_{19}$	2.8	481.66	-H	987.5530,945.5422,783.4909,621.4375,459.3842,375.2908	PPD-3Glc-Ace	√		
269	22.65	1031.5455	$C_{51}H_{84}O_{21}$	2.2	250.43	-H	987.5530,945.5422,783.4909,621.4375,459.3842,375.2908	PPD-Mal-3Glc	√	√	√
270	22.72	1165.6039[b]	$C_{55}H_{92}O_{23}$	2.4	366.16	+HCOO	1119.5923,1077.5852,945.5414,783.4906,621.4372,459.3844,375.2913	PPD-3Glc-Xyl-Ace		√	
271	22.98	1117.5468	$C_{54}H_{86}O_{24}$	2.8	340.02	-H	945.5431,783.4898,621.4377,459.3843,375.2907	PPD-3Glc-Dimal			√
272	22.98	1075.5698[b]	$C_{52}H_{86}O_{20}$	0.3	359.00	+HCOO	1029.5662,987.5543,945.5431,783.4898,621.4377,459.3843,375.2907	PPD-3Glc-2Ace			√
273	22.99	1073.5576[b]	$C_{53}H_{86}O_{22}$	3.5	353.13	-H	987.5579,945.5441,783.4910,621.4371,537.3444,459.3848	PPD-3Glc-Ace-Mal	√		
274	23.07	1165.6038[b]	$C_{55}H_{92}O_{23}$	2.3	362.60	+HCOO, -H	1119.5948,1077.5853,945.5425,783.4903,621.4367,459.3848,375.2906	PPD-3Glc-Xyl-Ace		√	

275	23.30	987.5546	$C_{50}H_{84}O_{19}$	1.2	333.94	-H	987.5520,784.4945,621.4380,475.3795,391.2857	PPT-2Glc-Rha		√	
276	23.34	1133.5772[b]	$C_{55}H_{90}O_{24}$	2.0	346.61	-H	987.5533,945.5422,765.4789,603.4271,459.3845，375.2908	PPD-3Glc-Rha-Ace			√
277	23.35	1033.5604[b]	$C_{50}H_{84}O_{19}$	1.5	347.65	+HCOO, -H	987.5533,945.5422,927.5311,783.4894,579.2841,459.3845,375.2908	PPD-3Glc-Ace			√
278	23.37	991.5507[a]	$C_{48}H_{82}O_{18}$	2.4	326.84	+HCOO, -H	945.5422,927.5311,783.4894,621.4372,459.3846,375.2908	Notoginsenoside K	√	√	√
279	23.40	1119.5936[b]	$C_{55}H_{92}O_{23}$	-1.8	369.69	-H	1119.5949,1077.5843,945.5422,783.4897,621.4372,459.3846	PPD-3Glc-Xyl-Ace			√
280	23.44	683.4393	$C_{36}H_{62}O_{9}$	2.5	442.02	+HCOO	637.4311,475.3793,391.2854	PPT-Glc	√		
281	23.52	1047.5771	$C_{52}H_{88}O_{21}$	2.4	484.94	-H	1047.5745,915.5330,783.4911,621.4378,459.3689,375.2905	PPD-2Glc-2Xyl	√	√	√
282	23.61	1117.5462[b]	$C_{54}H_{86}O_{24}$	2.3	258.33	-H	1031.5709,945.5432,783.4905,621.4373,459.3845,375.2907	PPD-3Glc-Dimal			√
283	23.61	1075.5715[b]	$C_{52}H_{86}O_{20}$	1.9	297.73	+HCOO	1029.5644,987.5538,945.5432,783.4905,621.4373,459.3845,375.2907	PPD-3Glc-2Ace			√
284	23.78	1031.5452	$C_{51}H_{84}O_{21}$	1.9	339.21	-H	945.5424,783.4892,621.4368,459.3841,375.2908	PPD-3Glc-Mal		√	
285	23.85	987.5562	$C_{50}H_{84}O_{19}$	2.8	338.30	-H	987.5593,945.5430,927.5316,783.4898,621.4375,459.3845	PPD-3Glc-Ace	√		
286	23.87	945.5425	$C_{48}H_{82}O_{18}$	-0.4	320.70	-H	945.5420,783.4892,621.4366,459.3841	PPD-3Glc		√	
287	23.87	1205.5994[b]	$C_{58}H_{94}O_{26}$	2.8	349.20	-H	1119.5990,1077.5865,945.5445,783.4907,621.4377,459.3846,375.2896	PPD-3Glc-Xyl-Mal-Ace			√
288	23.88	1221.6302[b]	$C_{58}H_{96}O_{24}$	2.3	370.63	+HCOO, -H	1107.5923,945.5430,783.4898,621.4375,459.3845,375.2907	PPD-4Glc-But	√		
289	23.92	961.5396	$C_{47}H_{80}O_{17}$	1.9	328.34	+HCOO	915.5317,783.4898,621.4375,459.3845,375.2907	PPD-2Glc-Xyl	√		
290	23.94	1093.5826	$C_{52}H_{88}O_{21}$	2.3	340.89	+HCOO	915.5317,783.4900,621.4375,459.3845,375.2907	PPD-2Glc-2Xyl	√		
291	24.15	991.5506	$C_{48}H_{82}O_{18}$	2.3	333.46	+HCOO	945.5440,783.4915,621.4372,459.3839	PPD-3Glc	√		
292	24.15	1075.5692[b]	$C_{52}H_{86}O_{20}$	-0.2	354.03	+HCOO	1029.5636,987.5512,945.5436,765.4794,621.4368,459.3838,375.2909	PPD-3Glc-2Ace			√
293	24.34	1205.5990[b]	$C_{58}H_{94}O_{26}$	2.4	350.70	-H	1119.5951,1077.5865,1059.5747,783.4907,621.4377,459.3845	PPD-3Glc-Xyl-Mal-Ace			√
294	24.55	961.5395[a]	$C_{47}H_{80}O_{17}$	1.8	247.30	+HCOO	915.5312,783.4893,621.4364,459.3841	Notoginsenoside Fe	√	√	√
295	24.61	1029.5298	$C_{50}H_{80}O_{19}$	2.1	334.28	+HCOO	915.5323,783.4912,621.4370,537.3432,459.3844,375.2901	PPD-2Glc-Xyl-But	√		
296	24.66	1093.5827[b]	$C_{52}H_{88}O_{21}$	2.5	345.54	+HCOO	1047.5747,784.4939,621.4364,441.3727	$(C_{30}H_{50}O_2+H_2O)$-2Glc-2Xyl		√	
297	24.70	1031.5454	$C_{51}H_{84}O_{21}$	2.1	319.98	-H	927.5313,765.4777,603.4266,459.3841	PPD-3Glc-Mal			√
298	24.77	961.5398	$C_{47}H_{80}O_{17}$	2.1	328.42	+HCOO, -H	915.5315,783.4904,621.4371,459.3839,375.2901	PPD-2Glc-Xyl	√	√	√
299	24.78	1029.5303[b]	$C_{50}H_{80}O_{19}$	2.6	333.45	+HCOO	915.5313,783.4893,622.4407,459.3837,375.2905	PPD-2Glc-Xyl-But	√		
300	24.89	767.4590	$C_{40}H_{66}O_{11}$	0.3	299.89	+HCOO, -H	721.4552,679.4437,475.3792,391.2855	PPT-Glc-2Ace		√	

301	24.90	811.4607	$C_{46}H_{68}O_{12}$	-3.8	292.55	-H	517.3900,475.3791,391.2845	PPT-Glc-Ace-Xyl	√		
302	24.98	1221.6293[b]	$C_{58}H_{96}O_{24}$	1.6	367.52	+HCOO	1107.5972,945.5344,783.4917,621.4373,459.3839,375.2907	PPD-4Glc-But	√		
303	25.00	1191.6195[b]	$C_{57}H_{94}O_{23}$	2.2	362.20	+HCOO, -H	1077.5877,915.5336,783.4908,621.4380,459.3842,375.2905	PPD-3Glc-Xyl-But			√
304	25.02	1001.5357[b]	$C_{50}H_{82}O_{20}$	3.0	334.15	-H	915.5336,783.4908,621.4380,459.3842,375.2905	PPD-2Glc-Xyl-Mal	√	√	√
305	25.03	957.5448[b]	$C_{49}H_{82}O_{18}$	2.0	329.17	-H	915.5338,783.4917,621.4373,459.3838,375.2907	PPD-2Glc-Xyl-Ace	√	√	
306	25.13	1277.6567	$C_{62}H_{102}O_{27}$	2.4	434.32	-H, +HCOO	1209.6310,1077.5855,945.5432,783.4900,621.4372,459.3842,375.2905	PPD-4Glc-Xyl-But			√
307	25.14	751.4657	$C_{41}H_{70}O_{12}$	2.6	433.46	-H	751.4629,619.4203,457.3685	5,6-didehydro-PPD-Glc-Xyl	√		
308	25.16	957.5460[b]	$C_{49}H_{82}O_{18}$	3.3	329.55	-H	957.5399,915.5333,784.4936,619.4201,457.3809	5,6-didehydro-PPD-2Glc-Xyl-Ace	√		
309	25.18	1001.5349[b]	$C_{50}H_{82}O_{20}$	2.2	326.60	-H	783.4900,621.4372,459.3842,375.2911	PPD-2Glc-Xyl-Mal	√		√
310	25.26	961.5397	$C_{47}H_{80}O_{17}$	2.1	248.56	+HCOO	915.5315,783.4898,621.4370,459.3835	PPD-2Glc-Xyl		√	
311	25.39	1001.5345[b]	$C_{50}H_{82}O_{20}$	1.8	317.27	-H	783.4899,621.4371,459.3836	PPD-2Glc-Xyl-Mal			√
312	25.41	1003.5478[b]	$C_{49}H_{82}O_{18}$	-0.5	337.08	+HCOO	957.5405,825.5013,783.4899,621.4371,459.3837,375.2900	PPD-2Glc-Xyl-Ace			√
313	25.52	1029.5286[b]	$C_{50}H_{80}O_{19}$	1.0	350.28	+HCOO	915.5305,783.4895,621.4364,459.3835,375.2900	PPD-2Glc-Xyl-But		√	
314	25.53	961.5393[a]	$C_{47}H_{80}O_{17}$	1.6	325.43	+HCOO, -H	915.5305,783.4895,621.4364,459.3835,375.2900	Notoginsenoside Fd		√	
315	25.61	1093.5815	$C_{52}H_{88}O_{21}$	1.4	342.85	+HCOO	1047.5731,783.4895,621.4364,459.3837,375.2896	PPD-2Glc-2Xyl		√	
316	25.62	1003.5491[b]	$C_{49}H_{82}O_{18}$	0.8	341.82	+HCOO	957.5409,915.5320,783.4914,621.4376,459.3839,375.2906	PPD-2Glc-Xyl-Ace	√		√
317	25.62	1001.5343[b]	$C_{50}H_{82}O_{20}$	1.6	341.28	-H	825.4999,783.4897,621.4366,459.3837	PPD-2Glc-Ace-GlurA			√
318	25.68	1107.5979[b]	$C_{53}H_{90}O_{21}$	2.0	408.50	+HCOO	1061.5937,929.5486,783.4897,621.4366,459.3837	PPD-2Glc-Xyl-Rha			√
319	25.97	1087.5353	$C_{53}H_{84}O_{23}$	2.0	336.89	-H	915.5311,783.4901,621.4371,459.3843,375.2907	PPD-2Glc-Xyl-Dimal		√	√
320	26.01	1001.5347[b]	$C_{50}H_{82}O_{20}$	2.0	331.85	-H	915.5332,783.4899,621.4363,459.3845,375.2911	PPD-2Glc-Xyl-Mal		√	√
321	26.01	1003.5486[b]	$C_{49}H_{82}O_{18}$	0.3	333.88	+HCOO	957.5432,915.5311,783.4900,621.4368,459.3843,375.2907	PPD-2Glc-Xyl-Ace		√	√
322	26.05	1191.6193	$C_{57}H_{94}O_{23}$	2.1	379.16	+HCOO, -H	1077.5853,915.5311,783.4900,621.4368,459.3842,375.2911	PPD-3Glc-Xyl-But			√
323	26.41	1001.5344[b]	$C_{50}H_{82}O_{20}$	1.7	258.13	-H	915.5324,621.4367,459.3843,375.2903	PPD-2Glc-Xyl-Mal		√	√
324	26.59	1001.5339[b]	$C_{50}H_{82}O_{20}$	1.2	318.73	-H	783.4883,621.4373,459.3845,375.2903	PPD-2Glc-Xyl-Mal		√	√
325	26.59	1003.5459[b]	$C_{49}H_{82}O_{18}$	-2.4	334.77	+HCOO	957.5428,915.5314,897.5209,783.4887,621.4370,459.3837,375.2903	PPD-2Glc-Xyl-Ace			√
326	26.66	975.5544	$C_{48}H_{82}O_{17}$	1.1	389.91	+HCOO, -H	929.5478,783.4876,621.4367,459.3839,375.2902	PPD-2Glc-Rha	√	√	√

327	27.13	961.5392[a]	$C_{47}H_{80}O_{17}$	1.5	331.58	+HCOO	915.5320,783.4893,621.4365,459.3841,375.2908	Notoginsenoside Ft1		√	
328	27.15	829.4962[a]	$C_{42}H_{72}O_{13}$	0.8	310.29	+HCOO	783.4874,731.4373,621.4362,551.3735,459.3836	Ginsenoside F2	√	√	

[a]: The components confirmed by comparison with the reference standards.

[b]: The components identified manually based on the MS information as no matching in the in-house library (not reported).

R: roots, SL: stems/leaves, F: flower buds.

√: The components identified in a part of *Panax notoginseng*

Mal: The components identified with a single malonyl substituent.

Dimalonyl: The components identified with two malonyl substituents.

Ace: The components identified with an acetyl substituent.

But: The components identified with a butenoyl substituent.

Table S5 Detailed information of 27 potential marker compounds diagnostic for differentiating among PNR. PNL, and PNF.

No.	VIP	t_R (min)	*m/z*	Assignment	CCS (Å^2)	MS^2 fragments	Identification
M1[a]	13.38	12.24	576.2968	$[M–2H+HCOOH]^{2–}$	423.55	1107.5985,945.5395,783.4784, 621.4359,459.3993,375.2926	ginsenoside Rb1
M2[a]	9.10	16.58	1123.5912	$[M–H+HCOOH]^{–}$	362.96	1077.5892,945.5406,783.4970, 621.4398,459.3781,375.2905	ginsenoside Rb3
M3[a]	8.81	13.95	627.3125	$[M–2H+HCOOH]^{2–}$	441.81	1209.6719,1077.5801,945.5423,783.4715, 621.4488,459.3777,375.2903	ginsenoside Ra1
M4[a]	7.21	10.73	642.3179	$[M–2H+HCOOH]^{2–}$	451.27	1239.6358,1107.5961,945.5424, 783.4921,621.4356.459.3818	notoginsenoside Fa
M5	7.03	11.95	627.3126	$[M–2H+HCOOH]^{2–}$	441.81	1210.6379,1077.5839,945.5434,783.5068, 621.4454,459.3803,375.2877	chikusetsusaponin FK4 or isomer
M6[a]	6.63	20.78	945.5432	$[M–H]^{–}$	331.48	945.5354,783.4889,621.4358, 459.3911,375.2876	ginsenoside Rd
M7[a]	6.62	13.81	561.2915	$[M–2H+HCOOH]^{2–}$	414.29	1077.5800,945.5476,783.4893, 621.4456,459.3859,375.2927	ginsenoside Rc
M8[a]	6.30	11.68	683.4381	$[M–H+HCOOH]^{–}$	283.79	683.4361,637.4287,475.4772,391.2901	20(*S*)-ginsenoside Rh1
M9	6.08	6.46	569.2890	$[M–2H+HCOOH]^{2–}$	409.31	1093.5817,961.5460,799.4857, 637.4294,475.3794	floralginsenoside P or isomer
M10	5.99	16.21	582.2968	$[M:]^{2–}$	423.41	1119.6089,1077.5890,945.5466, 783.4909,621.4309,459.3786	m-Rb3 or isomer
M11	5.68	17.22	1255.6331	$[M–H+HCOOH]^{–}$	367.33	1077.5849,945.5349,783.5016,621.4278, 459.4003	notoginsenoside Fc or isomer
M12	5.66	2.88	609.1465	/	231.03	609.1448,285.0389,255.0282,227.0343	kaempferol-2Glc

M13[a]	5.52	15.77	1123.5913	$[M–H+HCOOH]^-$	365.78	1123.5304,1077.5877,945.5410,783.4947, 621.4418,459.3927,375.2911	ginsenoside Rb2
M14	5.36	17.78	1165.5980	isotope peak of *m/z* 1163.5891	368.19	1077.5826,945.5394,783.4866,621.4321, 459.3837	m-Rb3 or isomer
M15[a]	5.23	10.25	815.4805	$[M–H+HCOOH]^-$	305.89	769.4738,637.4329,475.3793,391.2843	20(S)-notoginsenoside R2
M16[a]	5.19	14.57	693.3336	$[M–2H+HCOOH]^{2-}$	450.19	1077.5723,945.5231,783.4909,621.4246, 459.3758	notoginsenoside S
M17[a]	5.05	12.13	619.3151	$[M–2H]^{2-}$	451.79	1077.5880,945.5295,783.4737,621.4483, 459.3883	ginsenoside Ra3
M18	4.78	2.36	625.1414	/	233.27	625.1389,300.0269,271.0235,255.0283	quercetin-2Glc
M19	4.72	13.22	725.4485	$[M–H+HCOOH]^-$	288.44	725.4465,679.4378,637.4417,475.3846	20(*S*)-ginsenoside-Rh1-6'-acetate or isomer
M20[a]	4.70	11.40	829.4960	$[M–H+HCOOH]^-$	308.40	783.4881,637.4320,475.3772,391.2826	ginsenoside Rg2
M21[a]	4.66	14.96	1165.5972	isotope peak of *m/z* 1163.5844	365.36	1077.5747,945.5360,783.4906,621.4324, 459.3867	malonyl-ginsenoside Rc
M22[a]	4.61	4.71	847.4977	isotope peak of *m/z* 845.7562	302.78	845.4884,799.4858,637.4326,475.3795, 391.2825	ginsenoside Rg1
M23	4.26	15.36	582.2969	$[M:]^{2-}$	423.41	1119.5937,1077.5841,945.5383,783.4884, 621.4354,459.3844	m-Rb3 or isomer
M24[a]	4.18	9.76	642.3179	$[M–2H+HCOOH]^{2-}$	441.48	1239.6371,1107.5947,1077.5862,945.5432, 783.4886,621.4362,459.3848	notoginsenoside R4
M25	4.12	5.61	635.3101	$[M–2H+HCOOH]^{2-}$	436.75	1225.6201,1093.5805,961.5388,799.4847, 781.4737,637.4315,475.3790	chikusetsusaponin LM6 or isomer
M26	4.12	6.07	635.3099	$[M–2H+HCOOH]^{2-}$	436.75	1225.6187,1093.5783,961.5397,799.4840, 781.4732,637.4309,475.3786,375.2905	chikusetsusaponin LM6 or isomer

M27	4.03	10.85	977.5334	[M–H+HCOOH]$^-$	328.37	977.5291,931.5270,799.4940,637.4291, 475.3757	quinquenoside or isomer

[a]: the ginsenosides identified by comparing with the reference compounds.

Table S6 Method validation results for the UHPLC/UV approach enabling the quantitative assay of five ginsenosides.

(1) Linear regression data, limits of detection (LOD) and limits of quantification (LOQ) for five analytes

Ginsenoside	Calibration curves	Linear ranges (μg/mL)	LOD (μg /mL)	LOQ (μg /mL)	Correlation coefficients (r^2)
Noto-R1	y = 3.1054x + 18.903	34−12200	8.59	34.38	0.9996
G-Rg1	y = 3.3256x + 49.257	56−17200	14.06	56.25	0.9993
G-Rb1	y = 2.6927x + 8.7221	95−16080	23.75	47.50	0.9997
G-Rb2	y = 2.8777x−114.029	65−12080	16.25	65.00	0.9996
G-Rb3	y = 2.619x + 1.4327	127−14060	31.72	63.44	0.9998

(2) Precision results (n=3)

Ginsenoside	Content (μg/mL)					
	Day1	Day2	Day3		Inter-day RSD (%)	Intra-day (Day3) RSD (%)
Noto-R1	453.72	460.13	458.75	460.84	1.40	0.89
	447.03	456.49	465.83	454.85		
	446.38	455.98	461.39	455.50		
G-Rg1	1324.53	1323.14	1330.18	1352.58	1.23	0.70
	1305.04	1328.31	1345.66	1328.01		
	1293.34	1315.41	1339.50	1343.80		
G-Rb1	983.17	984.36	995.02	1017.08	0.99	0.93
	985.14	1003.45	1000.92	1003.89		
	981.94	980.20	1003.89	989.63		
G-Rb2	404.92	411.90	423.93	420.69	2.10	2.64
	403.39	414.47	398.04	424.45		
	400.43	417.70	405.47	419.55		
G-Rb3	759.44	762.38	768.64	783.84	0.43	1.55
	759.59	764.90	759.97	787.35		
	758.14	762.00	762.57	762.07		

(3) Repeatability results (n=6).

NO.	Content (μg/mL)				
	Noto-R1	G-Rg1	G-Rb1	G-Rb2	G-Rb3
1	73.55	214.41	371.77	151.66	440.35
2	74.16	212.61	376.45	156.28	451.50
3	69.75	219.94	366.54	154.37	437.41
4	69.36	220.42	379.17	148.53	441.84
5	73.03	215.34	377.01	145.02	456.54
6	70.26	214.38	370.40	149.23	443.74
RSD（%）	2.96	1.49	1.28	2.73	1.64

(4) Stability results.

Time (h)	Content (μg/mL)				
	Noto-R1	G-Rg1	G-Rb1	G-Rb2	G-Rb3
0	70.55	218.53	375.67	140.78	437.98
3	69.49	209.78	371.89	140.26	453.44
6	74.84	213.45	371.55	148.64	453.33
9	72.36	208.58	375.12	144.64	440.46
12	74.22	212.52	374.49	146.48	439.16
24	72.23	210.83	385.44	145.61	440.80
48	74.68	208.82	374.19	150.16	454.02
RSD (%)	2.87	1.64	1.24	2.55	1.69

(5) Recovery results (n=3).

Analyte	Original amount (μg)	Added amount (μg)	Measured Amount (μg)	Average recovery (%)	RSD (%)
Noto-R1	346.81	152.22	485.92	98.72	6.44
	346.81	152.22	501.05		
	346.81	152.22	504.27		
	346.81	304.44	665.28	102.50	2.96
	346.81	304.44	662.71		
	346.81	304.44	648.54		
	346.81	456.65	767.36	96.33	4.46
	346.81	456.65	784.75		
	346.81	456.65	807.94		
G-Rg1	977.40	540.00	1484.07	100.46	5.75
	977.40	540.00	1539.40		
	977.40	540.00	1536.09		
	977.40	1080.00	2010.89	98.00	3.22
	977.40	1080.00	2075.54		
	977.40	1080.00	2020.82		
	977.40	1620.00	2611.39	97.44	3.13
	977.40	1620.00	2544.33		
	977.40	1620.00	2512.16		
G-Rb1	1840.08	865.44	2712.44	101.56	3.17
	1840.08	865.44	2749.57		
	1840.08	865.44	2694.98		
	1840.08	1730.89	3594.08	101.80	1.25
	1840.08	1730.89	3627.13		
	1840.08	1730.89	3585.17		
	1840.08	2596.33	4440.07	99.33	0.94
	1840.08	2596.33	4424.47		
	1840.08	2596.33	4392.54		
G-Rb2	754.18	390.00	1109.32	94.81	7.50
	754.18	390.00	1155.88		
	754.18	390.00	1106.54		
	754.18	780.00	1551.34	101.64	5.54
	754.18	780.00	1588.52		
	754.18	780.00	1500.95		

	754.18	1170.00	1983.28		
	754.18	1170.00	2016.29	104.63	3.33
	754.18	1170.00	1935.33		
	2137.33	1097.20	3218.66		
	2137.33	1097.20	3292.74	100.31	4.39
	2137.33	1097.20	3202.24		
	2137.33	2194.40	4218.66		
G-Rb3	2137.33	2194.40	4266.77	94.95	2.05
	2137.33	2194.40	4177.04		
	2137.33	3291.60	5424.08		
	2137.33	3291.60	5316.03	97.59	1.96
	2137.33	3291.60	5309.15		

Table S7 Results for the quantitative assays of five ginsenosides among 45 batches of *P. notoginseng* samples.

Sample	Content (mg/g)				
	Noto-R1	**G-Rg1**	**G-Rb1**	**G-Rb2**	**G-Rb3**
PNR-1	14.25	28.12	20.78	-	-
PNR-2	8.07	31.08	21.88	-	-
PNR-3	6.42	27.54	24.34	-	-
PNR-4	8.70	31.32	24.21	-	-
PNR-5	5.72	32.41	28.26	-	-
PNR-6	8.93	26.30	21.40	-	-
PNR-7	8.25	29.21	21.28	-	-
PNR-8	6.59	27.03	24.01	-	-
PNR-9	6.46	28.50	18.76	-	-
PNR-10	5.56	23.21	18.67	-	-
PNR-11	6.02	28.35	19.82	-	-
PNR-12	5.73	25.82	21.51	-	-
PNR-13	11.89	46.09	36.30	-	-
PNR-14	10.86	47.67	41.64	-	-
PNR-15	11.65	43.54	32.64	-	-
PNL-1	-	-	3.26	2.80	14.61
PNL-2	-	-	2.48	2.79	15.94
PNL-3	-	-	2.87	3.00	17.37
PNL-4	-	-	2.60	3.47	22.10
PNL-5	-	-	3.31	4.04	23.63
PNL-6	-	-	3.14	2.65	13.77
PNL-7	-	-	1.88	0.56	1.88
PNL-8	-	-	3.07	3.58	19.77
PNL-9	-	-	2.36	1.27	6.66
PNL-10	-	-	1.97	1.30	6.70
PNL-11	-	-	2.81	4.29	27.02
PNL-12	-	-	3.31	4.07	24.85
PNL-13	-	-	4.75	5.10	29.85
PNL-14	-	-	1.91	2.40	13.77
PNL-15	-	-	2.95	2.05	11.49
PNF-1	0.31	-	22.35	10.93	32.81
PNF-2	0.66	-	20.08	11.51	35.97
PNF-3	-	-	24.30	14.72	48.34
PNF-4	-	-	17.09	10.77	32.65
PNF-5	1.11	-	11.93	7.02	23.76
PNF-6	-	-	21.67	13.50	41.90
PNF-7	-	-	15.92	10.51	33.58
PNF-8	-	-	19.83	13.01	39.94
PNF-9	1.86	-	15.42	11.20	35.04
PNF-10	1.97	-	14.00	10.02	30.56
PNF-11	-	-	16.03	10.63	34.37
PNF-12	-	-	10.53	7.14	23.69
PNF-13	-	-	13.42	9.26	29.63
PNF-14	1.11	-	9.01	5.45	18.37
PNF-15	-	-	16.21	9.51	26.63