

Supporting Information

Integration of ion-mobility high-resolution liquid chromatography/mass spectrometry-based untargeted metabolomics and desorption electrospray ionization-mass spectrometry imaging to unveil the ginsenosides variation induced by steaming for *Panax ginseng*, *P. quinquefolius* and *P. notoginseng*

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EXPERIMENTAL

Specific steaming steps of samples (taking PG as an example):

The specific evaporation steps of the sample were as follows: 1) washing: wash the soil and impurities on the surface of fresh ginseng with tap water and brush gently; 2) packing: washed ginseng medicinal materials wrapped in gauze into different small packages, 2/package, a total of 6 packages; 3) steaming: the packaged samples were placed in a pan with a caged drawer cloth, the temperature was set at 100°C, and the time was counted after water boiling. After steaming for 1 h, 2 h, 4 h, 6 h, 8 h, and 10 h, a package of PG was carefully removed; 4) drying: the steamed samples were taken out and dried in an oven at 60°C (lasting about 96 h), the raw samples were directly placed in a 45°C oven to dry after cleaning; 5) grinding: after drying, the sample was directly crushed by a crusher, through 60 mesh sieve, screening rate > 85%. PN and PQ were processed by the same method as PG, and 35 batches of samples were obtained for each medicinal material. 35 batches (105 batches: 35 × 3) of PG, PQ, and PN powder were stored in a dry and cool place for subsequent experiments.

Sample preparation of DESI-MSI:

Preparation of samples for mass spectrometry imaging: 1) samples with different steaming times were cut into small sections of about 1.5 cm from roughly the same position in the middle of the main root, and frozen at -80°C for about 10 min; 2) use the embedding medium (tissue freezing medium) to fix the sample axially on the sample holder of the appropriate size matched with the cryostat microtome (Leica CM3050 S, Leica Biosystems Nussloch GmbH, Germany), and the samples were cut into tissue sections with a thickness of 40 μm at -18°C; 3) tissue sections were slowly attached to the surface of an indium tin oxide (ITO)-coated glass slide (Bruker Daltonics, Bremen, Germany), take photos and save them as “tiff” files, then place the slides in a 4°C freezer until the data is scanned.

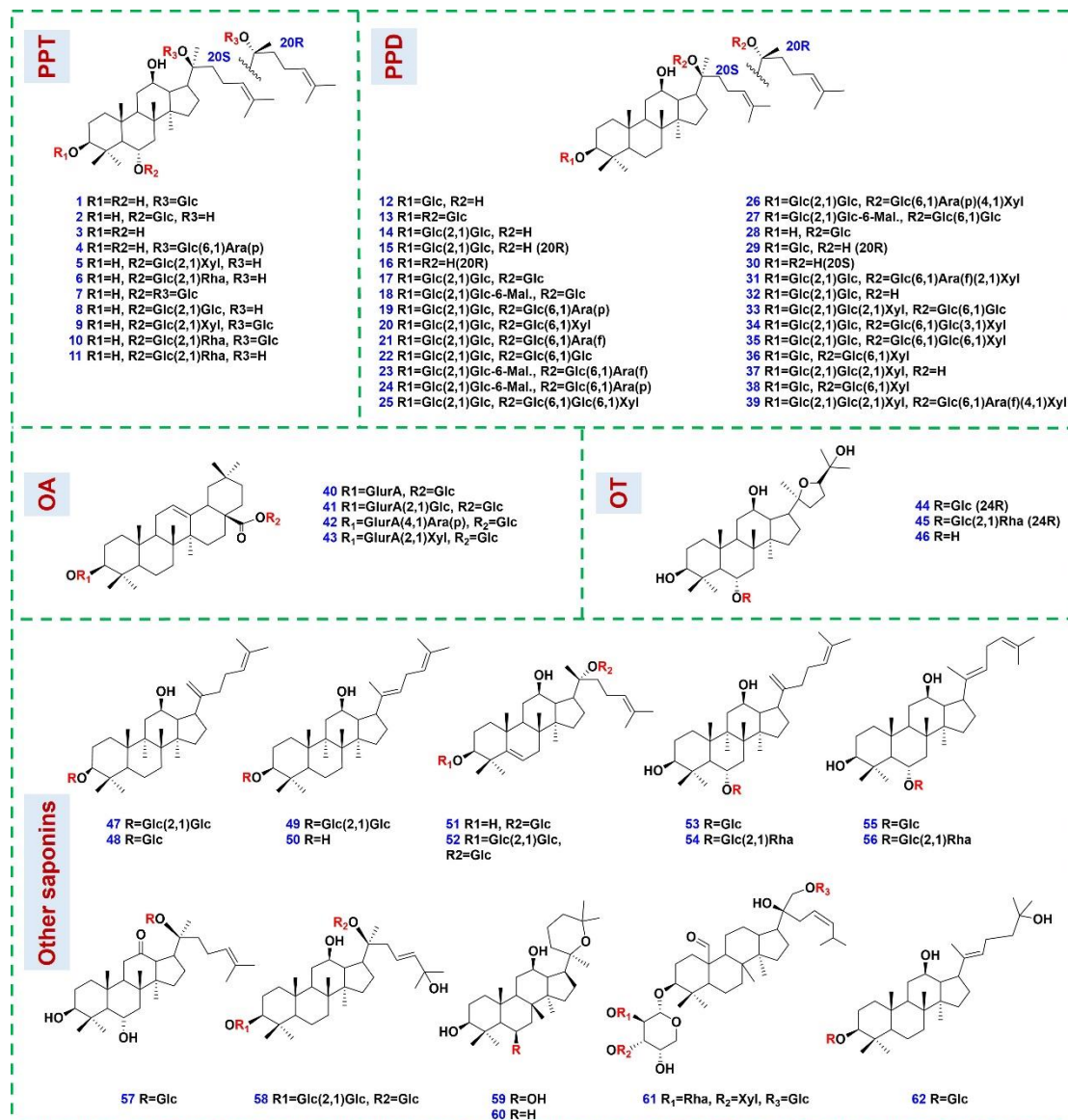


Figure S1 Chemical structures of 62 reference compounds of ginsenosides.

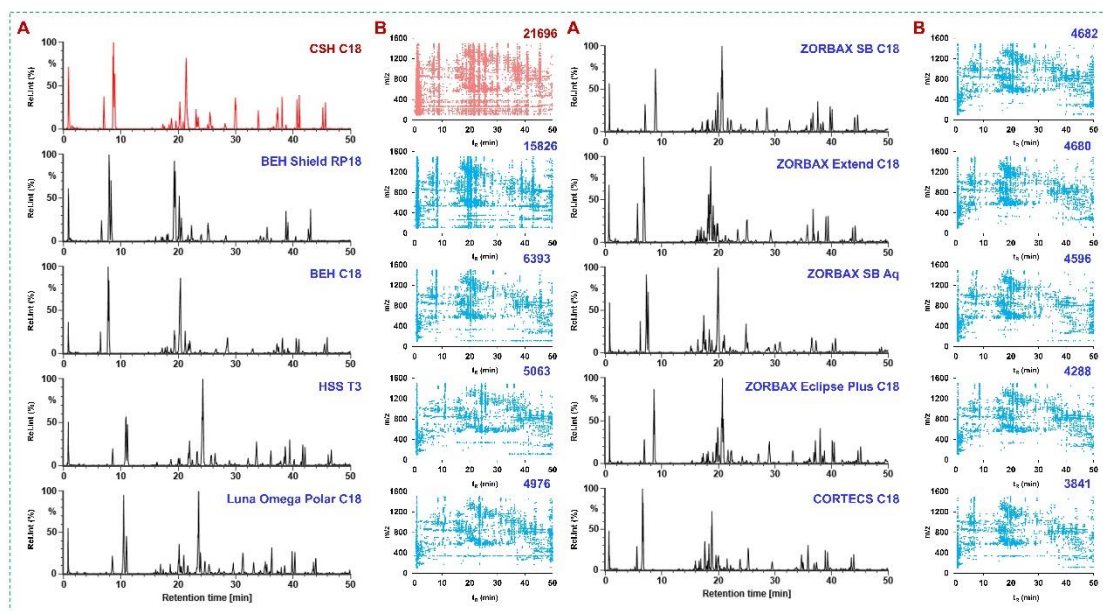


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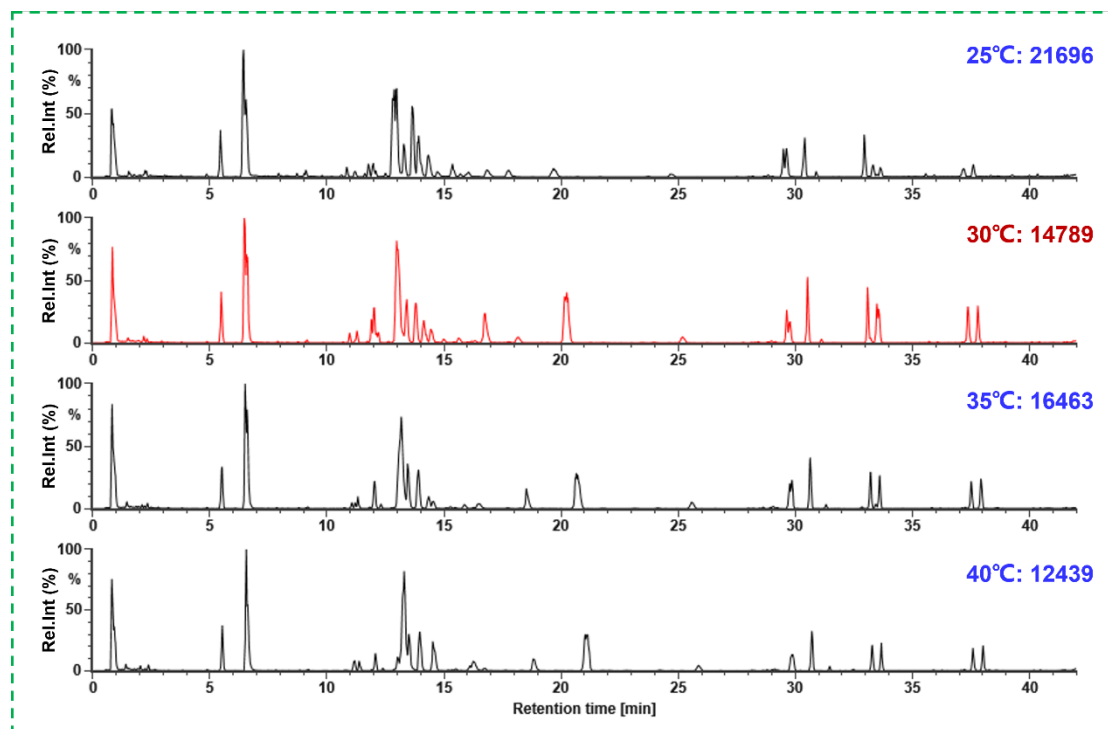


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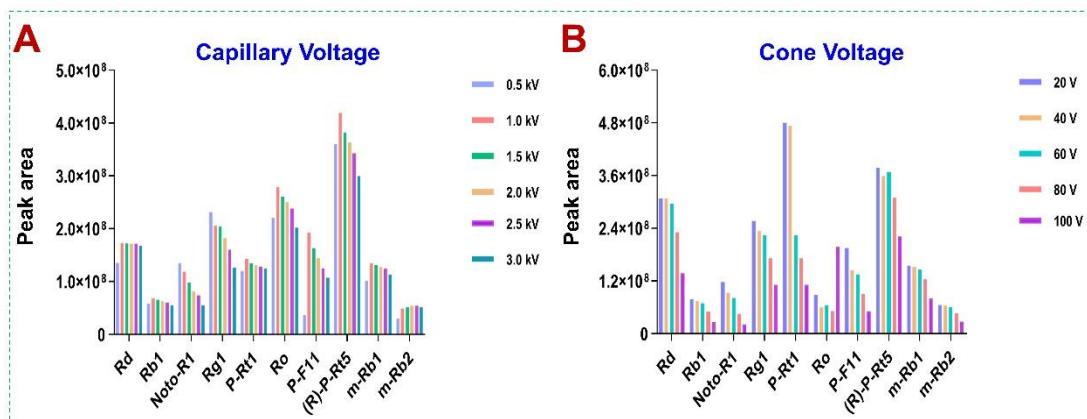


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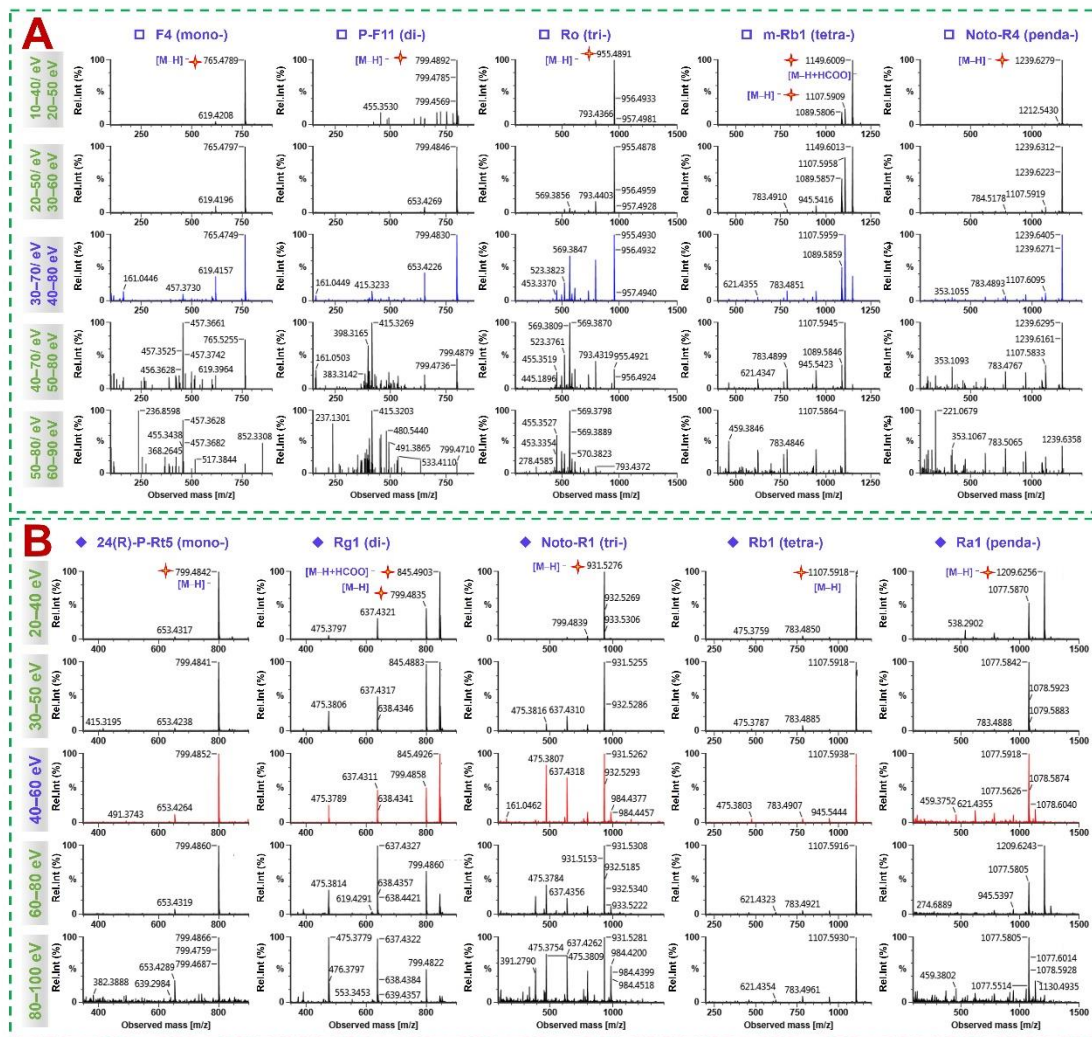


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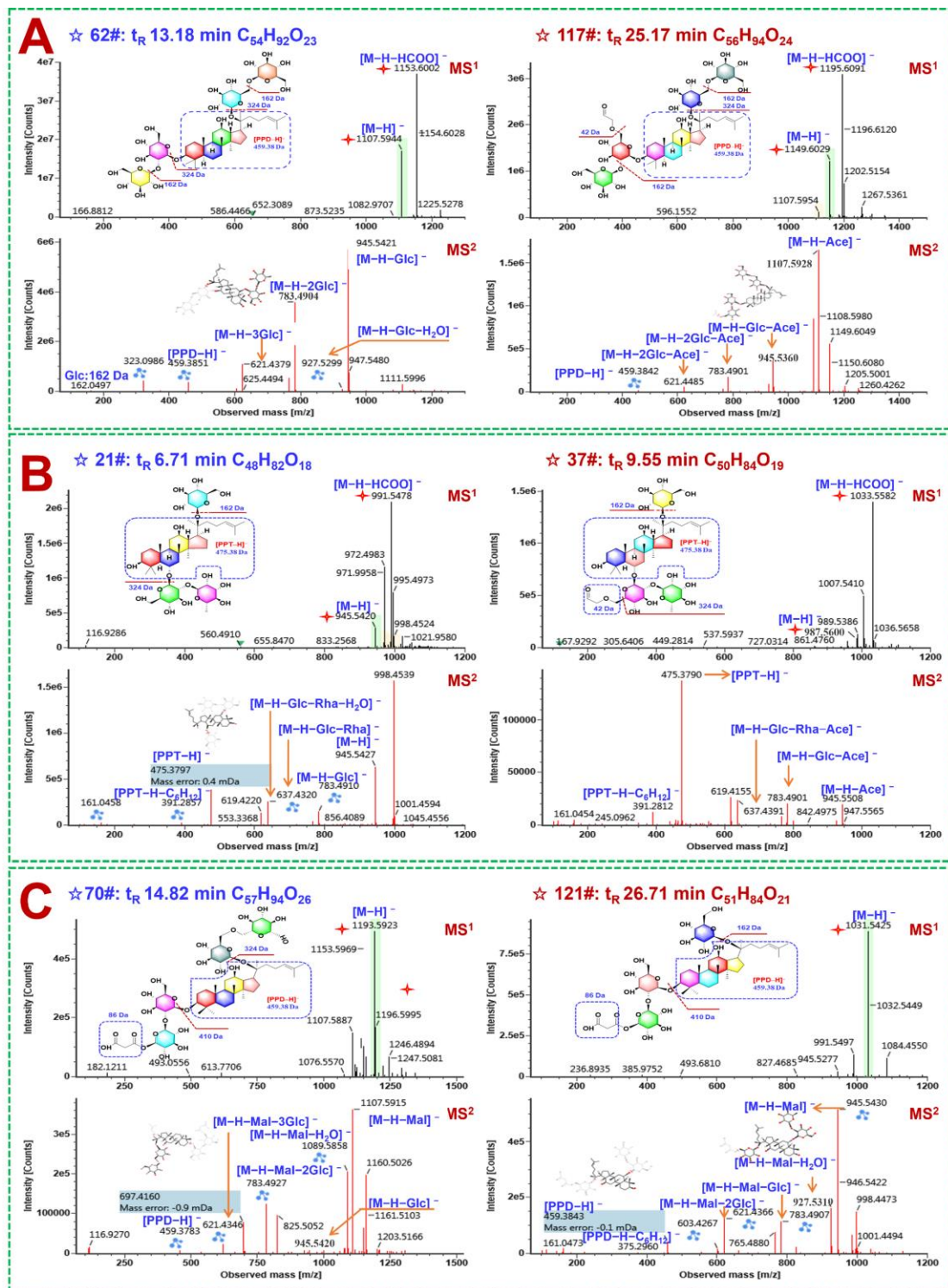


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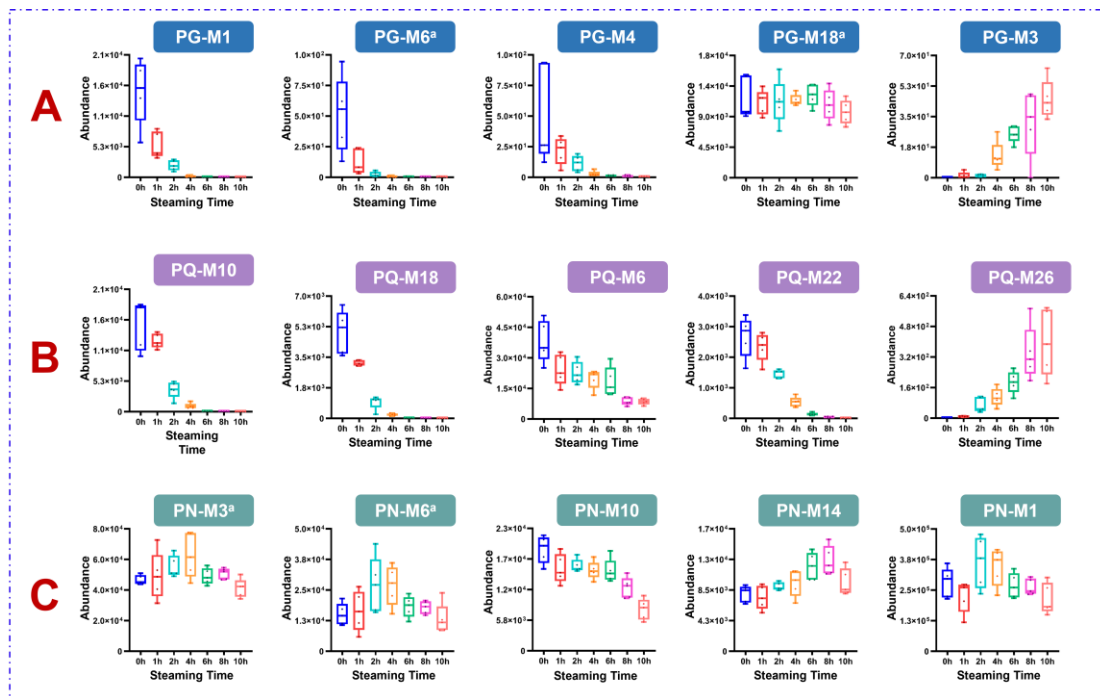


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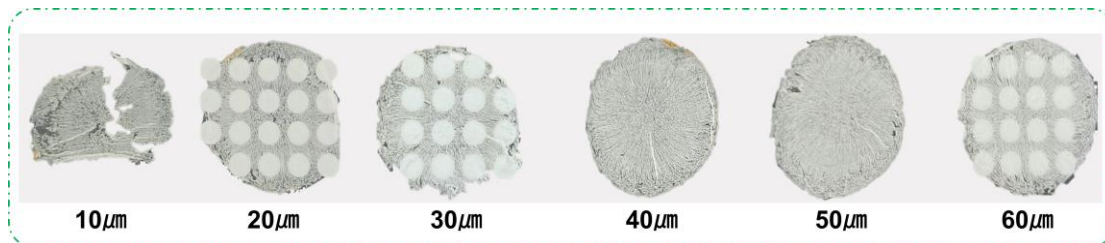


Figure S8 Optical scanning slices of PG for optimizing the thickness in DESI-MSI.

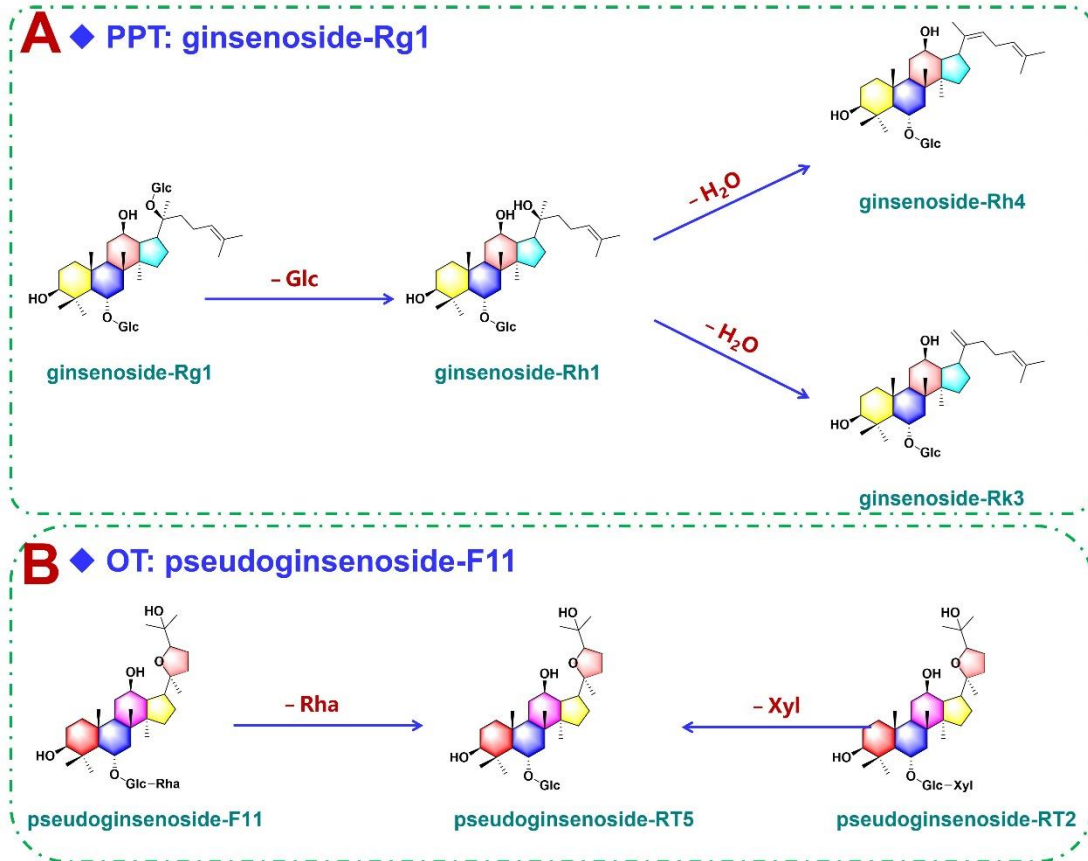


Figure S9 Transformation diagram of the PPT- and OT-type ginsenosides in PQ during the steaming process.

Table S1 Detailed information for the 62 ginsenoside reference compounds used in the current work.

No.	Trivial name	M.F.	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(<i>S</i>)-protopanaxatriol	C ₃₀ H ₅₂ O ₄	476.3866	
4	ginsenoside F3	C ₄₁ H ₇₀ O ₁₃	770.4816	
5	notoginsenoside R2	C ₄₁ H ₇₀ O ₁₃	770.4816	
6	ginsenoside Rg2	C ₄₂ H ₇₂ O ₁₃	784.4973	PPT
7	ginsenoside Rg1	C ₄₂ H ₇₂ O ₁₄	800.4922	
8	ginsenoside Rf	C ₄₂ H ₇₂ O ₁₄	800.4922	
9	notoginsenoside R1	C ₄₇ H ₈₀ O ₁₈	932.5345	
10	ginsenoside Re	C ₄₈ H ₈₂ O ₁₈	946.5501	
11	20(<i>R</i>)-ginsenoside Rg2	C ₄₂ H ₇₂ O ₁₃	784.4973	
12	ginsenoside Rh2	C ₃₆ H ₆₂ O ₈	622.4445	
13	ginsenoside F2	C ₄₂ H ₇₂ O ₁₃	784.4973	
14	20(<i>S</i>)-ginsenoside Rg3	C ₄₂ H ₇₂ O ₁₃	784.4973	
15	20(<i>R</i>)-ginsenoside Rg3	C ₄₂ H ₇₂ O ₁₃	784.4973	
16	20(<i>R</i>)-protopanaxadiol	C ₃₀ H ₅₂ O ₃	460.3916	
17	ginsenoside Rd	C ₄₈ H ₈₂ O ₁₈	946.5501	
18	malonyl-ginsenoside Rd	C ₅₁ H ₈₄ O ₂₁	1032.5505	
19	ginsenoside Rb2	C ₅₃ H ₉₀ O ₂₂	1078.5924	PPD
20	ginsenoside Rb3	C ₅₃ H ₉₀ O ₂₂	1078.5924	
21	ginsenoside Rc	C ₅₃ H ₉₀ O ₂₂	1078.5924	
22	ginsenoside Rb1	C ₅₄ H ₉₂ O ₂₃	1108.6029	
23	malonyl-ginsenoside Rc	C ₅₆ H ₉₂ O ₂₅	1164.5928	
24	malonyl-ginsenoside Rb2	C ₅₆ H ₉₂ O ₂₅	1164.5928	
25	notoginsenoside R4	C ₅₉ H ₁₀₀ O ₂₇	1240.6452	
26	ginsenoside Ra1	C ₅₈ H ₉₈ O ₂₆	1210.6346	

No.	Trivial name	M.F.	Exact Mass	Subclass
27	malonyl-ginsenoside Rb1	C ₅₇ H ₉₄ O ₂₆	1194.6033	
28	compound K	C ₃₆ H ₆₂ O ₈	622.4445	
29	20(<i>R</i>)-ginsenoside Rh2	C ₃₆ H ₆₂ O ₈	622.4445	
30	20(<i>S</i>)-protopanaxadiol	C ₃₀ H ₅₂ O ₃	460.3916	
31	ginsenoside Ra2	C ₅₈ H ₉₈ O ₂₆	1210.6346	
32	ginsenoside Rs3	C ₄₄ H ₇₄ O ₁₄	826.5079	
33	notoginsenoside Fa	C ₅₉ H ₁₀₀ O ₂₇	1240.6452	
34	ginsenoside Ra3	C ₅₉ H ₁₀₀ O ₂₇	1240.6452	
35	notoginsenoside Fc	C ₅₈ H ₉₈ O ₂₆	1210.6346	
36	notoginsenoside Fd	C ₄₇ H ₈₀ O ₁₇	916.5396	
37	notoginsenoside Ft1	C ₄₇ H ₈₀ O ₁₇	916.5396	
38	ginsenoside Rd2	C ₄₇ H ₈₀ O ₁₇	916.5396	
39	notoginsenoside S	C ₆₃ H ₁₀₆ O ₃₀	1342.6769	
40	chikusetsusaponin IVa	C ₄₂ H ₆₆ O ₁₄	794.4453	
41	ginsenoside Ro	C ₄₈ H ₇₆ O ₁₉	956.4981	OA
42	chikusetsusaponin IV	C ₄₇ H ₇₄ O ₁₈	926.4875	
43	pseudoginsenoside Rt1	C ₄₇ H ₇₄ O ₁₈	926.4875	
44	24(<i>R</i>)-pseudoginsenoside Rt5	C ₃₆ H ₆₂ O ₁₀	654.4343	
45	24(<i>R</i>)-pseudoginsenoside F11	C ₄₂ H ₇₂ O ₁₄	800.4922	OT
46	(20 <i>S</i> ,24 <i>R</i>)-Octillol	C ₃₀ H ₅₂ O ₅	492.3815	
47	ginsenoside Rk1	C ₄₂ H ₇₀ O ₁₂	766.4868	
48	ginsenoside Rk2	C ₃₆ H ₆₀ O ₇	604.4339	
49	ginsenoside Rg5	C ₄₂ H ₇₀ O ₁₂	766.4868	
50	ginsenoside Rh3	C ₃₆ H ₆₀ O ₇	604.4339	C17 side-
51	pseudoginsenoside Rh2	C ₃₆ H ₆₂ O ₈	622.4445	chain
52	ginsenoside Rk3	C ₃₆ H ₆₀ O ₈	620.4288	
53	ginsenoside Rg6	C ₄₂ H ₇₀ O ₁₂	766.4867	
54	ginsenoside Rh4	C ₃₆ H ₆₀ O ₈	620.4288	

No.	Trivial name	M.F.	Exact Mass	Subclass
55	ginsenoside F4	C ₄₂ H ₇₀ O ₁₂	766.4867	
56	vinaginsenoside R8	C ₄₈ H ₈₂ O ₁₉	962.5450	
57	panaxatriol	C ₃₀ H ₅₂ O ₄	476.3866	
58	panaxadiol	C ₃₀ H ₅₂ O ₃	460.3916	
59	ginsenoside Rh8	C ₃₆ H ₆₀ O ₉	636.4237	
60	ginsenoside Rh7	C ₃₆ H ₆₀ O ₉	636.4237	
61	5,6-didehydroginsenoside Rd	C ₄₈ H ₈₀ O ₁₈	944.5345	Others
62	gypenoside XLIX	C ₅₂ H ₈₆ O ₂₁	1046.5662	

Table S2 Information of 10 reversed-phase chromatographic columns for the stationary phase screening.

Number	Type	Specification/Manufacturer	Separation characteristics
1	HSS T3	2.1×100 mm, 1.8 μm; Waters	Polar modified octadecyl silane bonded silica gel chromatographic column, high strength silica gel particles, triple bond bonding to reduce carbon density; Enhance the retention of polar molecules and retain water-soluble compounds; Compatible with 100% water phase.
2	CORTECS C18	2.1×100 mm, 1.6 μm; Waters	Solid core particle phenyl chromatographic column can provide higher column efficiency; Realize the maximum separation with the highest column efficiency; Rapid separation, improve flux, and obtain peak shape and load for basic compounds; It can provide complementary selectivity for aromatic compounds; The bonded phase is stable without loss at low pH value.
3	CSH C18	2.1×100 mm, 1.7 μm; Waters	On the basis of ethylene bridged hybrid particles (BEH), a small amount of charge is controlled on its surface. It is the first-choice column for the analysis of basic drugs and peptides; The chromatographic column equilibrium is fast, the reproducibility between batches is superior, and the stability is good.
4	BEH Shield RP18	2.1×100 mm, 1.7 μm; Waters	Combined with ethylidene bridged hybrid particles, polarity embedded hydrophilic carbamate functional groups, fully capped; Enhance the retention of phenolic acid compounds; Resistant to 100% water, shielding silanol group, so that the peak shape of alkaline compounds is good; Offer different selectivity from C18.
5	BEH C18	2.1×100 mm, 1.7 μm; Waters	Ethylene bridged hybrid particle bonding C18, triple bond bonding; End groups seal the tail to ensure the peak shape of basic compounds, which is suitable for various analytes; Wide pH tolerance range.
6	Luna Omega Polar C18	2.1×100 mm, 1.6 μm; Phenomenex	It is a unique modified C18, which eliminates micropores on the surface of silica gel by heat treatment on the basis of traditional fully porous silica gel, and then adds polar groups on the surface of silica gel, which has 100% water phase stability, provides a choice for the balance retention of polar and hydrophobic compounds, and is suitable for the analysis of polar and nonpolar compounds.
7	Zorbax Extend C18	2.1×100 mm, 1.8 μm; Agilent	Spherical porous silica gel particles; Adopt unique double coordination C18-C1 bonding and double end-capping technology to ensure the stability of high pH separation; Improve the retention behavior, resolution and peak shape of basic compounds; Silica gel base, high column efficiency, higher column

Number	Type	Specification/Manufacturer	Separation characteristics
8	Zorbax Eclipse Plus C18	2.1×100 mm, 1.8 μm; Agilent	<p>efficiency and better peak shape than polymer matrix chromatography column.</p> <p>Spherical fully porous silica gel-based particles with double-terminated octadecylsilane chemically bonded phase; It can be used for the analysis of acid and neutral samples, especially for the separation of basic compounds with poor peak shape on other chromatographic columns.</p>
9	Zorbax SB-Aq	2.1×100 mm, 1.8 μm; Agilent	<p>Spherical fully porous silica gel particles with polarity enhanced octadecyl silica gel chemically bonded phase with three-dimensional protecting groups on the side groups. It can be used for highly acidic mobile phase and highly polar samples, and can be compatible with 100% pure water mobile phase.</p>
10	Zorbax SB-C18	2.1×100 mm, 1.8 μm; Agilent	<p>The StableBond packing used in this column is uncapped, uses unique, monofunctional silanes, has large diisobutyl side chain groups, is compatible with all common mobile phases, and is allowed to be used at high temperature and low pH value conditions.</p>

Table S3 Information of 10 ginsenoside indicators used for optimizing the ion-source parameters of Vion IM-QTOF.

Subclass	Trivial name	[M-H]⁻	[M-H+HCOOH]⁻
PPD	Rd	945.5429	991.5484
	Rb1	1107.5960	1153.6010
PPT	noto-R1	931.5273	977.5328
	Rg1	799.4850	845.4905
OA	pseudoginsenoside Rt1	925.4803	–
	Ro	955.4909	–
OT	p-F11	799.4850	845.4905
	24(R)-Rt5	653.4271	699.4326
Malonyl	m-Rb1	1193.5960	–
	m-Rb2	1163.5860	–

Table S4 Investigation on the intra-day precision of the established UHPLC/IM-QTOF-MS approach using 10 index components.

Trivial name	Peak area (<i>n</i>=6)						RSD (%)
noto-R1	28927430	27520159	30684989	26515053	35251962	33397048	11.54
Rg1	124304842	107358669	107782335	134094321	115980971	132204704	9.77
Re	161100706	160558674	154962869	161861656	179252182	173448641	5.55
Rd	155533668	159485252	154780147	173312393	179881371	169385284	6.24
Rb1	73676204	73914625	71629473	77460226	73111070	74419361	2.61
Rt1	1645807	1390496	1723440	1461010	1356658	1707401	10.61
Ro	97479371	97779352	104758276	103896661	101364533	82618651	8.27
p-F11	7210789	6983562	7561419	9519432	8540056	8141678	11.83
m-Rb1	45150791	45479480	44551876	45821570	37188242	45932240	7.69
m-Rb2	19026370	18658268	18586486	18857954	19301681	19021765	1.40

Table S5 Investigation on the inter-day precision of the established UHPLC/IM-QTOF-MS approach using 10 index components.

Trivial name	Peak area (<i>n</i> =6)									RSD (%)
	Day-1			Day-2			Day-3			
noto-R1	26515053	35251962	33397048	37564499	33752322	38538657	41090903	40239419	39746842	12.67
Rg1	134094321	115980971	132204704	107091663	117702334	136936252	112888775	128254508	132881433	8.76
Re	161861656	179252182	173448641	191978505	186280532	183101279	176325516	179941867	181601085	4.74
Rd	173312393	179881371	169385284	200304463	212950340	161820887	190104675	202579058	191631434	9.09
Rb1	77460226	73111070	74419361	85214004	77541637	75614072	79609531	80245196	78873386	4.61
Rt1	1461010	1356658	1707401	1846301	1864964	1687701	1880896	1839802	1825279	11.05
Ro	103896661	101364533	82618651	117816572	111723914	105240452	118965637	106767397	106557801	10.08
p-F11	9519432	8540056	8141678	11779174	9225858	10616877	11684773	9578043	8945858	13.36
m-Rb1	45821570	37188242	45932240	46176184	46187575	43224759	47734587	46913862	46935859	7.15
m-Rb2	18857954	19301681	19021765	17410696	18009738	16999711	16258202	16211058	16252021	7.14

Table S6 Investigation on repeatability of the established UHPLC/IM-QTOF-MS approach using 10 index components.

Trivial name	Peak area ($n=6$)						RSD (%)
noto-R1	22793259	25874551	22595662	20365824	23395250	21924815	7.97
Rg1	82406574	67598858	68715570	76528756	65599528	66807656	9.39
Re	153680658	155371612	144278986	157417272	132853310	157290175	6.51
Rd	132649672	122746134	126034348	118537266	126643869	123001307	3.81
Rb1	68055945	64518162	67663641	70766247	71847814	67267475	3.84
Rt1	1676267	1409961	1413602	1450087	1657552	1686814	8.87
Ro	66854823	57430083	59497710	63657336	59940359	68939105	7.23
p-F11	5161542	5843460	5287688	6513596	5754243	5091484	9.65
m-Rb1	55920010	43163021	43756681	48496376	49102289	42870053	10.73
m-Rb2	17939705	18539989	18994860	19373831	19337659	19795285	3.51

Table S7 Collision-cross section (CCS) of 48 reference compounds.

Trivial name	t_R (min)	m/z	Formula	CCS (\AA^2)
notoginsenoside R1	5.62	977.5311	C ₄₇ H ₈₀ O ₁₈	288.2074
ginsenoside Rg1	6.59	799.4840	C ₄₂ H ₇₂ O ₁₄	267.7457
ginsenoside Re	6.71	945.5420	C ₄₈ H ₈₂ O ₁₈	293.3994
vinaginsenoside R8	9.95	961.5377	C ₄₈ H ₈₂ O ₁₉	290.1148
24(R)-pseudoginsenoside F11	10.97	799.4857	C ₄₂ H ₇₂ O ₁₄	283.6003
24(R)-pseudoginsenoside Rt5	11.01	699.4355	C ₃₆ H ₆₂ O ₁₀	259.7744
ginsenoside Rf	11.31	799.4826	C ₄₂ H ₇₂ O ₁₄	270.0051
notoginsenoside R4	11.37	1239.6358	C ₅₉ H ₁₀₀ O ₂₇	319.5260
notoginsenoside Fa	12.00	1239.6370	C ₅₉ H ₁₀₀ O ₂₇	328.9218
notoginsenoside R2	12.16	815.4794	C ₄₁ H ₇₀ O ₁₃	272.5168
ginsenoside Ra2	12.80	1209.6237	C ₅₈ H ₉₈ O ₂₆	312.0647
ginsenoside F3	12.96	815.4785	C ₄₁ H ₇₀ O ₁₃	272.2038
ginsenoside Ra3	13.06	1239.6346	C ₅₉ H ₁₀₀ O ₂₇	320.3242
20(S)-ginsenoside Rg2	13.10	783.4905	C ₄₂ H ₇₂ O ₁₃	269.8051
ginsenoside Rb1	13.14	1107.5930	C ₅₄ H ₉₂ O ₂₃	309.8476
20(S)-ginsenoside Rg2	13.14	829.4950	C ₄₂ H ₇₂ O ₁₃	269.9872
20(S)-ginsenoside Rh1	13.22	683.4381	C ₃₆ H ₆₂ O ₉	245.2454
20(R)-ginsenoside Rg2	13.56	829.4951	C ₄₂ H ₇₂ O ₁₃	268.4625
ginsenoside Rc	14.33	1077.5842	C ₅₃ H ₉₀ O ₂₂	304.7788
ginsenoside Ra1	14.43	1209.6250	C ₅₈ H ₉₈ O ₂₆	315.8181
notoginsenoside Fc	14.46	1209.6269	C ₅₈ H ₉₈ O ₂₆	317.0309
malonylginsenoside Rb1	14.82	1193.5939	C ₅₇ H ₉₄ O ₂₆	309.7140
ginsenoside Rb2	16.27	1123.5894	C ₅₃ H ₉₀ O ₂₂	318.9846
20(S)-ginsenoside F1	16.34	637.4318	C ₃₆ H ₆₂ O ₉	247.9511
malonylginsenoside Rc	16.60	1163.5840	C ₅₆ H ₉₂ O ₂₅	321.2321
ginsenoside Rb3	16.72	1077.5822	C ₅₃ H ₉₀ O ₂₂	316.8699
ginsenoside Ro	18.15	955.4912	C ₄₈ H ₇₆ O ₁₉	287.5033

Trivial name	t_R (min)	m/z	Formula	CCS (\AA^2)
malonylginsenoside Rb2	18.83	1163.5847	$C_{56}H_{92}O_{25}$	319.8910
araloside A	20.43	925.4792	$C_{47}H_{74}O_{18}$	282.2671
ginsenoside Rd	20.61	945.5420	$C_{48}H_{82}O_{18}$	292.6827
pseudo-ginsenoside Rt1	21.27	925.4796	$C_{47}H_{74}O_{18}$	288.4036
chikusetsusaponin Iva	24.43	793.4380	$C_{42}H_{66}O_{14}$	261.1542
malonylginsenoside Rd	24.62	1031.5416	$C_{51}H_{84}O_{21}$	303.1792
notoginsenoside Fd	28.44	961.5365	$C_{47}H_{80}O_{17}$	288.0108
ginsenoside Rd2	29.01	961.5383	$C_{47}H_{80}O_{17}$	287.3132
ginsenoside Rg6	29.16	811.4853	$C_{42}H_{70}O_{12}$	283.5427
ginsenoside Rk3	29.76	665.4271	$C_{36}H_{60}O_8$	256.6714
ginsenoside F4	29.88	811.4844	$C_{42}H_{70}O_{12}$	288.7221
ginsenoside Rh4	30.59	665.4276	$C_{36}H_{60}O_8$	256.1908
ginsenoside F2	31.15	829.4956	$C_{42}H_{72}O_{13}$	268.5217
notoginsenoside Ft1	32.06	961.5366	$C_{47}H_{80}O_{17}$	281.6499
ginsenoside Rg3	33.15	783.4907	$C_{42}H_{72}O_{13}$	271.4352
20(R)-ginsenoside Rg3	33.54	829.4952	$C_{42}H_{72}O_{13}$	270.6995
ginsenoside Rk1	37.38	811.4845	$C_{42}H_{70}O_{12}$	281.8119
compound K (CK)	37.53	621.4376	$C_{36}H_{62}O_8$	240.8525
ginsenoside Rg5	37.78	811.4847	$C_{42}H_{70}O_{12}$	285.3987
20(S)-ginsenoside Rh2	38.58	667.4435	$C_{36}H_{62}O_8$	260.9541
20(R)-ginsenoside Rh2	38.86	667.4429	$C_{36}H_{62}O_8$	260.6128

Table S8 Information of ginsenosides identified from PG before and after the steaming.

No.	<i>t_R</i> (min)	<i>m/z</i>	Formula	Mass error (ppm)	CCS (Å ²)	Adduct	ESI-MS ²	Identification	Subclass
1	1.67	979.5423	C ₅₅ H ₈₀ O ₁₅	-0.10	293.8773	-H	671.4468, 653.4230, 491.3755, 221.1868, 131.0339	ginsengenin-S3 or its isomer ((PPT+O)-GlurA-Xyl-Glc-H ₂ O)	PPT
2	2.39	1007.5435	C ₄₈ H ₈₂ O ₁₉	0.83	294.3866	+HCOO	799.4757, 653.4322, 635.4194, 491.3816, 161.0475, 113.0222, 101.0240	ginsenoside Re7 or its isomer ((PPT+O)-2Glc-Rha)	PPT
3	3.71	1139.5742	C ₄₉ H ₉₀ O ₂₆	4.11	298.3600	+HCOO	1093.5654, 931.5388, 799.4857, 637.4244, 475.3754, 221.0769	floralginsenoside P or its isomer (PPT-3Glc-Xyl)	PPT
4	3.88	961.5374	C ₄₈ H ₈₂ O ₁₉	-0.31	285.2443	-H	961.5374, 637.4435, 513.8247, 475.3714	ginsenoside Re7 isomer (PPT-3Glc)	PPT
5	3.95	815.4792	C ₄₂ H ₇₂ O ₁₅	-0.86	262.4750	-H	815.4917, 727.2784, 653.4210, 491.3749	24(<i>R</i>)-majoroside R1 isomer ((PPT+O)-2Glc)	PPT
6	4.08	1153.5972	C ₅₄ H ₉₂ O ₂₃	-3.07	300.2432	+HCOO	1107.5869, 1063.5934, 945.5509, 783.4915, 637.4450, 475.3690	ginsenoside Re8 or its isomer (PPT-GlurA-2Glc-Xyl)	PPT
7	4.84	977.5316	C ₄₇ H ₈₀ O ₁₈	-0.54	282.8864	+HCOO	931.5425, 799.4783, 637.4268, 475.3863, 391.2924, 161.0454, 131.0359, 101.0203	notoginsenoside R1 isomer (PPT-2Glc-Xyl)	PPT
8	5.06	961.5371	C ₄₈ H ₈₂ O ₁₉	-0.62	288.5774	-H	799.4837, 637.4336, 475.3796, 391.2853, 179.0551	ginsenoside Re7 isomer (PPT-3Glc)	PPT
9	5.13	831.4747	C ₄₁ H ₇₀ O ₁₄	0.64	255.8187	+HCOO	785.4616, 653.4217, 491.3698, 391.2882, 389.2641, 161.0456	pseudoginsenoside RT2 (24 <i>R</i>) isomer ((PPT+O)-Glc-Xyl)	PPT
10	5.30	977.5310	C ₄₇ H ₈₀ O ₁₈	-1.18	279.7258	+HCOO	931.5080, 799.4661, 637.4325, 475.3788, 391.2768, 113.0217, 101.0273	notoginsenoside R1 isomer (PPT-2Glc-Xyl)	PPT
11 ^a	5.62	977.5311	C ₄₇ H ₈₀ O ₁₈	-1.07	288.8929	+HCOO	931.5252, 799.4836, 637.4312, 619.4193, 475.3788	notoginsenoside R1	PPT
12	5.82	1007.5465	C ₄₈ H ₈₂ O ₁₉	3.95	288.6769	+HCOO	961.5505, 799.4748, 637.4409, 553.3332, 475.3908	20-glucoginsenoside-Rf or its isomer (PPT-3Glc)	PPT
13	5.85	845.4891	C ₄₂ H ₇₂ O ₁₄	-1.00	261.3630	+HCOO	799.4735, 653.4144, 491.3762, 391.2843	20(<i>R</i>)-pseudoginsenoside F11 isomer ((PPT+O)-Glc-Rha)	PPT
14	6.18	977.5292	C ₄₇ H ₈₀ O ₁₈	-3.11	288.5587	+HCOO	931.5143, 637.4449, 475.3832, 391.2916, 161.0432, 131.0377	notoginsenoside R1 isomer (PPT-2Glc-Xyl)	PPT

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
15 ^a	6.59	799.4874	C ₄₂ H ₇₂ O ₁₄	3.13	262.6224	-H	621.4304, 553.3371, 475.3796, 391.2859	ginsenoside Rg1	PPT
16 ^a	6.71	945.5420	C ₄₈ H ₈₂ O ₁₈	-0.28	287.6636	-H	945.5427, 783.4910, 637.4321, 619.4220, 475.3796, 161.0457	ginsenoside Re	PPT
17	7.18	977.5285	C ₄₇ H ₈₀ O ₁₈	-3.86	288.2031	+HCOO	931.5122, 799.4982, 637.4302, 475.3791	notoginsenoside R1 isomer (PPT-2Glc-Xyl)	PPT
18	7.43	991.5476	C ₄₈ H ₈₂ O ₁₈	-0.21	296.7822	+HCOO	945.5527, 799.4830, 781.4709, 475.3723	ginsenoside Rg18 or its isomer (PPT-2Glc-Rha)	PPT
19	7.61	979.5479	C ₄₈ H ₈₄ O ₂₀	-0.51	296.4339	-H	817.4851, 655.4376, 475.3665, 179.0536	ginsenoside I (24S) or its isomer (PPT-3Glc-H ₂ O)	PPT
20 ^b	7.83	843.4746	C ₄₃ H ₇₂ O ₁₆	0.51	270.0849	-H	619.3721, 475.3552	PPT-2Glc-CO ₂	PPT
21	8.08	827.4772	C ₄₃ H ₇₂ O ₁₅	-3.26	267.1103	-H	827.4772, 637.4315, 475.3781, 391.2812, 161.0449	vinaginsenoside R2 isomer (PPT-Glc-Rha-CO ₂)	PPT
22	8.10	841.4942	C ₄₄ H ₇₄ O ₁₅	-1.54	267.9272	-H	621.4374, 475.3666, 391.2846, 329.2605	notoginsenoside Rt or its isomer (PPT-GlurA-Rha-CO ₂)	PPT
23 ^b	8.15	1019.5436	C ₄₉ H ₈₂ O ₁₉	0.92	294.7248	+HCOO	973.5593, 931.5016, 769.4689, 553.3404, 475.3782	PPT-2Glc-Xyl-Ace	PPT
24	8.28	1031.5447	C ₅₁ H ₈₄ O ₂₁	1.45	287.6027	-H	945.5519, 783.5144, 637.4415, 475.3820, 391.2897, 113.0273, 101.0220	malonyl ginsenoside Rd isomer (PPT-2Glc-Rha-Mal)	Mal
25	8.35	1139.5881	C ₅₃ H ₉₀ O ₂₃	2.83	314.0630	+HCOO	1093.5725, 799.5141, 781.4628, 475.3714	floralginsenoside P or its isomer (PPT-3Glc-Xyl)	PPT
26	8.44	961.5347	C ₄₇ H ₈₀ O ₁₇	-2.73	287.2857	+HCOO	915.5662, 753.4741, 607.4275, 475.3848, 391.2912	ginsenoside Rd2 isomer (PPT-Glc-Rha-Xyl)	PPT
27	8.50	1005.5287	C ₄₈ H ₈₀ O ₁₉	1.67	297.6077	+HCOO	959.5069, 797.4752, 635.4115, 473.3620, 455.3648, 101.0236	vinaginsenoside R20 or its isomer (C ₃₀ H ₅₀ O ₄ -3Glc)	C17side-chain
28	8.92	1031.5403	C ₅₁ H ₈₄ O ₂₁	-2.81	287.5061	-H	945.5281, 783.4909, 637.4311, 475.3798, 391.2841, 161.0483, 113.0252, 101.0291	malonyl ginsenoside Rd isomer (PPT-2Glc-Rha-Mal)	Mal
29	9.00	887.5002	C ₄₄ H ₇₄ O ₁₅	-0.24	274.5009	+HCOO	841.4952, 637.4291, 475.3724, 391.2799, 113.0277, 101.0207	notoginsenoside Rt or its isomer (PPT-2Glc-Ace)	PPT
30	9.14	1033.5508	C ₄₆ H ₈₄ O ₂₂	7.80	303.6482	+HCOO	987.5557, 945.5413, 783.5039, 637.4416, 475.3765, 391.2883, 161.0478, 113.0240	pseudoginsenoside Rs1 or its isomer (PPT-2Glc-Rha-Ace)	PPT
31	9.16	961.5386	C ₄₇ H ₈₀ O ₁₇	1.53	289.2122	+HCOO	915.5273, 783.4934, 637.4271, 475.3715, 391.2831, 161.0423, 101.0246	ginsenoside Rh24 isomer (PPT-Glc-Rha-Xyl)	PPT

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
32	9.25	887.5001	C ₄₄ H ₇₄ O ₁₅	-0.36	303.6482	+HCOO	841.4942, 637.4382, 475.3851, 391.2780, 161.0489, 113.0240	notoginsenoside Rt or its isomer (PPT-2Glc-Ace)	PPT
33	9.58	1007.5395	C ₄₈ H ₈₂ O ₁₉	-3.33	298.6282	+HCOO	961.5140, 799.4961, 619.4198, 375.2781, 221.0710, 161.0477, 113.0226	gypenoside XLVI isomer (PPD-GlurA-2Glc-H ₂ O-Bute)	PPD
34	9.58	1033.5608	C ₅₀ H ₈₄ O ₁₉	2.43	300.5923	+HCOO	987.5660, 945.5532, 783.5062, 637.4381, 475.3826, 391.2893, 161.0443	pseudoginsenoside Rs1 or its isomer (PPT-2Glc-Rha-Ace)	PPT
35	9.94	1007.5441	C ₄₈ H ₈₂ O ₁₉	1.46	299.0537	+HCOO	961.5433, 799.4843, 637.4325, 475.3723, 391.2877, 221.0677, 161.0478	20-glucoginsenoside-Rf or its isomer (PPT-3Glc)	PPT
36 ^b	10.13	971.4852	C ₄₈ H ₇₆ O ₂₀	0.02	268.1960	-H	637.4335, 475.3690, 391.2954	PPT-2Glc-Dimal	Mal
37	10.34	1033.5558	C ₅₀ H ₈₄ O ₁₉	-2.63	300.5045	+HCOO	987.5421, 945.5430, 783.4800, 637.4315, 475.3885, 191.0637	pseudoginsenoside Rs1 or its isomer (PPT-2Glc-Rha-Ace)	PPT
38 ^b	10.42	887.4988	C ₄₅ H ₇₆ O ₁₇	-1.80	275.2850	-H	637.4343, 553.3390, 475.3872, 391.2821	PPT-2Glc-2CO ₂	PPT
39	11.00	845.4879	C ₄₂ H ₇₂ O ₁₄	-2.50	269.0584	+HCOO	799.5121, 653.4391, 491.3737	20(R)-pseudoginsenoside F11 isomer (OT-Glc-Rha)	OT
40	11.15	913.5145	C ₄₇ H ₇₈ O ₁₇	-2.30	274.3818	-H	619.4226, 475.3879, 391.2857	notoginsenoside Ng1 or its isomer (PPT-2GlurA-Mal)	Mal
41 ^a	11.32	799.4846	C ₄₂ H ₇₂ O ₁₄	0.26	272.2003	-H	799.4845, 637.4318, 475.3793, 391.2847, 161.0455	ginsenoside Rf	PPT
42 ^a	11.37	1239.6358	C ₅₉ H ₁₀₀ O ₂₇	-1.69	205.9061	-H	1107.5945, 945.5507, 459.3896, 375.2953	notoginsenoside R4	PPD
43 ^b	11.51	1387.6718	C ₆₄ H ₁₀₈ O ₃₂	-1.95	334.0627	-H	1341.6710, 1209.6065, 1077.5709, 945.5710, 783.4761, 621.4394, 459.3727, 131.0343, 113.0239	PPD-3Glc-3Xyl	PPD
44	11.61	799.4845	C ₄₂ H ₇₂ O ₁₄	-0.50	280.3148	-H	637.4322, 475.3791	ginsenoside Rf or its isomer (PPT-2Glc)	PPT
45	11.74	1117.5399	C ₅₄ H ₈₆ O ₂₄	-3.31	315.9364	-H	1117.5408, 793.4240, 659.4049, 613.3726, 455.3526	malonyl floralginsenoside Rd6 isomer (OA-GlurA-3Glc)	OA
46	11.83	1239.6358	C ₅₉ H ₁₀₀ O ₂₇	-1.28	327.0074	-H	1239.6354, 1077.5869, 783.4804, 459.4113, 219.2148	ginsenoside Ra3 or its isomer (PPD-4Glc-Xyl)	PPD

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
47 ^a	12.16	769.4745	C ₄₁ H ₇₀ O ₁₃	0.89	267.9782	-H	769.4747, 637.4328, 475.3797, 161.0459	ginsenoside F3	PPT
48 ^a	12.16	815.4794	C ₄₁ H ₇₀ O ₁₃	0.13	269.2960	+HCOO	769.4747, 637.4328, 475.2028, 391.3034	notoginsenoside R2	PPT
49	12.29	1325.6386	C ₆₂ H ₁₀₂ O ₃₀	0.23	333.9526	-H	1239.6383, 1107.6234, 945.5413, 783.4854, 621.4275, 459.3794, 221.0788, 101.0256	ginsenoside Ra3 isomer (PPD-4Glc-Xyl-Mal)	Mal
50	12.38	1151.5827	C ₅₄ H ₉₀ O ₂₃	-2.08	315.0129	+HCOO	1105.5583, 943.5397, 781.4884, 459.3659, 221.0579, 161.0460, 101.0266	epoxynotoginsenoside A isomer (PPD-GlurA-2Glc-Rha)	PPD
51	12.42	1209.6273	C ₅₈ H ₉₈ O ₂₆	-0.08	320.1358	-H	1209.6245, 1047.5656, 783.4854, 621.4298, 459.3870, 179.0585, 101.0267	ginsenoside Ra1 isomer (PPD-3Glc-2Xyl)	PPD
52	12.45	815.4790	C ₄₁ H ₇₀ O ₁₃	-0.39	272.0914	+HCOO	769.4754, 637.4387, 475.3780, 391.2874, 125.0228	20(R)-notoginsenoside R2 or its isomer (PPT-Glc-Xyl)	PPT
53	12.54	1285.6380	C ₅₉ H ₁₀₀ O ₂₇	-3.95	320.0757	+HCOO	1239.6256, 1077.5950, 945.5513, 783.4745, 621.4334, 459.3998, 221.0713, 113.0255, 101.0201	ginsenoside Ra3 isomer (PPD-4Glc-Xyl)	PPD
54 ^a	12.80	1209.6237	C ₅₈ H ₉₈ O ₂₆	-2.55	316.7184	-H	1077.5845, 945.5695, 783.4913, 765.4784, 621.4413, 459.3659, 131.0348	ginsenoside Ra2	PPD
55	12.83	841.4937	C ₄₄ H ₇₄ O ₁₅	-2.14	277.3319	-H	799.5004, 637.4323, 475.3790, 391.2882	notoginsenoside Rt or its isomer (PPT-2Glc-Ace)	PPT
56	12.99	815.4784	C ₄₁ H ₇₀ O ₁₃	-1.17	272.5059	+HCOO	769.4766, 637.4265, 619.4106, 475.3812, 391.2852, 161.0397, 131.0401, 113.0217	20(R)-notoginsenoside R2 or its isomer (PPT-Glc-Xyl)	PPT
57 ^a	13.06	1239.6346	C ₅₉ H ₁₀₀ O ₂₇	-2.29	324.3973	-H	1077.5803, 891.5078, 667.3387, 459.1127	ginsenoside Ra3	PPD
58 ^b	13.14	1125.5743	C ₅₃ H ₉₀ O ₂₅	4.46	243.3308	-H	1107.5942, 945.5415, 783.4903, 621.4367, 459.3838, 221.0660, 161.0455, 101.0244	ginsenoside Rb4 or its isomer (PPD-4Glc-H ₂ O)	PPD
59 ^a	13.14	1107.5930	C ₅₄ H ₉₂ O ₂₃	-1.87	245.0291	-H	945.5415, 783.4903, 621.4367, 459.3838, 323.0976, 179.0563	ginsenoside Rb1	PPD
60 ^a	13.14	829.4950	C ₄₂ H ₇₂ O ₁₃	0.00	272.7008	+HCOO	783.4903, 637.4325, 475.3790, 323.0949	20(S)-Ginsenoside Rg2	PPT
61 ^a	13.22	683.4374	C ₃₆ H ₆₂ O ₉	0.51	249.2968	+HCOO	637.4292, 683.4400, 549.3355, 459.3858, 323.0983, 221.0666	20(S)-ginsenoside Rh1	PPT

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
62^a	13.56	829.4951	C ₄₂ H ₇₂ O ₁₃	0.15	274.3078	+HCOO	783.4895, 637.4334, 475.3794	20(<i>R</i>)-ginsenoside Rg2	PPT
63	13.93	683.4369	C ₃₆ H ₆₂ O ₉	-0.26	251.2280	+HCOO	637.4255, 553.3441, 475.3828, 391.2755	ginsenoside Rh1 or its isomer (PPT-Glc)	PPT
64^a	14.38	1123.5878	C ₅₃ H ₉₀ O ₂₂	-2.03	309.0430	+HCOO	1077.5824, 945.5412, 783.4897, 621.4369, 375.2991, 305.0899, 179.0578	ginsenoside Rc	PPD
65^a	14.49	1209.6239	C ₅₈ H ₉₈ O ₂₆	-2.41	315.7792	-H	1047.5723, 945.5405, 783.4902, 765.4800, 621.4369, 537.3436, 459.3852, 376.2950	ginsenoside Ra1	PPD
66	14.71	1325.6351	C ₆₂ H ₁₀₂ O ₃₀	-3.12	326.9772	-H	1239.6183, 1107.5831, 945.5314, 783.5058, 621.4327, 459.4025, 221.0709, 161.0450, 101.0274	ginsenoside Ra3 isomer (PPD-4Glc-Xyl-Mal)	Mal
67^a	14.85	1193.5939	C ₅₇ H ₉₄ O ₂₆	-1.36	311.9417	-H	1149.6042, 1107.5945, 945.5419, 783.4906, 621.4376, 459.3842, 323.0986,	malonyl ginsenoside Rb1	Mal
68	15.17	843.4758	C ₄₂ H ₇₀ O ₁₄	1.98	275.7123	+HCOO	797.4917, 475.6468, 215.8666	ginsenoside Rg11 or its isomer (PPT-GlurA-Rha)	PPT
69	15.30	1255.6314	C ₅₈ H ₉₈ O ₂₆	-0.78	322.4947	+HCOO	1209.6182, 1077.5870, 945.5724, 783.4918, 621.4420, 459.3924, 375.2880, 161.0422, 113.0232	ginsenoside Ra1 isomer (PPD-3Glc-2Xyl)	PPD
70	15.94	1123.5885	C ₅₃ H ₉₀ O ₂₂	-1.35	316.1044	+HCOO	1077.5846, 945.5406, 783.4893, 621.4395, 459.3848, 375.2870, 221.0731, 161.0453, 101.0247	ginsenoside Rb2 isomer (PPD-3Glc-Xyl)	PPD
71	16.00	1153.5269	C ₅₂ H ₈₄ O ₂₅	-0.84	246.4940	+HCOO	1107.5838, 945.5424, 783.4903, 621.4373, 459.3827, 221.9951	ginsenoside Rb4 or its isomer (PPD-4Glc)	PPD
72^a	16.00	1123.5885	C ₅₃ H ₉₀ O ₂₂	-1.41	316.8362	+HCOO	1077.5838, 945.5424, 783.4902, 621.4373, 537.3458, 459.3827	ginsenoside Rb2	PPD
73^a	16.41	683.4386	C ₃₆ H ₆₂ O ₉	2.36	246.6922	+HCOO	581.9354, 483.5605	20(<i>S</i>)-ginsenoside F1	PPT
74^b	16.55	1295.6248	C ₆₁ H ₁₀₀ O ₂₉	-1.82	329.5870	-H	1209.6218, 1077.5763, 945.5570, 783.4821, 621.4401, 459.3856, 161.0453, 101.0251	PPD-3Glc-2Xyl-Mal	Mal
75	16.62	1163.5832	C ₅₆ H ₉₂ O ₂₅	-1.94	305.2698	-H	1077.5831, 945.5422, 783.4949, 621.4386, 459.3834, 375.2981, 221.0668, 161.0447, 101.0239	malonyl ginsenoside Rb2 isomer (PPD-3Glc-Xyl-Mal)	Mal
76^a	16.72	1077.5822	C ₅₃ H ₉₀ O ₂₂	-2.66	314.1409	-H	1077.5837, 945.5421, 915.5282, 783.4896, 731.4485, 459.3847	ginsenoside Rb3	PPD

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
77	16.80	797.4670	C ₄₂ H ₇₀ O ₁₄	-2.82	273.1889	-H	737.9540, 569.4486, 475.3794	ginsenoside Rg11 or isomer (PPT-Rha-GlurA)	PPT
78	17.07	955.4857	C ₄₈ H ₇₆ O ₁₉	-4.86	290.4856	-H	955.4875, 793.4603, 631.3739, 455.3431	ginsenoside Rd isomer (OA-GlurA-2Glc)	OA
79 ^a	17.55	955.4902	C ₄₈ H ₇₆ O ₁₉	-0.12	289.7742	-H	955.4902, 793.4381, 731.4381, 659.4167, 613.3746, 455.0596, 227.1815	ginsenoside Ro	OA
80	17.56	1255.6315	C ₅₈ H ₉₈ O ₂₆	-0.65	323.1055	+HCOO	1209.6233, 1077.5806, 915.5331, 783.5006, 621.4414, 459.3819	ginsenoside Ra1 isomer (PPD-3Glc-2Xyl)	PPD
81	17.74	1153.6225	C ₅₈ H ₉₂ O ₂₀	0.54	312.7184	+HCOO	1107.6004, 945.5342, 783.4960, 621.4262, 459.3908, 161.0490	ginsenoside Rb4 or its isomer (PPD-4Glc)	PPD
82	17.84	1251.6391	C ₆₀ H ₁₀₀ O ₂₇	0.96	331.5783	-H	1209.6243, 1191.6154, 1029.5679, 927.5600, 783.4957, 459.3886	ginsenoside Ra5 or its isomer (PPD-3Glc-2Xyl-Ace)	PPD
83 ^b	18.41	1225.6102	C ₅₃ H ₉₆ O ₂₈	3.14	311.0871	+HCOO	1179.6081, 1047.5566, 929.5549, 787.5085, 459.3891, 191.0570, 113.0230	PPD-2Glc-3Xyl	PPD
84	18.52	1193.5951	C ₅₇ H ₉₄ O ₂₆	-0.80	326.5269	-H	1107.5928, 945.5616, 783.4895, 621.4378, 459.3848, 375.2707, 221.0642, 161.0449, 101.0223	malonyl ginsenoside Rb1 or its isomer (PPD-4Glc-Mal)	Mal
85	18.59	1149.6048	C ₅₆ H ₉₄ O ₂₄	-1.22	205.0978	-H	1107.5948, 1089.5844, 945.5400, 783.4918, 621.4395, 459.3868, 179.0560	quinquenoside R1 or its isomer (PPD-4Glc-Ace)	PPD
86	18.63	1195.6104	C ₅₆ H ₉₄ O ₂₄	-0.66	317.3455	+HCOO	1149.6418, 1107.5965, 945.5323, 783.4892, 621.4372, 459.3858, 161.0472, 113.0235, 101.0234	quinquenoside R1 or its isomer (PPD-4Glc-Ace)	PPD
87	18.74	1093.5799	C ₅₂ H ₈₈ O ₂₁	0.37	304.1312	+HCOO	1047.5738, 927.5325, 753.4803, 459.3811, 101.0246	notoginsenoside O or its isomer (PPD-2Glc-2Xyl)	PPD
88 ^a	18.83	1163.5847	C ₅₆ H ₉₂ O ₂₅	-0.15	314.8170	-H	1077.5844, 1059.5736, 1011.5520, 945.5423, 783.4917, 621.4353, 459.3840	malonyl ginsenoside Rb2	Mal
89	19.33	857.4881	C ₄₃ H ₇₂ O ₁₄	-2.22	278.1294	+HCOO	811.5079, 767.4967, 535.3152, 637.4228, 475.3920	20(S)-sanchirrhinoside A2 isomer (PPT-2Rha-CO ₂)	PPT
90	19.74	925.4788	C ₄₇ H ₇₄ O ₁₈	-1.52	288.6237	-H	925.4763, 763.4175, 455.3621, 191.0566, 101.0282	araloside A isomer (OA-GlurA-Xyl-Glc)	OA
91	19.91	1163.5849	C ₅₆ H ₉₂ O ₂₅	-0.43	315.6441	-H	1077.5890, 945.5468, 783.4938, 621.4450, 459.3869, 375.2907, 375.2907, 161.0449, 101.0244	malonyl ginsenoside Rb2 isomer (PPD-3Glc-Xyl-Mal)	Mal

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
92 ^a	20.43	925.4792	C ₄₇ H ₇₄ O ₁₈	-0.55	291.5648	-H	925.4713, 613.3691, 569.3861, 441.3567	araloside A	OA
93 ^a	20.65	945.5425	C ₄₈ H ₈₂ O ₁₈	0.18	293.8867	-H	945.5430, 783.4911, 621.4383, 459.3847	ginsenoside Rd	PPD
94 ^a	21.30	925.4795	C ₄₇ H ₇₄ O ₁₈	-0.76	287.4757	-H	925.4770, 763.4205, 701.4258, 613.3753, 569.3866	pseudo-ginsenoside Rt1	OA
95	21.47	1251.6349	C ₆₀ H ₁₀₀ O ₂₇	-2.44	324.9596	-H	1251.6316, 1209.6226, 1107.5952, 945.5320, 783.4995, 621.4383, 459.3698	ginsenoside Ra5 or its isomer (PPD-3Glc-2Xyl-Ace)	PPD
96	21.57	1093.5809	C ₅₂ H ₈₈ O ₂₁	1.34	311.4845	+HCOO	1047.5925, 945.5437, 783.4893, 621.4386, 459.3849, 191.0593	notoginsenoside O or its isomer (PPD-2Glc-2Xyl)	PPD
97	21.65	1163.5841	C ₅₆ H ₉₂ O ₂₅	-1.11	315.4081	-H	1059.5734, 947.5426, 915.5427, 783.4921, 459.3814	malonyl ginsenoside Rb2 isomer (PPD-3Glc-Xyl-Mal)	Mal
98	21.86	1165.5980	C ₅₅ H ₉₂ O ₂₃	-2.35	315.0930	+HCOO	1119.5909, 1077.5829, 945.5316, 783.4783, 621.4326, 459.3934, 375.2915, 161.0492, 101.0233	ginsenoside Rs11 or its isomer (PPD-3Glc-Xyl-Ace)	PPD
99	24.47	1163.5836	C ₅₆ H ₉₂ O ₂₅	-1.54	327.4197	-H	1121.6021, 945.5382, 783.4915, 621.4409, 459.3881	malonyl ginsenoside Rb2 isomer (PPD-3Glc-Xyl-Mal)	Mal
100	24.49	793.4384	C ₄₂ H ₆₆ O ₁₄	0.57	256.0672	-H	793.4393, 631.3842, 569.3778, 455.3545, 437.3362	zingibroside R1 or its isomer (OA-GlurA-Glc)	OA
101	24.65	1165.5978	C ₅₅ H ₉₂ O ₂₃	-2.47	323.7613	+HCOO	1119.5904, 1077.5904, 945.5573, 783.4837, 621.4359, 459.3761, 375.2977, 161.0465, 101.0243	ginsenoside Rs11 or its isomer (PPD-3Glc-Xyl-Ace)	PPD
102	24.70	987.5510	C ₅₀ H ₈₄ O ₁₉	-2.42	300.5465	-H	945.5420, 927.5316, 783.4891, 621.4369, 459.3847, 221.0732, 101.0247	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
103 ^a	24.70	1031.5410	C ₅₁ H ₈₄ O ₂₁	-1.65	303.7742	-H	945.5420, 927.5316, 783.4891, 621.4369, 459.3847	malonyl ginsenoside Rd	Mal
104	25.16	827.4793	C ₄₂ H ₇₀ O ₁₃	-0.02	272.4681	+HCOO	781.4813, 619.4243, 457.3642	12- <i>O</i> -glucoginsenoside Rh4 or its isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	C17side-chain
105	25.21	1195.6100	C ₅₆ H ₉₄ O ₂₄	-1.05	322.4250	+HCOO	1149.5992, 1107.5931, 945.5487, 783.4973, 621.4283, 459.3865, 221.0671, 161.0454	quinquenoside R1 or its isomer (PPD-4Glc-Ace)	PPD
106	25.69	945.5443	C ₄₈ H ₈₂ O ₁₈	1.54	289.6500	-H	783.4518, 621.4427, 459.4126	ginsenoside Rd isomer (PPD-3Glc)	PPD

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
107	25.78	1165.6010	C ₅₅ H ₉₂ O ₂₃	0.39	315.3948	+HCOO	1119.5782, 1077.5612, 945.5385, 783.5126, 621.4373, 459.3924	ginsenoside Rs11 or its isomer (PPD-3Glc-Xyl-Ace)	PPD
108	26.66	1221.6301	C ₅₈ H ₉₆ O ₂₄	2.84	324.0707	+HCOO	1175.6333, 1107.5867, 945.5113, 783.4915, 621.4321, 459.3840, 161.0456, 101.0265	ginsenoside Ra6 or its isomer (PPD-4Glc-Bute)	PPD
109	26.74	1031.5399	C ₅₁ H ₈₄ O ₂₁	-3.23	289.6118	-H	945.5429, 783.5090, 621.4374, 459.3787, 161.0450, 113.0251	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	Mal
110	26.92	827.4799	C ₄₂ H ₇₀ O ₁₃	0.75	281.5247	+HCOO	781.4729, 619.4121, 457.3643	12- <i>O</i> -glucoginsenoside Rh4 or its isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	C17side-chain
111	27.42	1165.6009	C ₅₅ H ₉₂ O ₂₃	0.25	317.6226	+HCOO	1119.5953, 1077.5712, 945.5495, 783.4864, 621.4378, 459.3807, 161.0482, 113.0230	ginsenoside Rs11 or its isomer (PPD-3Glc-Xyl-Ace)	PPD
112	28.02	961.5368	C ₄₇ H ₈₀ O ₁₇	-0.48	287.0338	+HCOO	915.5342, 621.4249, 459.3843, 375.2938, 131.0347	ginsenoside Rd2 isomer (PPD-2Glc-Xyl)	PPD
113	28.13	1033.5559	C ₅₀ H ₈₄ O ₁₉	-2.49	302.6550	+HCOO	987.5452, 945.5348, 783.4897, 621.4569, 459.3839	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
114	28.30	1191.6138	C ₅₇ H ₉₄ O ₂₃	-2.20	319.6838	+HCOO	1145.6255, 1077.5921, 945.5539, 783.5074, 621.4409, 459.3792	ginsenoside Ra7 or its isomer (PPD-3Glc-Xyl-Bute)	PPD
115	28.41	1031.5439	C ₅₁ H ₈₄ O ₂₁	1.16	297.9203	-H	945.5431, 783.4892, 621.4384, 459.3836, 375.2856, 161.0461, 113.0249	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	Mal
116	28.49	961.5362	C ₄₇ H ₈₀ O ₁₇	-1.07	288.1366	+HCOO	915.5242, 783.4832, 621.4374, 459.3833, 375.2901, 161.0451, 113.0214, 101.0284	ginsenoside Rd2 isomer (PPD-2Glc-Xyl)	PPD
117	28.59	987.5500	C ₅₀ H ₈₄ O ₁₉	-3.42	302.6278	-H	945.5415, 783.4899, 621.4374, 459.3839, 143.0404	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
118	28.61	1165.5982	C ₅₅ H ₉₂ O ₂₃	-2.10	329.5176	+HCOO	1119.5874, 1077.5657, 945.5276, 783.4991, 621.4314, 459.3905	ginsenoside Rs11 or its isomer (PPD-3Glc-Xyl-Ace)	PPD
119	28.69	1117.5415	C ₅₄ H ₈₆ O ₂₄	-1.93	297.9487	-H	945.5377, 783.4992, 621.4314, 459.3733, 113.0246	malonyl floralginsenoside Rd6 or its isomer (PPD-3Glc-Dimal)	Mal
120 ^a	29.01	961.5383	C ₄₇ H ₈₀ O ₁₇	1.25	289.9918	+HCOO	915.5198, 865.4187, 621.4456, 459.3810	ginsenoside Rd2	PPD

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
121 ^a	29.16	811.4853	C ₄₂ H ₇₀ O ₁₂	1.18	268.1091	+HCOO	765.4816, 675.3482, 457.3703, 113.0247	ginsenoside Rg6	C17side-chain
122	29.23	1191.6161	C ₅₇ H ₉₄ O ₂₃	-0.17	324.7034	+HCOO	1145.6307, 1077.5959, 945.5640, 783.4972, 621.4282, 459.3826	ginsenoside Ra7 or its isomer (PPD-3Glc-Xyl-Bute)	PPD
123	29.42	1033.5574	C ₅₀ H ₈₄ O ₁₉	-1.03	303.2366	+HCOO	987.5396, 945.4574, 783.4869, 621.1182, 459.3873	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
124 ^a	29.76	665.4271	C ₃₆ H ₆₀ O ₈	1.00	246.9631	+HCOO	571.3203	ginsenoside Rk3	C17side-chain
125	29.87	811.4845	C ₄₂ H ₇₀ O ₁₂	0.09	273.9539	+HCOO	765.4660, 619.4211, 457.3681, 439.3564, 161.0407, 113.0235, 101.0222	ginsenoside Rg6 isomer (C ₃₀ H ₅₀ O ₃ -Glc-Rha)	C17side-chain
126	30.03	987.5494	C ₅₀ H ₈₄ O ₁₉	-4.11	303.3422	-H	945.5430, 783.4924, 621.4379, 459.3812, 161.0450	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
127	30.43	1033.5592	C ₅₀ H ₈₄ O ₁₉	0.78	310.0754	+HCOO	987.5467, 945.5454, 783.4894, 621.4358, 459.3701	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
128 ^a	30.62	665.4280	C ₃₆ H ₆₀ O ₈	2.41	250.9585	+HCOO	613.3321, 531.3056, 457.3661	ginsenoside Rh4	C17side-chain
129	30.73	975.5532	C ₄₈ H ₈₂ O ₁₇	0.32	291.6078	+HCOO	929.3003, 783.5035, 621.4463, 459.3796, 375.2933, 161.0427	notoginsenoside R1 isomer (PPD-2Glc-Rha)	PPD
130	30.93	975.5520	C ₄₈ H ₈₂ O ₁₇	-1.01	298.3664	+HCOO	783.5004, 621.4355, 459.3812, 375.3036	notoginsenoside R1 isomer (PPD-2Glc-Rha)	PPD
131	31.04	1059.5757	C ₅₂ H ₈₆ O ₁₉	1.68	312.0393	+HCOO	1013.5558, 945.4467, 783.4832, 621.4317, 459.3835, 161.0422, 101.0240	quinquenoside I or its isomer (PPD-3Glc-Bute)	PPD
132 ^b	31.51	1003.5459	C ₄₉ H ₈₂ O ₁₈	-2.03	303.1865	+HCOO	957.5208, 915.5357, 783.4788, 621.4387, 459.3823, 375.2821, 161.0466	PPD-2Glc-Xyl-Ace	PPD
133	32.46	827.4796	C ₄₂ H ₇₀ O ₁₃	0.36	274.2274	+HCOO	781.4764, 457.3776, 373.2716	12- <i>O</i> -glucoginsenoside Rh4 or its isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	C17side-chain
134 ^b	32.56	1075.5680	C ₅₂ H ₈₆ O ₂₀	-0.85	312.8562	+HCOO	1029.5581, 987.5793, 945.5330, 783.4849, 621.4363, 459.3774, 161.0441	PPD-3Glc-2Ace	PPD

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
135 ^a	33.17	829.4953	C ₄₂ H ₇₂ O ₁₃	0.35	272.0082	+HCOO	783.4905, 621.4379, 537.3434, 459.3849	ginsenoside Rg3	PPD
136 ^a	33.55	829.4960	C ₄₂ H ₇₂ O ₁₃	1.29	269.0744	+HCOO	783.4909, 735.3906, 621.4383, 605.3975, 453.3378, 375.3391,	20(R)-ginsenoside Rg3	PPD
137 ^b	33.68	791.4228	C ₄₂ H ₆₄ O ₁₄	1.26	272.1113	-H	659.4431, 497.3576, 455.3523, 101.0264	OA-Glc-Xyl-Ace	OA
138	33.87	793.4387	C ₄₂ H ₆₆ O ₁₄	0.98	272.3516	-H	793.4394, 631.4008, 455.3537, 437.3477, 161.0442, 113.0230, 101.0233	zingibroside R1 or its isomer (OA-GlurA-Glc)	OA
139	34.04	825.4997	C ₄₄ H ₇₄ O ₁₄	-1.05	276.3848	-H	783.4896, 621.4296, 459.3830, 375.2893, 125.0269, 101.0249	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
140	34.23	793.4402	C ₄₂ H ₆₆ O ₁₄	3.50	277.8827	-H	631.3664, 455.3560	zingibroside R1 or its isomer (OA-GlurA-Glc)	OA
141	34.39	801.5004	C ₄₂ H ₇₄ O ₁₄	-0.20	270.3668	-H	783.4826, 621.4439, 459.3865, 375.2853, 131.0318, 101.0238	20(S)-ginsenoside Rf2 isomer (PPT-2Glc-H ₂ O)	PPD
142	34.41	825.5010	C ₄₄ H ₇₄ O ₁₄	0.63	275.5017	-H	783.4826, 621.4439, 569.3867, 459.3854, 161.9168, 101.9052	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
143	34.98	871.5071	C ₄₄ H ₇₄ O ₁₄	1.97	281.3530	+HCOO	783.5001, 621.4582, 459.2947	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
144	35.06	925.4784	C ₄₇ H ₇₄ O ₁₈	-2.01	303.3047	-H	731.4379, 637.3180, 569.3852, 455.3438, 437.3328	araloside A isomer (OA-Rha-GlurA-2H ₂ O-Bute-CO ₂)	OA
145	35.14	871.5039	C ₄₄ H ₇₄ O ₁₄	-1.94	290.6874	+HCOO	825.4977, 783.4739, 621.4324, 459.3825, 375.2971	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
146	35.18	799.4820	C ₄₁ H ₇₀ O ₁₂	-3.18	271.6940	+HCOO	753.4714, 621.4345, 459.3818, 375.2858	ginsenoside Mc or its isomer (PPD-Glc-Xyl)	PPD
147	35.55	799.4829	C ₄₁ H ₇₀ O ₁₂	-2.04	264.0833	+HCOO	753.4668, 621.4362, 459.3863	ginsenoside Mc or its isomer (PPD-Xyl)	PPD
148	35.67	763.4270	C ₄₁ H ₆₄ O ₁₃	-0.52	269.4075	-H	763.4387, 613.3672, 569.3926, 455.3579, 437.3404	pseudoginsenoside RP1 isomer (OA-Glc-Rha)	OA
149	35.79	825.5003	C ₄₄ H ₇₄ O ₁₄	-0.25	280.9750	-H	783.4910, 621.4389, 459.3855, 375.2895, 125.0233, 101.9340	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
150	36.02	797.4657	C ₄₂ H ₇₀ O ₁₄	-4.44	270.1338	-H	553.2920, 455.3616	ginsenoside Rg11 or its isomer (OA-2Glc-H ₂ O)	OA
151	36.16	825.5007	C ₄₄ H ₇₄ O ₁₄	0.17	279.8954	-H	783.4881, 621.4419, 459.3822, 375.2901, 161.1751	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
152 ^b	36.50	809.4682	C ₄₃ H ₇₀ O ₁₄	-0.64	291.9589	-H	627.3844, 537.3550, 455.3491	OA-Glc-Xyl-Ace-H ₂ O	OA
153	36.51	807.4563	C ₄₃ H ₆₈ O ₁₄	3.32	287.1953	-H	763.4665, 627.3844, 537.3550, 455.3495, 101.9318	chikusetsusaponin IVa methyl ester or its isomer (OA-Glc-Rha-CO ₂)	OA
154	36.92	871.5044	C ₄₄ H ₇₄ O ₁₄	-1.33	277.8333	+HCOO	825.4960, 783.5051, 621.4296, 459.3817, 375.3160, 161.0414	ginsenoside Rs3 or isomer (PPD-2Glc-Ace)	PPD

No.	t_R (min)	m/z	Formula	Mass error (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
155 ^a	37.40	811.4848	C ₄₂ H ₇₀ O ₁₂	0.52	281.0793	+HCOO	765.4804, 603.4271, 527.3011, 497.3548	ginsenoside Rk1	C17side-chain
156 ^a	37.56	667.4425	C ₃₆ H ₆₂ O ₈	0.64	244.7200	+HCOO	573.3194, 361.0953	compound K	PPD
157	37.78	1215.6705	C ₆₅ H ₁₀₀ O ₂₁	1.70	329.3682	-H	955.4915, 793.4273, 523.3786, 455.3512	polyacetyleneginsenoside-Ro or its isomer (OA-2GlurA-2Glc-2Ace)	OA
158 ^a	37.81	765.4796	C ₄₂ H ₇₀ O ₁₂	0.17	283.2776	-H	765.4791, 603.4260, 483.3872, 441.3779	ginsenoside Rg5	C17side-chain
159 ^a	38.58	667.4435	C ₃₆ H ₆₂ O ₈	2.25	261.9800	+HCOO	585.3758, 393.5552, 279.2332, 191.8451	20(<i>S</i>)-ginsenoside Rh2	PPD
160 ^b	38.65	631.3862	C ₃₆ H ₅₆ O ₉	2.56	245.4856	-H	631.3836, 455.3516, 113.6973	OA-GlurA	OA
161 ^a	38.89	667.4415	C ₃₆ H ₆₂ O ₈	-0.97	261.1400	+HCOO	615.3587, 559.5748, 459.3857, 125.8741	20(<i>R</i>)-ginsenoside Rh2	PPD
162	39.50	807.4886	C ₄₄ H ₇₂ O ₁₃	-1.77	292.5260	-H	765.4769, 639.2593, 603.4401, 391.5832	ginsenoside Rs4 or its isomer (PPT-GlurA-2H ₂ O-Glc-Ace)	PPT
163	40.18	807.4908	C ₄₄ H ₇₂ O ₁₃	1.02	288.2640	-H	765.47878, 747.4586, 603.4282, 527.2958, 441.3709	ginsenoside Rs4 or its isomer (C ₃₀ H ₅₀ O ₂ -2Glc-Ace)	C17side-chain
164	40.47	807.4912	C ₄₄ H ₇₂ O ₁₃	1.49	292.4049	-H	765.4803, 747.4596, 603.4275, 441.3671, 161.0290	ginsenoside Rs4 or its isomer (C ₃₀ H ₅₀ O ₂ -2Glc-Ace)	C17side-chain

^a Identified by comparison with the reference standards; ^b Ingredients not found in the "in-house ginsenoside library".

Table S9 Information of ginsenosides identified from PQ before and after the steaming.

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
1	1.67	1025.5511	C ₄₈ H ₈₄ O ₂₀	-2.25	294.2480	+HCOO	979.5478, 799.4832, 671.4402, 491.3661, 161.0536	ginsengenin-S3 or its isomer ((PPT+O)-2Glc-2H ₂ O-Mal-Ace)	PPT
2	2.36	961.5375	C ₄₈ H ₈₂ O ₁₉	0.35	293.4059	-H	799.4907, 781.4709, 635.4294, 391.2821	ginsenoside Re7 or its isomer (PPT-GlurA-Rha-Glc-H ₂ O-Bute)	PPT
3 ^b	2.50	1009.5576	C ₄₈ H ₈₄ O ₁₉	-0.83	296.5175	+HCOO	963.5542, 783.4886, 637.4295, 475.3791, 391.2853, 161.0442	PPT-2Glc-Rha-H ₂ O	PPT
4	2.75	1023.5361	C ₄₈ H ₈₂ O ₂₀	-1.53	291.3650	+HCOO	977.5177, 765.4302, 619.4037, 457.3401, 161.0400	ginsengenin-S4 isomer (C ₃₀ H ₅₀ O ₃ -Glc-Rha-GlurA-2H ₂ O)	Others
5	2.93	863.5003	C ₄₂ H ₇₄ O ₁₅	-0.12	266.0640	+HCOO	817.4935, 671.4355, 491.3783, 161.0464, 101.0243	quinquenoside L9 isomer ((PPT+O)-Glc-Rha-H ₂ O)	PPT
6	3.02	991.5292	C ₅₁ H ₇₈ O ₁₆	2.64	290.6694	+HCOO	945.4909, 765.4444, 607.0037, 457.3407	ginsenoside Rg18 isomer (C ₃₀ H ₅₀ O ₃ -GlurA-Glc-Xyl-H ₂ O)	Others
7	3.21	961.5335	C ₄₈ H ₈₂ O ₁₉	-4.47	285.0130	-H	815.4844, 653.4267, 635.4085, 491.3792, 101.8539	ginsenoside Re7 or its isomer ((PPT+O)-2Glc-Rha)	PPT
8 ^b	3.29	849.4825	C ₄₁ H ₇₂ O ₁₅	-2.86	259.0037	+HCOO	803.4657, 671.4336, 509.3811, 491.3549	(PPT+O)-Glc-Xyl-H ₂ O	PPT
9	3.36	863.5005	C ₄₂ H ₇₄ O ₁₅	0.12	266.5045	+HCOO	817.4952, 671.4389, 509.3856, 391.2858	quinquenoside L9 isomer (PPT-GlurA-Rha-Bute-2H ₂ O)	PPT
10	4.08	1153.5996	C ₅₄ H ₉₂ O ₂₃	-0.90	300.5144	+HCOO	1107.5902, 945.5185, 783.4813, 637.4487, 475.3770, 391.2873, 221.0761, 161.0451, 101.0235	ginsenoside Re8 isomer (PPT-3Glc-Rha)	PPT
11	4.52	1153.5980	C ₅₄ H ₉₂ O ₂₃	-2.35	304.7124	+HCOO	1107.5920, 945.5258, 783.4883, 637.4234, 475.3754, 391.2868, 221.0740, 161.0400, 113.0239	ginsenoside Re8 isomer (PPT-3Glc-Rha)	PPT
12	4.84	977.5311	C ₄₇ H ₈₀ O ₁₈	-1.07	279.3779	+HCOO	931.5245, 799.4857, 637.4162, 475.3796, 391.2857, 161.0437, 101.0245	notoginsenoside R1 isomer (PPT-2Glc-Xyl)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
13	5.04	847.5071	C ₄₂ H ₇₄ O ₁₄	2.00	254.4308	+HCOO	801.5078, 637.4354, 607.4165, 475.3996,	floralginsenoside C isomer (PPT-Xyl-GlurA-H ₂ O)	PPT
14	5.39	977.5292	C ₄₇ H ₈₀ O ₁₈	-3.11	281.4226	+HCOO	931.5462, 799.4810, 637.4338, 475.3829	notoginsenoside R1 isomer (PPT-2Glc-Xyl)	PPT
15	5.46	847.5066	C ₄₂ H ₇₄ O ₁₄	1.37	275.0254	+HCOO	801.4974, 655.4746, 535.3922, 475.3897	floralginsenoside C or isomer (PPT-Rha-Glc-H ₂ O)	PPT
16 ^a	5.61	977.5305	C ₄₇ H ₈₀ O ₁₈	-1.72	289.3317	+HCOO	931.5243, 637.4298, 475.3786, 391.2801, 391.2801, 161.0448	notoginsenoside R1	PPT
17	5.89	845.4910	C ₄₂ H ₇₂ O ₁₄	1.38	260.5027	+HCOO	799.4972, 653.4177, 491.3730, 131.0340	24(R)-pseudoginsenoside F11 isomer ((PPT+O)-Glc-Rha)	PPT
18	6.20	977.5337	C ₄₇ H ₈₀ O ₁₈	1.72	284.4563	+HCOO	931.5360, 637.4196, 475.3824, 391.2840, 101.0352	notoginsenoside R1 isomer (PPT-2Glc-Xyl)	PPT
19	6.36	991.5473	C ₄₈ H ₈₂ O ₁₈	-0.53	292.3096	+HCOO	945.5224, 783.4787, 637.4251, 475.3778, 391.2812, 161.0404	ginsenoside Rg18 or its isomer (PPT-2Glc-Rha)	PPT
20 ^a	6.61	845.4899	C ₄₂ H ₇₂ O ₁₄	0.00	266.4300	+HCOO	799.5374, 637.4621, 475.4028,	ginsenoside Rg1	PPT
21 ^a	6.71	945.5422	C ₄₈ H ₈₂ O ₁₈	-0.74	286.4129	-H	783.4896, 637.4320, 475.3792, 391.2852, 161.0453, 101.0243	ginsenoside Re	PPT
22	6.97	845.4898	C ₄₂ H ₇₂ O ₁₄	-0.13	272.1065	+HCOO	799.4772, 727.2917, 457.3608	ginsenoside Rg1 isomer (C ₃₀ H ₅₀ O ₂ -2Glc-H ₂ O)	Others
23	7.10	831.4749	C ₄₁ H ₇₀ O ₁₄	0.89	268.6587	+HCOO	785.4681, 653.4317, 533.3819, 491.3875, 161.0420, 101.0242	pseudoginsenoside RT2 (24R) isomer ((PPT+O)-Glc-Xyl)	PPT
24	7.40	991.5441	C ₄₈ H ₈₂ O ₁₈	-3.91	292.7958	+HCOO	945.5798, 799.4753, 637.4309, 475.3812, 391.2818, 161.0458, 113.0309	ginsenoside Rg18 or its isomer (PPT-2Glc-Rha)	PPT
25	7.58	1025.5531	C ₄₈ H ₈₄ O ₂₀	-0.20	302.7812	+HCOO	989.5274, 799.4798, 637.4181, 491.3655, 161.0472	ginsengenin-S3 or its isomer ((PPT+O)-Glc-2Rha-CO ₂)	PPT
26	8.14	991.5454	C ₄₈ H ₈₂ O ₁₈	-2.54	313.5486	+HCOO	945.5625, 783.4740, 621.4266, 475.3758, 391.2913, 101.0297	ginsenoside Rg18 or its isomer (PPT-2Glc-Rha)	PPT
27	8.28	1031.5431	C ₅₁ H ₈₄ O ₂₁	0.39	287.3672	-H	945.5402, 927.5327, 799.4768, 637.4403, 475.3767, 161.0450, 101.0269	malonyl ginsenoside Rd isomer (PPT-Rha-2Glc-Mal)	Mal
28	8.46	961.5354	C ₄₇ H ₈₀ O ₁₇	-1.97	286.8439	+HCOO	915.5288, 753.4910, 607.4176, 475.3798, 391.2865	ginsenoside Rd2 isomer (PPT-Glc-Rha-Xyl)	PPT
29	8.69	1031.5423	C ₅₁ H ₈₄ O ₂₁	-0.40	313.7505	-H	945.5779, 783.4846, 621.4009, 475.3866, 391.2817, 113.0281	malonyl ginsenoside Rd isomer (PPT-Rha-2Glc-Mal)	Mal

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
30 ^b	8.89	1171.6105	C ₅₄ H ₉₄ O ₂₄	-0.62	323.3967	+HCOO	1125.6065, 963.5603, 783.4756, 621.4295, 475.3657, 221.0674, 161.0452, 101.0241	PPT-Rha-3Glc-H ₂ O	PPT
31	8.94	1033.5564	C ₅₀ H ₈₄ O ₁₉	-2.03	295.8685	+HCOO	987.5658, 945.5602, 783.4715, 637.4339, 475.3834, 391.2857, 161.0475, 113.0232	pseudoginsenoside Rs1 or its isomer (PPT-2Glc-Rha-Ace)	PPT
32	9.08	1139.5806	C ₅₄ H ₉₂ O ₂₅	-4.30	320.3953	-H	1093.5665, 969.4632, 797.4628, 635.4264, 459.2157	notoginsenoside K isomer (PPD-3Glc-GlurA-H ₂ O)	PPD
33	9.16	961.5371	C ₄₇ H ₈₀ O ₁₇	-0.11	290.3490	+HCOO	915.5237, 783.4815, 637.4356, 475.3757, 391.2821, 161.0442, 113.0249, 101.0273	ginsenoside Rd2 isomer (PPT-Glc-Rha-Xyl)	PPT
34	9.18	815.4815	C ₄₂ H ₇₂ O ₁₅	2.08	262.3790	-H	639.4415, 621.4006, 475.3761, 457.3755	ginsenoside Rg12 or its isomer (C ₃₀ H ₅₀ O ₃ -Rha-GlurA-2H ₂ O)	C17side-chain
35 ^b	9.27	887.5006	C ₄₅ H ₇₆ O ₁₇	0.21	272.4357	-H	637.4211, 619.4225, 475.3855, 391.2856, 161.0475, 101.00237	PPT-2Glc-2CO ₂	PPT
36	9.41	863.4991	C ₄₂ H ₇₄ O ₁₅	-1.59	273.3862	+HCOO	817.4816, 655.4438, 637.4257, 491.3684	quiquenoside L9 isomer ((PPT+O)-Glc-Rha-H ₂ O)	PPT
37	9.55	1033.5582	C ₅₀ H ₈₄ O ₁₉	-0.20	298.1181	+HCOO	987.5660, 945.5508, 783.4901, 637.4391, 475.3790, 391.2812, 221.1531, 161.0454	pseudoginsenoside Rs1 or its isomer (PPT-2Glc-Rha-Ace)	PPT
38	9.61	861.4851	C ₄₂ H ₇₂ O ₁₅	0.37	272.7879	+HCOO	815.4708, 653.4352, 491.3808, 161.0434, 113.0229, 101.0245	24(R)-majoroside R1 isomer ((PPT+O)-2Glc)	PPT
39	9.78	863.4978	C ₄₂ H ₇₄ O ₁₅	-3.18	268.5913	+HCOO	817.4828, 655.4436, 537.3318, 375.2922	quiquenoside L9 isomer (PPD-Glc-GlurA-Bute-2H ₂ O)	PPD
40 ^a	9.95	961.5377	C ₄₈ H ₈₂ O ₁₉	0.00	299.9141	-H	915.5369, 799.4878, 637.4311, 475.3871, 22.0660, 101.0226	vinaginsenoside R8	PPD
41	9.99	829.4957	C ₄₂ H ₇₂ O ₁₃	0.89	270.9579	+HCOO	783.5059, 637.4271, 6194186, 475.3745, 161.0440	20(R)-ginsenoside Rg2 isomer (PPT-Glc-Rha)	PPT
42	10.33	1033.5581	C ₅₀ H ₈₄ O ₁₉	-0.30	300.9873	+HCOO	987.5395, 945.5297, 783.5063, 637.4334, 475.3810, 391.2722, 161.0418, 101.0249	pseudoginsenoside Rs1 or its isomer (PPT-2Glc-Rha-Ace)	PPT
43	10.45	1007.5412	C ₄₈ H ₈₂ O ₁₉	-1.56	293.9378	+HCOO	961.5312, 799.4921, 637.4326, 475.3738, 161.0453	20-glucoginsenoside-Rf or its isomer (PPT-3Glc)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
44	10.72	831.4753	C ₄₁ H ₇₀ O ₁₄	1.40	265.8490	+HCOO	785.4700, 653.4173, 491.3740, 131.0396, 115.0398	pseudoginsenoside RT2 (24R) or its isomer (OT-Glc-Xyl)	OT
45 ^b	10.86	1007.5435	C ₄₉ H ₈₄ O ₂₁	0.84	296.3489	-H	921.3486, 843.5233, 681.4558, 475.3822	20-glucoginsenoside-Rf isomer (PPT-2Glc-Rha-CO ₂ -H ₂ O)	PPT
46 ^a	10.97	799.4857	C ₄₂ H ₇₂ O ₁₄	1.00	266.8220	-H	799.4854, 653.4268, 415.3215	24(R)-pseudoginsenoside F11	OT
47 ^a	11.01	699.4355	C ₃₆ H ₆₂ O ₁₀	5.36	245.0100	+HCOO	579.0591	24(R)-pseudoginsenoside RT5	OT
48	11.19	863.5010	C ₄₂ H ₇₄ O ₁₅	-2.94	279.0521	+HCOO	817.4861, 655.4416, 491.3616, 131.0384	quinquenoside L9 isomer (OT-Glc-Rha-H ₂ O)	OT
49 ^a	11.31	799.4826	C ₄₂ H ₇₂ O ₁₄	-2.88	276.2618	-H	637.4405, 475.3719, 391.2866	ginsenoside Rf	PPT
50	11.45	1117.5405	C ₅₄ H ₈₆ O ₂₄	-2.77	310.1954	-H	955.4674, 749.4364, 637.4552, 455.3616, 161.0439	ginsenoside Rb1 isomer (OA-3Glc-Xyl-CO ₂)	OA
51 ^b	11.54	1249.5842	C ₅₉ H ₉₄ O ₂₈	-0.87	343.2062	-H	1117.5328, 925.4590, 793.4188, 731.4349, 551.3732, 455.3490	OA-GlurA-Glc-2Xyl-Ace-H ₂ O	OA
52	11.64	845.4871	C ₄₂ H ₇₂ O ₁₄	-3.50	276.1858	+HCOO	799.4915, 637.4369, 475.3753, 391.2908, 101.0273	ginsenoside Rf isomer (PPT-2Glc)	PPT
53	11.73	1117.5422	C ₅₄ H ₈₆ O ₂₄	-1.25	313.1792	-H	937.4857, 835.4526, 793.4385, 613.3749, 455.3549, 323.1023, 221.0659	ginsenoside Rb1 isomer (OA-GlurA-3Glc)	OA
54	11.84	1315.6491	C ₆₀ H ₁₀₂ O ₂₈	-3.39	324.5765	+HCOO	1269.6466, 1107.5995, 945.5543, 783.5114, 621.4279, 459.3836, 221.0655, 161.0431, 101.0239	ginsenoside Rb5 or its isomer (PPD-5Glc)	PPD
55 ^a	12.13	815.4801	C ₄₁ H ₇₀ O ₁₃	1.04	269.9430	+HCOO	769.4614, 637.4271, 475.3789, 391.2860, 161.045	notoginsenoside R2	PPT
56	12.20	1091.5997	C ₅₄ H ₉₂ O ₂₂	-0.92	311.2398	-H	929.5416, 767.4907, 605.4456, 443.5433, 101.9342	notoginsenoside I or its isomer (C ₃₀ H ₅₂ O ₂ -4Glc)	Others
57	12.33	1151.5847	C ₅₄ H ₉₀ O ₂₃	-0.27	312.8015	+HCOO	1105.5813, 943.5487, 781.4847, 619.4174, 457.3715, 221.0756, 161.0440, 101.0272	epoxynotoginsenoside A or isomer (C ₃₀ H ₅₀ O ₃ -4Glc)	C17side-chain
58	12.41	989.5322	C ₄₈ H ₈₀ O ₁₈	0.11	299.5493	+HCOO	943.5314, 763.4546, 619.4132, 457.3596	chikusetsusaponin FK2 or its isomer (C ₃₀ H ₅₀ O ₃ -3Glc)	Others
59	12.66	1087.5318	C ₅₃ H ₈₄ O ₂₃	-1.10	309.0387	-H	937.4697, 763.4321, 631.3844, 613.3762, 455.3562	stipuleanoside R2 or its isomer (OA-GlurA-Xyl-2Glc)	OA
60 ^a	12.96	815.4785	C ₄₁ H ₇₀ O ₁₃	-1.04	274.3145	+HCOO	637.4274, 475.3772	ginsenoside F3	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
61 ^a	13.12	829.4957	C ₄₂ H ₇₂ O ₁₃	0.89	271.1236	+HCOO	783.4905, 637.4321, 475.3794, 391.2855	20(S)-Ginsenoside Rg2	PPT
62 ^a	13.18	1107.5944	C ₅₄ H ₉₂ O ₂₃	-1.08	310.7186	-H	945.5421, 783.4904, 621.4379, 459.3851, 323.0986	ginsenoside Rb1	PPD
63 ^a	13.22	683.4381	C ₃₆ H ₆₂ O ₉	1.57	248.4510	+HCOO	621.4380, 459.3851	20(S)-ginsenoside Rh1	PPD
64 ^a	13.54	829.4955	C ₄₂ H ₇₂ O ₁₃	0.64	273.3622	+HCOO	783.4903, 637.4326, 475.3793	20(R)-ginsenoside Rg2	PPT
65	13.73	1153.5951	C ₅₄ H ₉₂ O ₂₃	-4.97	313.2782	+HCOO	1107.6158, 945.5335, 783.5043, 621.4440, 459.3914, 221.0698, 161.0453	ginsenoside Rb4 or its isomer (PPD-4Glc)	PPD
66	13.91	683.4382	C ₃₆ H ₆₂ O ₉	1.73	251.8558	+HCOO	637.4307, 475.3810, 391.2882, 161.0433	ginsenoside Rh1 or its isomer (PPT-Glc)	PPT
67 ^a	14.33	1077.5842	C ₅₃ H ₉₀ O ₂₂	-0.84	306.2525	-H	1077.5846, 945.5425, 783.4910, 621.4378, 459.3836, 221.0667, 161.0454, 101.0245	ginsenoside Rc	PPD
68 ^a	14.46	1209.6269	C ₅₈ H ₉₈ O ₂₆	-0.33	314.5877	-H	1107.5905, 615.7417, 465.6027, 323.0995	notoginsenoside Fc	PPD
69	14.67	955.4894	C ₄₈ H ₇₆ O ₁₉	-0.92	287.1824	-H	793.4512, 749.4316, 569.3740, 455.3651	ginsenoside Rd isomer (OA-2Glc-Xyl-CO ₂)	OA
70 ^a	14.82	1193.5923	C ₅₇ H ₉₄ O ₂₆	-1.84	313.0041	-H	1149.6039, 1107.5915, 945.5420, 783.4893, 621.4346, 459.3783	malonyl ginsenoside Rb1	Mal
71	15.12	847.5052	C ₄₂ H ₇₄ O ₁₄	-0.37	269.4097	+HCOO	801.5155, 621.4330, 475.3720, 221.0691, 161.0427, 101.0233	floralginsenoside C or its isomer (PPT-Rha-Glc-H ₂ O)	PPT
72	15.18	1195.6095	C ₅₆ H ₉₄ O ₂₄	-4.61	325.6625	+HCOO	1149.6050, 1107.5855, 945.5434, 783.4856, 621.4380, 459.3824, 221.0681, 161.0440, 101.0236	quinquenoside R1 or its isomer (PPD-4Glc-Ace)	PPD
73	15.32	1193.5959	C ₅₇ H ₉₄ O ₂₆	-0.08	311.9049	-H	1107.6004, 945.5452, 783.4834, 621.4463, 459.3718, 161.0457, 113.0218, 101.0268	malonyl ginsenoside Rb1 or its isomer (PPD-4Glc-Mal)	Mal
74	15.34	955.4900	C ₄₈ H ₇₆ O ₁₉	-0.94	293.2067	-H	793.4247, 749.4514, 603.4256, 459.3827, 221.0639	ginsenoside Ro isomer (PPD-2Glc-Mal-Ace-CO ₂)	PPD
75	15.57	1193.5923	C ₅₇ H ₉₄ O ₂₆	-3.1	315.1018	-H	1107.5915, 1089.5858, 825.5067, 783.4927, 697.4160, 621.4346, 459.3783	malonylginsenoside Rb1 or its isomer (PPD-4Glc-Mal)	Mal
76	15.69	873.4853	C ₄₃ H ₇₂ O ₁₅	0.60	275.6639	+HCOO	827.4751, 785.4846, 653.4148, 491.3859, 161.0494, 113.0275, 101.0261	vinaginsenoside R2 or its isomer (OT-Glc-Xyl-Ace)	OT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
77	15.77	955.4916	C ₄₈ H ₇₆ O ₁₉	1.31	294.1512	-H	775.4323, 731.4527, 613.3912, 455.3511	ginsenoside Rd isomer (OA-Rha-Glc-H ₂ O-Mal-2CO ₂)	OA
78	15.90	1193.5930	C ₅₇ H ₉₄ O ₂₆	-2.51	312.8046	-H	1107.5938, 1077.5842, 945.5411, 783.4914, 621.4360, 459.3787	malonylginsenoside Rb1 or its isomer (PPD-4Glc-Mal)	Mal
79	15.91	1123.5894	C ₅₃ H ₉₀ O ₂₂	-0.56	320.7004	+HCOO	1077.5831, 945.5331, 783.4844, 621.4364, 459.3907, 161.0424, 131.0365, 101.0254	ginsenoside Rb2 isomer (PPD-3Glc-Xyl)	PPD
80	15.95	801.4972	C ₄₂ H ₇₄ O ₁₄	-4.37	264.0994	-H	639.4446, 477.3938, 375.3902, 213.0310, 177.1283	20(S)-ginsenoside Rf2 isomer (PPD-2Xyl-Glc)	PPD
81 ^a	16.27	1123.5894	C ₅₃ H ₉₀ O ₂₂	-0.56	311.0400	+HCOO	1077.5846, 945.5543, 753.4811, 621.4349, 459.3749, 221.0643	ginsenoside Rb2	PPD
82 ^a	16.37	683.4375	C ₃₆ H ₆₂ O ₉	0.63	245.9449	+HCOO	591.3884, 503.2553, 475.3905	20(S)-ginsenoside Rh1	PPT
83	16.48	845.4867	C ₄₂ H ₇₂ O ₁₄	-4.00	268.4266	+HCOO	799.4842, 637.4359, 613.3972, 475.3781	ginsenoside Rf isomer (PPT-2Glc)	PPT
84	16.50	1195.6079	C ₅₆ H ₉₄ O ₂₄	-2.87	321.6655	+HCOO	1149.6015, 1107.5799, 945.5378, 783.4856, 621.4404, 459.3789, 221.0563, 161.0427, 101.0241	quinquenoside R1 or its isomer (PPD-4Glc-Ace)	PPD
85 ^a	16.60	1163.5840	C ₅₆ H ₉₂ O ₂₅	-1.03	308.3210	-H	1077.5838, 945.5422, 783.4384, 621.4377, 459.3832	malonyl ginsenoside Rc	Mal
86	16.66	1087.5319	C ₅₃ H ₈₄ O ₂₃	-1.01	322.0215	-H	955.5015, 749.4380, 523.3856, 375.2883	stipuleanoside R2 isomer (PPD-3Xyl-Glc-CO ₂ -Bute-Ace)	PPD
87 ^a	16.68	1077.5837	C ₅₃ H ₉₀ O ₂₂	-1.30	313.5302	-H	1077.5838, 945.5422, 783.4898, 731.4384, 621.4377, 455.3628	ginsenoside Rb3	OA
88	16.83	1153.5977	C ₅₄ H ₉₂ O ₂₃	-2.62	305.6577	+HCOO	1107.5929, 945.4205, 767.0965, 621.0839, 475.0271	ginsenoside Re8 isomer (PPT-Rha-2Glc)	PPT
89 ^a	17.47	955.4905	C ₄₈ H ₇₆ O ₁₉	-0.42	287.7698	-H	793.4386, 731.4380, 569.3850, 523.3799, 455.3534	ginsenoside Ro	OA
90	17.68	1087.5310	C ₅₃ H ₈₄ O ₂₃	-1.93	324.5390	-H	925.4848, 745.4358, 569.3889, 455.3544, 113.0218	stipuleanoside R2 isomer (OA-3Glc-Mal-Ace-H ₂ O)	OA
91	17.72	1107.5933	C ₅₄ H ₉₂ O ₂₃	-2.08	311.9302	-H	945.5427, 783.4897, 621.4387, 459.3826, 221.0642, 161.0453	ginsenoside Rb1 isomer (PPD-4Glc)	PPD
92	17.88	955.4903	C ₄₈ H ₇₆ O ₁₉	-0.03	297.4557	-H	793.4491, 613.3745, 455.3576, 161.0563, 113.0213	ginsenoside Rd isomer (OA-GlurA-Glc)	OA
93	18.13	955.4907	C ₄₈ H ₇₆ O ₁₉	-0.21	301.1898	-H	793.4383, 731.4327, 455.3539, 161.0476, 131.0370	ginsenoside Rd isomer (OA-GlurA-Glc)	OA

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
94	18.36	861.4843	C ₄₂ H ₇₂ O ₁₅	-0.61	267.7848	+HCOO	815.4747, 699.3893, 537.3442, 475.3795	Vinaginsenoside R15 isomer (PPT-Rha-Xyl-H ₂ O-CO ₂)	PPT
95	18.57	1193.5963	C ₅₇ H ₉₄ O ₂₆	0.20	325.8468	-H	1107.5941, 945.5416, 783.4940, 621.4357, 459.3834, 375.2855, 161.0431, 101.0233	malonylginsenoside Rb1 or its isomer (PPD-4Glc-Mal)	Mal
96 ^a	18.79	1163.5839	C ₅₆ H ₉₂ O ₂₅	-1.38	319.7333	-H	1077.5861, 945.5474, 783.4845, 621.4410, 459.3743	malonyl ginsenoside Rb2	Mal
97	19.19	845.4910	C ₄₂ H ₇₂ O ₁₄	1.38	271.3717	+HCOO	799.4843, 637.4441, 475.3795	ginsenoside Rf isomer (PPT-2Glc)	PPT
98	19.28	857.4895	C ₄₃ H ₇₂ O ₁₄	-0.49	275.5172	+HCOO	811.4823, 799.4843, 621.4376, 569.3843, 391.2928, 161.0457	20(S)-sanchirrhinoside A2 isomer (PPT-2Glc-Bute-CO ₂)	PPT
99	19.33	975.5523	C ₄₈ H ₈₂ O ₁₇	-0.65	292.3328	+HCOO	929.5628, 767.5110, 605.4454, 441.3826, 161.0512, 113.0308, 101.0231	notoginsenoside R1 isomer (C ₃₀ H ₅₀ O ₂ -GlurA-Xyl-H ₂ O)	Others
100	19.61	1195.6107	C ₅₆ H ₉₄ O ₂₄	-0.43	319.6437	+HCOO	1149.6113, 1107.5980, 945.4851, 783.4851, 621.4373, 459.3739, 221.0663, 161.0453, 101.0242	quinquenoside R1 or its isomer (PPD-4Glc-Ace)	PPD
101	19.80	1163.5834	C ₅₆ H ₉₂ O ₂₅	-1.80	314.5457	-H	1077.5710, 945.5307, 783.4762, 621.4385, 459.3906, 375.2915, 161.0396, 101.0221	malonyl ginsenoside Rb2 isomer (PPD-3Glc-Xyl-Mal)	Mal
102	19.91	991.5470	C ₄₈ H ₈₂ O ₁₈	-0.85	294.9189	+HCOO	945.5398, 783.4910, 621.4393, 459.3847, 161.0458, 131.0358, 101.0253	ginsenoside Rd isomei (PPD-3Glc)	PPD
103	20.11	793.4380	C ₄₂ H ₆₆ O ₁₄	0.76	265.2537	-H	631.3680, 455.3489	zingibroside R1 or its isomer (OA-GlurA-Glc)	OA
104	20.25	993.5245	C ₄₈ H ₈₂ O ₂₁	-3.12	288.3462	-H	793.4368, 631.3984, 455.3538	floralginsenoside K isomer (OA-GlurA-Glc-Xyl-Bute)	OA
105 ^a	20.36	925.4794	C ₄₇ H ₇₄ O ₁₈	-0.97	182.5739	-H	793.4368, 569.3851, 455.3538,	araloside A	OA
106 ^a	20.60	945.5423	C ₄₈ H ₈₂ O ₁₈	-0.53	290.2213	-H	783.5422, 621.4373, 459.3845, 375.2903	ginsenoside Rd	PPD
107	20.89	845.4909	C ₄₂ H ₇₂ O ₁₄	1.25	287.8310	+HCOO	799.4926, 619.4100, 457.3627	ginsenoside Rg1 isomer (C ₃₀ H ₅₀ O ₃ -2Glc-H ₂ O)	Others
108 ^a	21.27	925.4796	C ₄₇ H ₇₄ O ₁₈	-0.76	286.4209	-H	763.4282, 619.4336, 455.3548	pseudo-ginsenoside Rt1	OA

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
109	21.46	1193.5928	C ₅₇ H ₉₄ O ₂₆	-2.68	318.8409	-H	1107.5921, 945.5431, 783.4915, 603.4304, 459.3865	malonylginsenoside Rb1 or its isomer (PPD-4Glc-Mal)	Mal
110	21.66	1163.5808	C ₅₆ H ₉₂ O ₂₅	-4.04	316.6829	-H	1077.5878, 945.5418, 783.4866, 621.4370, 459.3835, 221.0666, 161.0384, 101.0284	malonyl ginsenoside Rb2 isomer (PPD-3Glc-Xyl-Mal)	Mal
111	21.72	1165.5980	C ₅₅ H ₉₂ O ₂₃	-2.32	315.2177	+HCOO	1119.5911, 1077.5781, 945.5404, 783.4723, 621.4363, 459.3853, 161.0433, 101.0251	ginsenoside Rs11 or its isomer (PPD-3Glc-Xyl-Ace)	PPD
112	22.13	989.5329	C ₄₈ H ₈₀ O ₁₈	0.85	287.8784	+HCOO	943.5164, 799.4926, 783.1519, 621.4299, 459.3975	chikusetsusaponin FK2 isomer (PPD-Glc-GlurA-Rha)	PPD
113	22.67	871.5059	C ₄₄ H ₇₄ O ₁₄	0.48	280.0750	+HCOO	825.4993, 697.4243, 475.3750	ginsenoside Rs3 isomer (PPT-Glc-Rha-Ace)	PPT
114	24.31	1237.6221	C ₅₉ H ₉₈ O ₂₇	0.33	333.0618	-H	1107.5815, 945.5469, 783.4907, 621.4422, 459.3816	notoginsenoside LK3 isomer (PPD-3Glc-2Rha)	PPD
115 ^a	24.43	793.4380	C ₄₂ H ₆₆ O ₁₄	0.00	259.1592	-H	631.3857, 569.3853, 455.3534	chikusetsusaponin Iva	OA
116 ^a	24.62	1031.5416	C ₅₁ H ₈₄ O ₂₁	-1.55	302.6217	-H	987.5508, 945.5424, 783.4902, 621.4376, 459.3845	malonyl ginsenoside Rd	Mal
117	25.17	1149.6029	C ₅₆ H ₉₄ O ₂₄	-2.87	323.9421	-H	1107.5931, 1089.5809, 945.5360, 783.4901, 621.4485, 459.3842	quinquenoside R1 or its isomer (PPD-4Glc-Ace)	PPD
118	25.61	945.5421	C ₄₈ H ₈₂ O ₁₈	-0.74	288.3055	-H	783.4896, 621.4370, 459.3839, 441.3727, 341.1091	ginsenoside Rd isomer (PPD-3Glc)	PPD
119	25.90	987.5502	C ₅₀ H ₈₄ O ₁₉	-3.24	307.7466	-H	825.4992, 783.4878, 603.4152, 459.3824	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
120	26.63	1175.6192	C ₅₈ H ₉₆ O ₂₄	-1.76	323.9548	-H	1107.5935, 783.4905, 621.4369, 459.3855	ginsenoside Ra6 or its isomer (PPD-4Glc-Bute)	PPD
121	26.71	1031.5425	C ₅₁ H ₈₄ O ₂₁	-0.68	290.5323	-H	945.5430, 783.4907, 621.4366, 459.3843, 375.2960, 221.0707, 161.0473, 101.0259	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	Mal
122	26.96	1033.5564	C ₅₀ H ₈₄ O ₁₉	-2.03	308.7589	+HCOO	987.5582, 945.5428, 783.4833, 621.4411, 459.3853, 375.3037, 161.0456, 101.0255	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
123	27.08	961.5369	C ₄₇ H ₈₀ O ₁₇	-0.33	293.9127	+HCOO	915.5369, 753.4835, 621.4366, 459.3855	ginsenoside Rd2 isomer (PPD-2Glc-Xyl)	PPD
124 ^b	27.38	1165.6007	C ₅₅ H ₉₂ O ₂₃	0.09	319.7359	+HCOO	1119.5808, 1077.5958, 945.5501, 783.4796, 621.4380, 459.3925	ginsenoside Rs11 or its isomer (PPD-3Glc-Xyl-Ace)	PPD
125	27.76	991.5487	C ₄₈ H ₈₂ O ₁₈	0.95	296.4900	+HCOO	945.5490, 783.4932, 765.5063, 621.4500, 459.3769, 161.0399	ginsenoside Rd isomer (PPD-3Glc)	PPD

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
126	27.98	961.5374	C ₄₇ H ₈₀ O ₁₇	0.22	288.4871	+HCOO	915.5267, 783.4832, 621.4375, 459.3827, 293.0914, 125.0251	ginsenoside Rd2 isomer (PPD-2Glc-Xyl)	PPD
127	28.35	1031.5426	C ₅₁ H ₈₄ O ₂₁	-0.08	297.8167	-H	945.5434, 783.4885, 621.4334, 459.3841, 375.2854, 161.0449, 101.0257	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	Mal
128	28.44	961.5373	C ₄₇ H ₈₀ O ₁₇	0.11	289.9476	+HCOO	915.5311, 621.4371, 537.3337, 459.3852, 179.0510	ginsenoside Rd2 isomer (PPD-2Glc-Xyl)	PPD
129	28.59	1033.5568	C ₅₀ H ₈₄ O ₁₉	-1.62	303.4739	+HCOO	987.5507, 945.5399, 783.4900, 621.4376, 459.3842, 375.2901, 221.0639, 161.0445	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
130 ^b	28.69	1073.5518	C ₅₃ H ₈₆ O ₂₂	-1.34	311.8028	-H	945.5371, 783.4841, 621.4502, 459.3745, 161.0414, 101.0244	PPD-3Glc-Mal-Ace	Mal
131 ^b	28.75	997.5058	C ₅₀ H ₇₈ O ₂₀	5.01	309.6920	-H	793.4344, 659.4305, 613.3711, 569.3839, 455.3479	OA-2Glc-2Ace	OA
132	28.78	829.4959	C ₄₂ H ₇₂ O ₁₃	1.15	275.4685	+HCOO	783.5030, 621.4799, 457.3239	3 β ,12 β ,25-trihydroxydammar-(E)-20(22)-ene-6-O- α -L-rhamnopyranosyl-(1 \rightarrow 2)- β -D- glucopyranoside or isomer (C ₃₀ H ₅₀ O ₃ -Glc-Rha- H ₂ O)	C17side- chain
133	28.90	1031.5418	C ₅₁ H ₈₄ O ₂₁	-0.88	291.0413	-H	945.5448, 783.4676, 621.4188, 459.3833	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	Mal
134 ^a	29.12	811.4850	C ₄₂ H ₇₀ O ₁₂	0.78	267.9316	+HCOO	765.4794, 619.4192, 543.2978, 457.3698, 125.0239, 101.9365	ginsenoside Rg6	C17side- chain
135	29.38	1033.5563	C ₅₀ H ₈₄ O ₁₉	-2.13	302.9242	+HCOO	987.5539, 945.5416, 783.4901, 621.4347, 459.3850, 375.2882, 131.5024	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
136	29.39	961.5362	C ₄₇ H ₈₀ O ₁₇	-1.09	286.5769	+HCOO	915.5314, 836.3967, 621.4347, 459.3830, 375.2882, 161.0427, 113.0247	ginsenoside Rd2 isomer (PPD-2Glc-Xyl)	PPD
137	29.46	829.4961	C ₄₂ H ₇₂ O ₁₃	1.40	262.8143	+HCOO	783.4906, 457.3666	3 β ,12 β ,25-trihydroxydammar-(E)-20(22)-ene-6-O- α -L-rhamnopyranosyl-(1 \rightarrow 2)- β -D- glucopyranoside or isomer (C ₃₀ H ₅₀ O ₃ -Glc-Rha- H ₂ O)	C17side- chain

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
138 ^a	29.72	665.4275	C ₃₆ H ₆₀ O ₈	1.61	247.5220	+HCOO	613.3112, 531.3158, 457.3711, 279.2278,	ginsenoside Rk3	C17side-chain
139 ^a	29.90	811.4851	C ₄₂ H ₇₀ O ₁₂	0.91	273.4275	+HCOO	765.4804, 619.4212, 601.4135, 457.3689, 125.0263, 113.9407	ginsenoside F4	C17side-chain
140	30.01	1033.5578	C ₅₀ H ₈₄ O ₁₉	-0.61	304.4936	+HCOO	987.5534, 945.5447, 783.4867, 621.4366, 459.3850	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
141	30.23	1175.6215	C ₅₈ H ₉₆ O ₂₄	-0.34	328.2245	-H	1107.5943, 1089.5725, 823.4168, 459.3863, 305.0826	ginsenoside Ra6 or its isomer (PPD-4Glc-Bute)	PPD
142	30.38	987.5510	C ₅₀ H ₈₄ O ₁₉	-2.43	306.0402	-H	945.5416, 927.5323, 783.4911, 621.4379, 459.3865	quinquenoside III or its isomer (PPD-3Glc-Ace)	PPD
143 ^a	30.59	665.4270	C ₃₆ H ₆₀ O ₈	0.81	251.4256	+HCOO	613.3112, 531.3158, 457.3711, 125.8730, 101.9357	ginsenoside Rh4	C17side-chain
144	30.68	929.5499	C ₄₈ H ₈₂ O ₁₇	2.15	294.1325	-H	857.5320, 783.4903, 621.4356, 537.3598, 459.3907, 101.0241	notoginsenosides NL-C2 or its isomer (PPD-2Glc-Rha)	PPD
145	30.99	1059.5725	C ₅₂ H ₈₆ O ₁₉	-1.48	313.5153	+HCOO	1013.5612, 945.5348, 783.4836, 621.4365, 459.3838	quinquenoside I or its isomer (PPD-3Glc-But)	PPD
146	31.02	827.4767	C ₄₂ H ₇₀ O ₁₃	-3.33	273.1508	+HCOO	781.4665, 629.1141, 443.9656	12-O-glucoginsenoside Rh4 isomer (C ₃₀ H ₅₂ O ₂ -Glc)	C17side-chain
147 ^a	31.15	829.4956	C ₄₂ H ₇₂ O ₁₃	0.77	275.3446	+HCOO	783.4893, 537.3436, 459.3853, 313.2428, 131.0373, 101.9312	ginsenoside F2	PPD
148	31.21	781.4773	C ₄₂ H ₇₀ O ₁₃	3.71	264.7443	-H	619.4185, 537.3435, 457.3696, 279.2381	ginsenoside La or isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	C17side-chain
149 ^b	31.44	1003.5493	C ₄₉ H ₈₂ O ₁₈	1.57	305.9453	+HCOO	957.5328, 915.5316, 783.4789, 621.4375, 459.3828, 375.2857, 161.0407, 101.0220	PPD-2Glc-Xyl-Ace	PPD
150 ^b	31.50	1003.5488	C ₄₉ H ₈₂ O ₁₈	1.04	300.8958	+HCOO	957.5367, 915.5338, 783.4830, 621.4371, 459.3843, 375.2867	PPD-2Glc-Xyl-Ace	PPD
151	31.86	1003.5458	C ₅₀ H ₈₄ O ₂₀	-2.59	298.3825	-H	915.5616, 783.4918, 621.4495, 459.3845	6-acetyl ginsenoside Rg3 isomer (PPD-2Glc-Xyl-2CO ₂)	PPD
152	32.08	871.5027	C ₄₄ H ₇₄ O ₁₄	-3.39	289.4155	+HCOO	825.4761, 783.4982, 585.0595, 459.3931	ginsenoside Rs3 or isomer (PPD-2Glc-Ace)	PPD
153	32.33	829.4931	C ₄₂ H ₇₂ O ₁₃	-2.43	289.7699	+HCOO	783.4768, 745.3704, 621.4305, 459.3829	ginsenoside Rg3 isomer (PPD-2Glc)	PPD

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
154	32.43	827.4789	C ₄₂ H ₇₀ O ₁₃	-0.51	275.2047	+HCOO	781.4843, 619.4140, 457.3691, 131.0348, 101.0277	12- <i>O</i> -glucoginsenoside Rh4 or its isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	C17side- chain
155	32.52	1075.5683	C ₅₃ H ₈₈ O ₂₂	-1.02	317.0536	-H	929.5392, 783.5043, 621.4398, 459.3862, 375.2913, 161.0482	PPD-2Glc-2Rha	PPD
156	32.62	871.5050	C ₄₅ H ₇₆ O ₁₆	-0.59	286.5538	-H	793.4342, 621.4406, 459.3902	notoginsenosides NL-A4 isomer (PPD-2Glc- 2CO ₂)	PPD
157	32.71	1015.5506	C ₅₀ H ₈₂ O ₁₈	2.89	300.0949	+HCOO	969.5314, 837.4111, 783.4977, 621.4364, 459.3837, 375.2972, 161.0414	ginsenoside Ro methyl ester isomer (PPD-Glc- 2Xyl-2Ace)	PPD
158 ^a	33.15	829.4946	C ₄₂ H ₇₂ O ₁₃	-0.51	271.2890	+HCOO	783.4894, 621.4366, 537.3424, 459.3839, 375.2895	ginsenoside Rg3	PPD
159 ^a	33.54	829.4952	C ₄₂ H ₇₂ O ₁₃	0.26	268.5401	+HCOO	783.4903, 621.4370, 537.3428, 459.3844, 375.2905	20(<i>R</i>)-ginsenoside Rg3	PPD
160	33.58	925.4794	C ₄₇ H ₇₄ O ₁₈	-0.97	301.8052	-H	745.4236, 675.3389, 459.3841, 161.0450	ginsenoside Re6 isomer (PPD-GlurA-Glc-Ace- Bute-H ₂ O)	PPD
161	33.83	793.4383	C ₄₂ H ₆₆ O ₁₄	1.01	270.8622	-H	731.4419, 613.3753, 455.3523, 161.0414, 113.0240, 101.0249	zingibroside R1 or its isomer (OA-GlurA-Glc)	OA
162	34.01	825.5001	C ₄₄ H ₇₄ O ₁₄	-0.61	272.4086	-H	783.4901, 621.4384, 537.3413, 459.3843, 375.2890, 161.0454	ginsenoside Rs3 or its isomer (PPD-2Glc1-Ace)	PPD
163	34.21	781.4732	C ₄₂ H ₇₀ O ₁₃	0.00	290.0559	+HCOO	793.4422, 781.4732, 619.4295, 375.4548	ginsenoside Rg10 or its isomer (C ₃₆ H ₅₀ O ₈ -Glc)	C17 side- chain
164	34.40	825.5005	C ₄₄ H ₇₄ O ₁₄	-0.12	273.6719	-H	783.4884, 621.4372, 459.3842, 375.2837, 113.0297	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
165	34.63	827.4832	C ₄₂ H ₇₀ O ₁₃	4.99	266.9208	+HCOO	781.4721, 621.4342, 603.4227, 457.3703	12- <i>O</i> -glucoginsenoside Rh4 or isomer (C ₃₀ H ₅₀ O ₃ - 2Glc)	C17side- chain
166	34.86	829.4915	C ₄₂ H ₇₂ O ₁₃	-4.47	274.3062	+HCOO	783.4838, 621.4249, 459.3855, 375.2850	ginsenoside Rg3 isomer (PPD-2Glc)	PPD
167	35.04	925.4788	C ₄₇ H ₇₄ O ₁₈	-1.51	303.9981	-H	881.4183, 749.4469, 569.3862, 455.3516	araloside A isomer (OA-Glc-2Xyl-CO ₂)	OA
168	35.11	871.5051	C ₄₄ H ₇₄ O ₁₄	-0.48	286.5699	+HCOO	825.4802, 783.4836, 621.4345, 459.3822, 375.2923, 161.0487, 101.0265	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
169	35.14	799.4849	C ₄₁ H ₇₀ O ₁₂	0.66	269.5732	+HCOO	753.4774, 621.4355, 459.3841, 375.2916, 113.0252, 101.0249	ginsenoside Mc or its isomer (PPD-Glc-Xyl)	PPD
170	35.30	829.4962	C ₄₂ H ₇₂ O ₁₃	1.53	270.9366	+HCOO	783.4857, 621.4401, 459.3847, 375.2876, 161.0403, 113.0242	ginsenoside Rg3 isomer (PPD-2Glc)	PPD

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
171	35.48	825.4996	C ₄₄ H ₇₄ O ₁₄	-1.33	284.4664	-H	783.4883, 621.4331, 375.2896, 167.0355, 123.0470	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
172	35.63	763.4252	C ₄₁ H ₆₄ O ₁₃	-3.01	270.6391	-H	687.4169, 613.3819, 569.3941, 455.3513, 113.0226	pseudoginsenoside RP1 or its isomer (OA-GlurA-Xyl)	OA
173	35.77	825.5005	C ₄₄ H ₇₄ O ₁₄	-0.12	282.5302	-H	783.4904, 621.4372, 459.3845, 125.0301	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
174	35.87	793.4382	C ₄₂ H ₆₆ O ₁₄	1.03	275.6892	-H	631.3805, 455.3442, 393.3096, 113.0233	zingibroside R1 or its isomer (OA-GlurA-Glc)	OA
175	36.11	825.5005	C ₄₄ H ₇₄ O ₁₄	-0.12	282.8141	-H	783.4906, 621.4223, 605.3973, 459.3982	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
176	36.91	825.4989	C ₄₄ H ₇₄ O ₁₄	-2.06	284.1828	-H	783.4877, 621.4410, 603.4187, 375.2900, 161.0430	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
177 ^a	37.38	811.4845	C ₄₂ H ₇₀ O ₁₂	0.13	282.7339	+HCOO	765.4796, 603.4268, 527.3012, 441.3739	ginsenoside Rk1	C17side-chain
178 ^a	37.54	667.4426	C ₃₆ H ₆₂ O ₈	0.80	246.7200	+HCOO	559.7212, 419.2196	compound K	PPD
179	37.76	811.4847	C ₄₂ H ₇₀ O ₁₂	0.39	285.8246	+HCOO	765.4772, 603.4429, 459.5240, 441.3610, 161.0428, 113.0240, 101.0243	ginsenoside Rg6 isomer (C ₃₀ H ₅₀ O ₂ -2Glc)	C17side-chain
180 ^a	37.79	765.4795	C ₄₂ H ₇₀ O ₁₂	0.00	280.7800	-H	603.4275, 441.3726, 125.0227, 113.0248	ginsenoside Rg5	C17side-chain
181	38.19	807.4899	C ₄₄ H ₇₂ O ₁₃	-0.12	278.1396	-H	765.4784, 603.4378, 441.3670, 161.0510, 113.0283, 101.0234	ginsenoside Rs4 or its isomer (C ₃₀ H ₅₀ O ₂ -2Glc-Ace)	C17side-chain
182	38.30	959.5007	C ₅₁ H ₇₆ O ₁₇	0.35	283.5716	-H	831.3805, 759.2840, 523.3882, 391.2228	vinaginsenoside R20 isomer (PPT-2Glc-Xyl-CO ₂ -Bute)	PPT
183	38.41	913.5190	C ₄₆ H ₇₆ O ₁₅	3.34	299.4439	+HCOO	867.5279, 783.4932, 459.3761	ginsenoside Re6 or its isomer (PPD-2Glc-2Ace)	PPD
184	38.44	811.4822	C ₄₂ H ₇₀ O ₁₂	-2.87	286.3218	+HCOO	765.4789, 459.3761	ginsenoside Rg6 isomer (PPD-2Xyl-Ace)	PPD
185 ^a	38.54	667.4428	C ₃₆ H ₆₂ O ₈	1.13	260.8200	+HCOO	481.9075	20(S)-ginsenoside Rh2	PPD
186	38.62	807.4899	C ₄₄ H ₇₂ O ₁₃	-0.12	287.0214	-H	765.4805, 603.4263, 441.3779, 161.0461, 101.0256	ginsenoside Rs4 or its isomer (C ₃₀ H ₅₀ O ₂ -2Glc-Ace)	C17side-chain
187 ^b	38.63	631.3850	C ₃₆ H ₅₆ O ₉	0.66	245.8145	-H	555.3721, 455.3543, 113.0229	OA-GlurA	OA

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
188^a	38.86	667.4429	C ₃₆ H ₆₂ O ₈	1.29	261.5600	+HCOO	529.2677, 407.0773	20(<i>R</i>)-ginsenoside Rh2	PPD
189^b	39.11	631.3844	C ₃₆ H ₅₆ O ₉	-0.37	245.6669	-H	555.3681, 455.3506	OA-GlurA	OA
190	39.91	807.4901	C ₄₄ H ₇₂ O ₁₃	0.12	295.5211	-H	765.4886, 603.4519, 455.3476, 279.2326	spinasaponin A methyl ester isomer (OA-Glc-Ace-Mal-H ₂ O-CO ₂)	OA
191	40.45	807.4892	C ₄₄ H ₇₂ O ₁₃	-0.99	292.6263	-H	765.4794, 6034247, 441.3744, 125.0257, 113.0241	ginsenoside Rs4 or its isomer (C ₃₀ H ₅₀ O ₂ -2Glc-Ace)	C17side-chain
192	41.25	833.5187	C ₅₀ H ₇₄ O ₁₀	-2.01	266.5865	-H	571.2878, 391.2304, 161.5509	vinaginsenoside R21 (24 <i>S</i>) isomer (PPT-Glc-GlurA-H ₂ O-Mal)	PPT

^a Identified by comparison with the reference standards; ^b Ingredients not found in the "in-house ginsenoside library".

Table S10 Information of ginsenosides identified from PN before and after the steaming.

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
1 ^b	1.53	879.4952	C ₄₃ H ₇₆ O ₁₈	-0.12	270.1473	-H	671.4368, 635.4269, 509.3759, 391.2846	PPT-2GlurA-2Bute	PPT
2	2.18	995.5413	C ₄₇ H ₈₂ O ₁₉	-1.47	293.0307	+HCOO	949.5395, 769.4757, 637.4291, 607.4207, 457.3824, 161.0428, 113.0255, 101.0236	notoginsenoside NL-E1 or its isomer (C ₃₀ H ₅₀ O ₃ -2Glc-Xyl-2H ₂ O)	C17side-chain
3	2.23	861.4852	C ₄₂ H ₇₂ O ₁₅	0.49	270.5423	+HCOO	815.4739, 653.4377, 503.1762, 491.3657	24(R)-majoroside R1 isomer ((PPT+O)-2Glc)	PPT
4 ^b	2.44	1009.5548	C ₄₉ H ₈₅ O ₂₁	2.39	293.3795	+HCOO	963.5136, 783.4781, 653.4161, 491.3653, 101.0236	(PPT+O)-2Rha-Glc-H ₂ O	PPT
5 ^b	2.62	877.4793	C ₄₃ H ₇₄ O ₁₈	-0.44	273.4229	-H	747.1585, 511.4001, 443.4051	C ₃₀ H ₅₂ O ₂ -GlurA-Dimal-Ace-CO ₂	Others
6	2.78	859.4682	C ₄₂ H ₇₀ O ₁₅	1.11	269.9590	+HCOO	813.4748, 727.1522, 491.6648, 443.3789	notoginsenoside SY4 isomer ((PPT+O)-Rha-GlurA)	PPT
7	3.20	1169.5989	C ₅₄ H ₉₂ O ₂₄	3.03	304.5396	+HCOO	1123.5885, 961.5536, 799.4706, 637.4226, 475.315, 221.0136	6-O-[β -D-glucopyranosyl-(1 \rightarrow 2)- β -D-glucopyranosyl]-20-O-[β -D-glucopyranosyl-(1 \rightarrow 4)- β -D-glucopyranosyl]-20(S)-protopanaxatriol isomer (PPT-4Glc)	PPT
8	3.47	1139.5822	C ₅₃ H ₉₀ O ₂₃	-2.56	298.4080	+HCOO	1093.5777, 961.5340, 637.4333, 475.3811, 323.1009, 109.4646	ginsenoside Rb3 isomer (PPD-3Glc-Xyl)	PPT
9	3.88	961.5365	C ₄₈ H ₈₂ O ₁₉	-1.35	281.8759	-H	799.4882, 637.4322, 475.3791, 323.0940, 245.0700, 143.0358	notoginsenoside R3 or its isomer (PPT-3Glc)	PPT
10	4.09	1107.5904	C ₅₄ H ₉₂ O ₂₃	-4.69	299.9046	-H	945.5411, 799.4856, 637.4332, 475.3766, 323.0916, 193.7572, 143.0353	ginsenoside Re8 or its isomer (PPT-3Glc-Rha)	PPT
11	4.32	1007.5414	C ₄₈ H ₈₂ O ₁₉	-1.35	284.7329	+HCOO	961.5349, 799.5149, 637.4289, 475.3772	notoginsenoside R6 or its isomer (PPT-3Glc)	PPT
12 ^b	4.46	833.4913	C ₄₁ H ₇₂ O ₁₄	1.78	256.1242	+HCOO	787.4973, 655.4381, 637.4376, 491.8094, 161.0468, 113.5846, 101.0246	(PPT+O)-Rha-Xyl-H ₂ O	PPT
13	4.52	1153.6006	C ₅₄ H ₉₂ O ₂₃	0.00	300.8320	+HCOO	1107.5939, 961.5192, 783.5085, 637.4194, 475.3877	ginsenoside Re8 isomer (PPT-Glc-2Rha-2Bute-Ace)	PPT
14	4.67	701.4471	C ₃₆ H ₆₄ O ₁₀	-0.76	237.7905	+HCOO	655.4535, 391.2765, 273.1893	ginsenoside Rh12 isomer (PPT-2Xyl)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
15	4.84	1007.5439	C ₄₈ H ₈₂ O ₁₉	1.25	285.9817	+HCOO	961.5477, 799.4742, 475.3790, 391.2832, 161.0426, 113.0240, 101.0227	notoginsenoside R6 or its isomer (PPT-3Glc)	PPT
16	5.13	831.4745	C ₄₁ H ₇₀ O ₁₄	0.38	258.0328	+HCOO	785.4631, 653.4301, 491.3730, 389.2723, 307.2624	pseudoginsenoside RT2 (24R) isomer ((PPT+O)-Glc-Xyl)	PPT
17	5.28	977.5307	C ₄₇ H ₈₀ O ₁₈	-1.50	281.4020	+HCOO	931.5269, 799.4754, 637.4325, 475.3800, 391.2832, 275.1531	notoginsenoside R1 or its isomer (PPT-2Glc-Xyl)	PPT
18	5.53	977.5327	C ₄₇ H ₈₀ O ₁₈	0.64	286.0317	+HCOO	931.5391, 769.4594, 637.4336, 475.3797, 391.2846, 349.2699, 161.0451, 101.0243	notoginsenoside R1 or its isomer (PPT-2Glc-Xyl)	PPT
19	5.77	1007.5435	C ₄₈ H ₈₂ O ₁₉	0.83	288.4316	+HCOO	961.5379, 799.4839, 475.3755, 391.2887, 161.0456, 101.0240	notoginsenoside R6 or its isomer (PPT-3Glc)	PPT
20	5.85	845.4897	C ₄₂ H ₇₂ O ₁₄	-0.25	261.6947	+HCOO	799.4821, 653.4224, 491.3729,	24(R)-pseudoginsenoside F11 isomer ((PPT+O)-Glc-Rha)	PPT
21	6.17	977.5320	C ₄₇ H ₈₀ O ₁₈	-0.11	284.7214	+HCOO	931.5282, 799.4657, 637.4327, 475.3798, 391.2834, 257.1611, 161.0451, 101.0260	notoginsenoside R1 or its isomer (PPT-2Glc-Xyl)	PPT
22	6.28	1121.5721	C ₅₄ H ₉₀ O ₂₄	-2.50	244.5443	-H	959.5245, 797.4663, 637.4323, 553.3268, 391.2849, 373.2724, 261.2597	notoginsenoside B isomer (PPT-3Glc-Rha-GlurA-2Ace)	PPT
23	6.41	1169.5984	C ₅₄ H ₉₂ O ₂₄	2.58	314.5736	+HCOO	1123.6065, 961.5509, 799.4754, 637.4269, 475.3954, 221.0607, 113.0258	6-O-[β -D-glucopyranosyl-(1 \rightarrow 2)- β -D-glucopyranosyl]-20-O-[β -D-glucopyranosyl-(1 \rightarrow 4)- β -D-glucopyranosyl]-20(S)-protopanaxatriol isomer (PPT-4Glc)	PPT
24 ^a	6.59	799.4840	C ₄₂ H ₇₂ O ₁₄	-1.13	205.4975	-H	637.4326, 475.3796, 391.2851, 273.9767	ginsenoside Rg1	PPT
25 ^a	6.70	945.5420	C ₄₈ H ₈₂ O ₁₈	-0.85	285.8238	-H	783.4894, 637.4894, 475.3791, 391.2851, 161.0454	ginsenoside Re	PPT
26	6.92	1003.5477	C ₅₀ H ₈₄ O ₂₀	-0.60	290.9381	-H	943.5367, 825.5165, 781.4679, 605.6287, 491.3661	6-acetyl ginsenoside Rg3 isomer ((PPT+O)-2Glc-Mal-2Ace-H ₂ O)	PPT
27	7.19	1007.5435	C ₄₈ H ₈₂ O ₁₉	0.83	289.6646	+HCOO	961.5226, 799.4807, 621.4153, 475.3805	notoginsenoside R6 or its isomer (PPT-3Glc)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
28	7.26	947.5247	C ₄₆ H ₇₈ O ₁₇	3.44	276.8730	+HCOO	901.5102, 769.4554, 619.4131, 457.3372	notoginsenoside Rw1 isomer (C ₃₀ H ₅₀ O ₃ -Glc-2Xyl-H ₂ O)	Others
29	7.34	699.4328	C ₃₇ H ₆₄ O ₁₂	1.18	247.6544	-H	587.4450, 475.3787	dammar-9(11),24-dien-3 β -ol-3 α -L-arabinosyl-7 α -octanoate isomer (PPT-Dimal-2CO ₂)	PPT
30	7.52	845.4900	C ₄₂ H ₇₂ O ₁₄	0.13	267.0211	+HCOO	799.4819, 621.4271, 459.3869	notoginsenoside U isomer (PPD-Rha-GlurA-H ₂ O)	PPD
31	7.64	1169.5935	C ₅₄ H ₉₂ O ₂₄	-1.78	313.2135	+HCOO	1123.5854, 961.5306, 799.4854, 637.4350, 475.3794, 391.2944, 221.0691, 161.0447, 101.0246	6-O-[β -D-glucopyranosyl-(1 \rightarrow 2)- β -D-glucopyranosyl]-20-O-[β -D-glucopyranosyl-(1 \rightarrow 4)- β -D-glucopyranosyl]-20(S)-protopanaxatriol isomer (PPT-4Glc)	PPT
32	7.91	947.5205	C ₄₆ H ₇₈ O ₁₇	-1.22	284.9547	+HCOO	901.5145, 607.4213, 475.3786, 391.2870, 349.2811, 161.0498, 113.0252, 101.0235	notoginsenoside Rw1 or its isomer (PPT-2Xyl-Glc)	PPT
33	8.04	841.4957	C ₄₄ H ₇₄ O ₁₅	0.24	262.4159	-H	637.4206, 553.3430, 517.3897, 475.3841, 339.3760, 161.0419, 113.0254	notoginsenoside Rt or its isomer (PPT-2Glc-Ace)	PPT
34	8.28	1031.5428	C ₅₁ H ₈₄ O ₂₁	-0.48	286.0586	-H	945.5420, 783.4947, 475.3752, 391.2807, 161.0448, 113.0275, 101.0298	malonylginsenoside Rd isomer (PPT-2Glc-Rha-Mal)	Mal
35	8.32	947.5208	C ₄₆ H ₇₈ O ₁₇	-0.89	285.2338	+HCOO	901.5143, 637.4305, 553.3414, 475.3804, 391.2882, 161.0444, 101.0252	notoginsenoside Rw1 or its isomer (PPT-2Xyl-Glc)	PPT
36 ^b	8.67	1019.5408	C ₄₉ H ₈₂ O ₁₉	-1.95	297.4703	+HCOO	973.5274, 931.5332, 769.4856, 637.4293, 475.3796, 391.2804, 161.0399, 113.0250, 101.0223	PPT-2Glc-Xyl-Ace	Mal
37	8.76	1007.5414	C ₄₈ H ₈₂ O ₁₉	-1.35	298.3667	+HCOO	961.5364, 799.4788, 637.4261, 475.3777, 391.2841, 161.0449, 113.0206, 101.0217	notoginsenoside R6 or its isomer (PPT-3Glc)	PPT
38	8.95	1031.5449	C ₅₁ H ₈₄ O ₂₁	1.55	293.4060	-H	945.5280, 927.5349, 783.4906, 637.4752, 475.3823, 375.4996	malonylginsenoside Rd isomer (PPT-2Glc-Rha-Mal)	Mal
39	9.01	841.4949	C ₄₄ H ₇₄ O ₁₅	-0.71	268.2354	-H	637.4275, 475.3828, 391.2815	notoginsenoside Rt or its isomer (PPT-2Glc-Ace)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
40	9.18	815.4797	C ₄₁ H ₇₀ O ₁₃	0.52	263.2397	+HCOO	769.4837, 637.4325, 475.3779, 391.2926, 161.0465, 113.0236, 101.0254	ginsenoside F3 isomer (PPT-Glc-Xyl)	PPT
41	9.33	1185.5899	C ₅₄ H ₉₂ O ₂₅	-0.44	316.1242	+HCOO	1139.5918, 961.5477, 799.4786, 475.3795	notoginsenoside K isomer (PPT-3Glc-2Bute-Ace)	PPT
42	9.42	841.4955	C ₄₄ H ₇₄ O ₁₅	0.00	267.0770	-H	637.4317, 603.3815, 475.3786	notoginsenoside Rt or its isomer (PPT-2Glc-Ace)	PPT
43	9.56	1007.5425	C ₄₈ H ₈₂ O ₁₉	-0.21	298.4764	+HCOO	961.5367, 781.4743, 637.4296, 475.3782	notoginsenoside R6 or its isomer (PPT-3Glc)	PPT
44	9.73	815.4797	C ₄₁ H ₇₀ O ₁₃	0.52	261.0483	+HCOO	769.4715, 655.4397, 491.3759	ginsenoside F3 isomer ((PPT+O)-Rha-Xyl)	PPT
45	9.78	863.4991	C ₄₂ H ₇₄ O ₁₅	-1.59	268.4685	+HCOO	817.5038, 655.4397, 475.3800	quinquenoside L9 isomer (PPT-2Glc-H ₂ O)	PPT
46	9.85	745.3985	C ₄₃ H ₅₆ O ₈	4.72	253.5044	+HCOO	699.3947, 637.4329, 475.3800	dammar-9(11),24-dien-3 β -ol-3 α -L-arabinosyl-7 α -octanoate isomer (PPT-Glc-CO ₂ -H ₂ O)	PPT
47	9.94	961.5358	C ₄₈ H ₈₂ O ₁₉	-1.98	295.1046	-H	799.4849, 637.4329, 475.3794, 323.0991, 193.0493, 113.0243	notoginsenoside R3 or its isomer (PPT-3Glc)	PPT
48	10.08	959.5218	C ₄₇ H ₇₈ O ₁₇	0.22	282.0297	+HCOO	913.5416, 619.4253, 457.3753, 161.0443, 113.0289, 101.0237	notoginsenoside Ng1 or isomer (C ₃₀ H ₅₀ O ₃ -2Glc-Xyl)	C17side-chain
49 ^b	10.24	1009.5548	C ₅₅ H ₈₀ O ₁₄	2.39	297.3842	+HCOO	963.5525, 801.5106, 783.4859, 621.4326, 475.3772, 221.0669, 161.0409, 101.0227	PPT-Rha-2Glc-H ₂ O	PPT
50	10.39	829.4930	C ₄₂ H ₇₂ O ₁₃	-2.55	267.4937	+HCOO	783.4877, 637.4314, 621.4314, 475.3881, 391.2806, 279.2332	20(R)-Ginsenoside Rg2 isomer (PPT-Rha-Glc)	PPT
51	10.48	1023.5353	C ₄₈ H ₈₂ O ₂₀	-2.35	301.9134	+HCOO	977.5597, 797.5111, 765.4405, 603.3952, 441.3279	notoginsenoside E isomer (C ₃₀ H ₅₀ O ₂ -2Glc-GlurA-2H ₂ O)	C17side-chain
52	10.72	845.4903	C ₄₂ H ₇₂ O ₁₄	0.50	264.9386	+HCOO	799.4736, 637.4263, 475.3881	notoginsenoside U isomer (PPT-Glc-Bute-CO ₂)	PPT
53	10.77	1371.6770	C ₆₂ H ₁₀₂ O ₃₀	-2.04	336.9801	+HCOO	1325.5715, 1107.5893, 945.5382, 783.4831, 621.4425, 459.3884, 221.0640, 161.0507	malonylginsenoside Ra3 or its isomer (PPD-4Glc-Xyl-Mal)	PPD
54	10.89	845.4895	C ₄₂ H ₇₂ O ₁₄	-0.50	259.0907	+HCOO	799.5136, 637.4503, 475.3760, 391.2883, 221.0623, 113.0260, 101.0265	notoginsenoside U or its isomer (PPT-2Glc)	PPT
55	10.97	1315.6527	C ₆₀ H ₁₀₂ O ₂₈	-0.55	325.0435	+HCOO	1269.6524, 1107.6006, 945.5512, 783.4911, 621.4442, 459.3722, 161.0448, 101.0309	ginsenoside Rb5 or its isomer (PPD-5Glc)	PPD

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
56	11.16	913.5160	C ₄₆ H ₇₆ O ₁₅	-0.12	271.6849	+HCOO	867.5191, 637.4338, 475.3795, 391.2878, 113.0250	ginsenoside Re6 or its isomer (PPT-2Glc-Bute)	PPT
57	11.28	977.5324	C ₄₇ H ₈₀ O ₁₈	0.32	278.9433	+HCOO	931.5359, 799.5076, 637.4242, 475.3675, 221.0590, 161.0550, 101.0258	notoginsenoside R1 or its isomer (PPT-2Glc-Xyl)	PPT
58 ^a	11.31	799.4851	C ₄₂ H ₇₂ O ₁₄	0.25	274.1938	-H	637.4323, 475.3789, 113.0350	ginsenoside Rf	PPT
59 ^a	11.37	1239.6353	C ₅₉ H ₁₀₀ O ₂₇	-2.10	207.9292	-H	1107.5932, 945.5418, 783.4398, 621.4398, 459.3865, 293.0824, 275.0771	notoginsenoside R4	PPD
60	11.60	845.4897	C ₄₂ H ₇₂ O ₁₄	-0.25	277.8195	+HCOO	799.4839, 637.4349, 475.3793	notoginsenoside U or its isomer (PPT-2Glc)	PPT
61	11.63	1269.6492	C ₆₀ H ₁₀₂ O ₂₈	0.55	328.2669	-H	945.5783, 621.4524, 475.3768	ginsenoside Rb5 isomer (PPT-4Glc-Rha)	PPT
62	11.75	947.5207	C ₄₆ H ₇₈ O ₁₇	-1.00	288.5676	+HCOO	901.4924, 769.4603, 637.4268, 475.3797, 391.2862, 113.0261, 101.0248	notoginsenoside Rw1 or its isomer (PPT-2Xyl-Glc)	PPT
63	11.90	1151.5837	C ₅₄ H ₉₀ O ₂₃	-1.18	312.7104	+HCOO	1105.5637, 929.5470, 641.6102, 459.3857	epoxynotoginsenoside A isomer (PPD-2Glc-Rha-GlurA)	PPD
64 ^a	12.00	1239.6370	C ₅₉ H ₁₀₀ O ₂₇	-0.73	209.1995	-H	1107.5944, 945.5409, 783.4893, 621.4383, 459.3857, 375.2902, 221.0669, 161.0461, 101.0256	notoginsenoside Fa	PPD
65 ^a	12.14	815.4798	C ₄₁ H ₇₀ O ₁₃	0.65	268.6183	+HCOO	769.4746, 619.4228, 475.3794, 331.2658	ginsenoside F3	PPT
66	12.31	1105.5802	C ₅₄ H ₉₀ O ₂₃	0.09	308.0361	-H	943.5276, 781.4975, 457.3836, 161.0452	epoxynotoginsenoside A or its isomer (C ₃₀ H ₅₀ O ₃ -4Glc)	C17side-chain
67 ^a	12.42	815.4802	C ₄₁ H ₇₀ O ₁₃	1.17	271.3180	+HCOO	769.5890, 637.4194, 475.3793, 389.2689	notoginsenoside R2	PPT
68	12.56	769.4770	C ₄₁ H ₇₀ O ₁₃	3.51	269.9768	-H	637.4284, 595.1609, 475.3793, 279.2355	20(R)notoginsenoside R2 or its isomer (PPT-Glc-Xyl)	PPT
69	12.69	683.4363	C ₃₇ H ₆₄ O ₁₁	-0.97	248.0056	-H	619.4125, 553.3255, 457.3354	notoginsenoside SP20 isomer (C ₃₀ H ₅₀ O ₃ -Rha-2H ₂ O-CO ₂)	OT
70	12.94	815.4802	C ₄₁ H ₇₀ O ₁₃	-1.82	269.4477	+HCOO	769.4870, 637.4307, 475.3794, 391.2857, 161.0448, 113.0265, 101.0240	notoginsenoside R2 isomer (PPT-Glc-Xyl)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
71	13.06	619.3153	C ₃₃ H ₄₈ O ₁₁	5.59	205.9181	-H	459.3829, 375.2856	ginsenoside Rh16 isomer (PPD-GlurA-Bute)	PPD
72 ^a	13.10	783.4905	C ₄₂ H ₇₂ O ₁₃	0.64	269.9109	-H	619.4229, 529.3927, 439.3592, 411.1628, 311.0986, 179.0561	20(S)-Ginsenoside Rg2	PPT
73 ^a	13.21	1107.5942	C ₅₄ H ₉₂ O ₂₃	-1.26	309.9995	-H	945.5422, 783.4905, 621.4375, 459.3849, 341.1030, 263.0794, 167.0405	ginsenoside Rb1	PPD
74 ^a	13.53	829.4960	C ₄₂ H ₇₂ O ₁₃	1.28	273.6401	+HCOO	783.4907, 637.4331, 475.3799, 329.2338, 113.9419	20(R)-Ginsenoside Rg2	PPT
75	13.90	683.4389	C ₃₆ H ₆₂ O ₉	2.82	344.9810	+HCOO	637.4327, 545.3930, 475.3796, 101.0251	ginsenoside Rh1 or isomer (PPT-Glc)	PPT
76 ^a	14.31	1123.5900	C ₅₃ H ₉₀ O ₂₂	0.00	310.8251	+HCOO	1077.5848, 947.5429, 765.4716, 621.4384, 459.3892, 311.0930	ginsenoside Rc	PPD
77	14.37	857.4908	C ₄₃ H ₇₂ O ₁₄	1.11	277.9940	+HCOO	811.4858, 769.4652, 637.4298, 475.3796, 391.2804, 161.0415, 101.0230	yesanchinoside A (24S) isomer (PPT-Glc-Xyl-Ace)	PPT
78	14.41	1209.6255	C ₅₈ H ₉₈ O ₂₆	-1.49	314.6365	-H	1077.5646, 945.5474, 783.4784, 621.4414, 459.4094, 161.0426, 113.0235, 101.2781	ginsenoside Ra1 isomer (PPD-3Glc-2Xyl)	PPD
79	14.42	1107.5946	C ₅₄ H ₉₂ O ₂₃	-0.90	308.3887	-H	945.5443, 783.4900, 765.4863, 621.4345, 459.3914, 323.0986, 293.0896, 191.0573, 101.0237	ginsenoside Rb1 isomer (PPD-4Glc)	PPD
80 ^a	14.43	1209.6250	C ₅₈ H ₉₈ O ₂₆	-1.98	254.9766	-H	1107.5958, 1077.5824, 945.5449, 783.4900, 459.3847, 375.2832, 279.2282, 191.0563, 161.0429	ginsenoside Ra1	PPD
81	14.65	1325.6376	C ₆₂ H ₁₀₂ O ₃₀	-0.53	325.6882	-H	1239.6171, 1107.6141, 945.5501, 783.4692, 621.4537, 459.3852, 221.0654, 161.0460, 113.0245	malonylginsenoside Ra3 or its isomer (PPD-4Glc-Xyl-Mal)	Mal
82 ^a	14.79	1193.5940	C ₅₇ H ₉₄ O ₂₆	-1.68	238.6466	-H	1107.5939, 945.5429, 783.4904, 621.4362, 459.3863, 341.1084, 227.0505	malonyl ginsenoside Rb1	Mal
83	15.08	857.4905	C ₄₄ H ₇₄ O ₁₆	0.12	273.5733	-H	767.6952, 693.3497, 475.3766, 473.3635, 401.3512, 101.9374	yesanchinoside A (24S) isomer (PPT-Xyl-Rha-Mal-H ₂ O)	PPT
84	15.22	1149.6048	C ₅₆ H ₉₄ O ₂₄	-1.30	325.0721	-H	1107.9717, 783.4882, 621.4361, 459.3858, 323.0960, 179.0561	6"-O-acetylginsenoside Rb1 or its isomer (PPD-4Glc-Ace)	PPD
85	15.55	1107.5913	C ₅₄ H ₉₂ O ₂₃	-3.43	312.8466	-H	945.5440, 783.4822, 697.4188, 459.7560	ginsenoside Rb1 isomer (PPD-4Glc)	OA

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
86	15.65	825.4981	C ₄₄ H ₇₄ O ₁₄	-3.15	269.6732	-H	783.4919, 637.4423, 475.3767, 391.2908, 279.2269	20(S)-6'-O-acetyl-ginsenoside Rg2 or its isomer (PPT-Glc-Rha-Ace)	PPT
87	15.85	1123.5886	C ₅₃ H ₉₀ O ₂₂	-1.30	318.9303	+HCOO	1077.5759, 945.5397, 783.4895, 621.4366, 459.3858, 161.0462, 113.0274, 101.0231	ginsenoside Rb3 isomer (PPD-4Glc)	PPD
88	15.89	1193.5940	C ₅₇ H ₉₄ O ₂₆	-1.68	310.1600	-H	1077.5832, 945.5409, 783.4909, 621.4364, 459.3845, 311.0956, 251.0796, 191.0562, 161.0451, 113.0247	malonyl ginsenoside Rb1 isomer (PPD-4Glc-Mal)	Mal
89	15.91	849.4982	C ₄₆ H ₇₄ O ₁₄	-2.83	267.9908	-H	801.4876, 799.4642, 639.4396, 475.3794, 407.3344, 161.0451, 113.0250	chikusetsusaponin IVa butyl ester isomer (PPT- 2Glc-Xyl-H ₂ O)	PPD
90	16.08	679.4430	C ₃₈ H ₆₄ O ₁₀	0.59	245.0777	-H	637.4299, 475.3791, 307.1116, 101.9322	3-β-acetoxyl ginsenoside F1 or its isomer (PPT- Glc-Ace)	PPT
91	16.25	1123.5884	C ₅₃ H ₉₀ O ₂₂	-2.32	309.6774	+HCOO	1077.5832, 945.5317, 783.4727, 621.4382, 459.3865, 179.0551	ginsenoside Rb3 isomer (PPD-3Glc-Xyl)	PPD
92 ^a	16.34	637.4318	C ₃₆ H ₆₂ O ₉	-0.63	244.4589	-H	547.3212, 475.3752, 391.2870, 113.0229	20(S)-ginsenoside F1	PPT
93	16.41	841.4937	C ₄₄ H ₇₄ O ₁₅	-2.14	266.2916	-H	799.4975, 517.3970, 475.3788, 433.2860, 221.0648, 113.0233, 101.0245	notoginsenoside Rt isomer (PPT-Rha-2Ace- Dimal)	PPT
94	16.61	1123.5902	C ₅₃ H ₉₀ O ₂₂	0.19	314.0124	+HCOO	1077.5871, 945.5383, 783.4885, 621.4321, 459.3921, 161.0491, 101.0235	ginsenoside Rb3 isomer (PPD-3Glc-Xyl)	PPD
95	16.65	1087.5337	C ₅₃ H ₈₄ O ₂₃	0.64	318.4092	-H	955.4781, 749.4405, 731.4395, 455.3538, 119.0333	stipuleanoside R2 isomer (OA-Glc-Xyl-Rha-Ace- H ₂ O)	OA
96	16.72	785.4696	C ₄₀ H ₆₈ O ₁₂	1.08	261.4690	+HCOO	739.4671, 607.4235, 475.3790, 375.2911	(20S)-6-O-[β-D-xylopyranosyl-(1→2)-β-D- xylopyranosyl] dammar-24-ene-3β,6α,12β,20- tetrol or its isomer (PPT-2Xyl)	PPT
97	16.74	843.4754	C ₄₂ H ₇₀ O ₁₄	1.50	274.8145	+HCOO	797.4601, 635.4064, 475.8593	12-one-pseudoginsenoside F11 isomer (PPT-Rha- GlurA)	PPT
98	17.08	975.5496	C ₅₅ H ₇₈ O ₁₂	2.80	286.2764	+HCOO	929.5653, 783.5009, 637.4246, 475.3812	notoginsenosides NL-C1 isomer (PPT-Glc-2Rha)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
99	17.15	977.5355	C ₄₇ H ₈₀ O ₁₈	3.65	297.7689	+HCOO	931.5536, 799.5071, 637.4161, 475.3717, 391.2877, 161.0437, 101.0268	notoginsenoside R1 or its isomer (PPT-2Glc-Xyl)	PPT
100	17.33	1077.5850	C ₅₃ H ₉₀ O ₂₂	-0.09	317.7680	-H	945.5418, 915.5317, 783.4914, 765.4876, 621.4381, 459.3863	ginsenoside Rb3 isomer (PPD-3Glc-Xyl)	PPD
101	17.48	955.4900	C ₄₈ H ₇₆ O ₁₉	-0.84	289.1661	-H	793.4413, 731.4364, 631.3728, 455.3504, 161.0465	ginsenoside Ro isomer (OA-2Glc-GlurA)	OA
102	17.64	1087.5333	C ₅₃ H ₈₄ O ₂₃	0.28	325.1549	-H	925.4818, 763.4321, 569.3849, 551.3742, 455.3534, 113.0265	stipuleanoside R2 isomer (OA-3Glc-Rha)	OA
103	17.95	1123.5874	C ₅₃ H ₉₀ O ₂₂	-2.41	304.9528	+HCOO	1077.5736, 945.5527, 783.4885, 621.4514, 459.3759, 221.0667, 161.0437, 101.0241	ginsenoside Rb3 isomer (PPD-3Glc-Xyl)	PPD
104 ^a	18.15	955.4912	C ₄₈ H ₇₆ O ₁₉	0.42	236.2568	-H	793.4389, 569.3864, 455.3595	ginsenoside Ro	OA
105	18.66	1195.6089	C ₅₆ H ₉₄ O ₂₄	-2.00	321.6457	+HCOO	1149.6057, 1107.5933, 945.5497, 783.4900, 621.4354, 459.3826, 221.0654, 161.0493, 101.0210	6"-O-acetylginsenoside Rb1 isomer (PPD-4Glc-Ace)	PPD
106	19.09	845.4911	C ₄₂ H ₇₂ O ₁₄	1.50	272.7396	+HCOO	799.4876, 637.4237, 475.3740, 391.2863	notoginsenoside U or its isomer (PPT-2Glc)	PPD
107	19.20	975.5523	C ₄₈ H ₈₂ O ₁₇	-0.65	297.6808	+HCOO	929.5349, 767.5045, 605.4482, 443.3914, 161.0506, 113.0244, 101.0269	notoginsenosides NL-C1 isomer (C ₃₀ H ₅₀ O ₂ -3Glc)	others
108	19.26	857.4897	C ₄₃ H ₇₂ O ₁₄	-0.25	276.9538	+HCOO	811.4848, 769.4789, 637.4253, 475.3803, 113.0267	20(S)-sanchirrhinoside A2 or isomer (PPT-Glc-Xyl-Ace)	PPT
109	19.63	1195.6057	C ₅₆ H ₉₄ O ₂₄	-4.78	322.9326	+HCOO	1149.5961, 1107.6193, 945.5198, 783.5067, 621.4373, 459.3907, 375.3009, 161.0465, 101.0278	6"-O-acetylginsenoside Rb1 isomer (PPD-4Glc-Ace)	PPT
110	19.80	725.4482	C ₃₈ H ₆₄ O ₁₀	0.88	256.4850	+HCOO	679.4425, 581.4027, 475.3751	3-β-acetoxyl ginsenoside F1 or its isomer (PPT-Glc-Ace)	PPD
111	19.85	845.4896	C ₄₂ H ₇₂ O ₁₄	-0.38	270.8264	+HCOO	799.4792, 475.3759	notoginsenoside U or its isomer (PPT-2Glc)	PPT
112	19.91	991.5484	C ₄₈ H ₈₂ O ₁₈	0.63	296.6561	+HCOO	945.5492, 783.5075, 621.4409, 459.3869, 375.2823, 161.0453, 101.0259	ginsenoside Rd isomer (PPD-3Glc)	PPT
113	20.04	793.4352	C ₄₂ H ₆₆ O ₁₄	-3.53	261.9961	-H	693.3689, 637.4350, 475.3869	zingibroside R1 isomer (PPT-Rha-Dimal)	PPD
114	20.32	925.4785	C ₄₇ H ₇₄ O ₁₈	-1.84	292.6125	-H	793.4223, 613.3793, 569.3861, 455.3611	elatoside A or its isomer (OA-Glc-Xyl-GlurA)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
115 ^a	20.61	945.5420	C ₄₈ H ₈₂ O ₁₈	-0.27	289.0175	-H	783.4898, 765.4798, 621.4374, 459.3843, 161.0452, 101.0243	ginsenoside Rd	OA
116	21.58	991.5494	C ₄₈ H ₈₂ O ₁₈	1.69	296.9004	+HCOO	945.5352, 783.5008, 621.4342, 459.4523, 161.0420, 101.0229	ginsenoside Rd isomer (PPD-3Glc)	PPD
117	21.77	871.5062	C ₄₄ H ₇₄ O ₁₄	0.85	280.7506	+HCOO	825.5040, 637.4456, 475.3886, 391.2960	ginsenoside Rs isomer (PPT-Glc-Rha-Ace)	PPT
118 ^b	22.29	725.4480	C ₃₉ H ₆₆ O ₁₂	0.61	255.0921	-H	549.3186, 475.3775	PPT-Glc-2CO ₂	PPT
119	22.79	725.4480	C ₃₈ H ₆₄ O ₁₀	0.59	255.2194	+HCOO	679.4198, 475.3754, 391.2796, 101.0295	3- β -acetoxyl ginsenoside F1 or its isomer (PPT-Glc-Ace)	PPT
120 ^a	24.46	793.4361	C ₄₂ H ₆₆ O ₁₄	-1.59	260.0498	-H	631.3867, 569.3838, 455.3492	chikusetsusaponin IVa	OA
121	24.56	1031.5398	C ₅₁ H ₈₄ O ₂₁	-3.3	310.8227	-H	945.5392, 783.4919, 621.4614, 459.3835, 375.2842, 161.0476	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	Mal
122	25.11	1195.6091	C ₅₆ H ₉₄ O ₂₄	-1.83	326.2658	+HCOO	1149.5973, 1107.5937, 945.5433, 783.4823, 621.4509, 459.3943, 161.0429, 113.0215	6"-O-acetylginsenoside Rb1 isomer (PPD-4Glc-Ace)	PPD
123	25.27	1077.5809	C ₅₃ H ₉₀ O ₂₂	-3.35	303.0569	-H	945.5415, 783.5034, 621.4384, 459.3980	ginsenoside Rb3 isomer (PPD-3Glc-Xyl)	PPD
124	25.58	945.5422	C ₄₈ H ₈₂ O ₁₈	-0.63	288.1544	-H	891.3250, 758.4809, 691.4384, 621.4368, 459.3834	PPD-3Glc	PPD
125	25.79	1031.5429	C ₅₁ H ₈₄ O ₂₁	-0.39	306.2586	-H	945.5415, 783.4927, 621.4209, 459.3744, 375.2875, 161.0463, 101.0226	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	Mal
126	26.70	1031.5439	C ₅₁ H ₈₄ O ₂₁	0.68	286.6152	-H	945.5497, 783.4801, 621.4325, 459.3848, 375.2905, 221.0662, 113.0252	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	Mal
127	26.83	827.4807	C ₄₂ H ₇₀ O ₁₃	1.79	279.7727	+HCOO	781.4746, 619.4339, 499.3681, 457.3587, 161.0467, 113.0249	sanchirrhinoside B or its isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	C17side-chain
128	27.06	961.5356	C ₄₇ H ₈₀ O ₁₇	-1.75	293.6685	+HCOO	915.5292, 753.4942, 621.4346, 603.4288, 459.3776	notoginsenoside Fd isomer (PPD-2Glc-Xyl)	PPD
129	27.76	991.5469	C ₄₈ H ₈₂ O ₁₈	-0.95	297.8682	+HCOO	945.5352, 783.4809, 621.4364, 475.3798	ginsenoside Re isomer (PPT-Rha-2Glc)	PPT
130	27.88	769.4376	C ₄₀ H ₆₆ O ₁₄	0.29	254.5325	-H	665.3296, 475.3808, 391.2820	20(R) notoginsenoside R2 isomer (PPT-Rha-Xyl)	PPT
131	27.90	679.4429	C ₃₈ H ₆₄ O ₁₀	0.44	255.9638	-H	637.4214, 475.3802, 391.2837, 347.2597	3- β -acetoxyl ginsenoside F1 or its isomer (PPT-Glc-Ace)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
132	28.12	1033.5560	C ₅₀ H ₈₄ O ₁₉	-2.43	301.0122	+HCOO	987.5233, 945.5368, 783.5015, 621.4311, 459.3959, 113.0195	6''-O-acetylginsenoside Rg3 or its isomer (PPD-3Glc-Ace)	PPD
133	28.29	797.4693	C ₄₁ H ₆₈ O ₁₂	0.67	267.5127	+HCOO	751.4642, 619.4220, 457.3752, 161.0431, 113.0235, 101.0219	notoginsenoside T5 or its isomer (C ₃₀ H ₅₀ O ₃ -Glc-Xyl)	C17side-chain
134 ^a	28.44	961.5365	C ₄₇ H ₈₀ O ₁₇	-0.76	291.5007	+HCOO	915.5306, 783.4904, 621.4378, 459.3847, 441.3663, 269.1040	notoginsenoside Fd	PPD
135	28.61	1033.5563	C ₅₀ H ₈₄ O ₁₉	-2.13	306.4846	+HCOO	987.5619, 945.5319, 783.4758, 621.4365, 459.3910, 375.2886, 161.0551, 101.0217	6''-O-acetylginsenoside Rg3 or its isomer (PPD-3Glc-Ace)	PPD
136	28.89	1031.5430	C ₅₁ H ₈₄ O ₂₁	0.26	295.2898	-H	945.5313, 879.5052, 621.4207, 459.3814, 221.0687	malonylginsenoside Rd isomer (PPD-3Glc-Mal)	Mal
137	29.12	811.4841	C ₄₂ H ₇₀ O ₁₂	-0.39	268.9418	+HCOO	765.4793, 619.4202, 601.4121, 457.3615	ginsenoside F4 isomer (C ₃₀ H ₅₀ O ₃ -Glc-Rha)	C17side-chain
138	29.21	725.4485	C ₃₈ H ₆₄ O ₁₀	1.32	255.1420	+HCOO	679.4308, 475.3671, 113.0235	3-β-acetoxyl ginsenoside F1 or its isomer (PPT-Glc-Ace)	PPT
139	29.29	797.4684	C ₄₁ H ₆₈ O ₁₂	-0.53	273.6348	+HCOO	751.4642, 619.4205, 457.3686, 447.3080	notoginsenoside T5 or its isomer (C ₃₀ H ₅₀ O ₃ -Glc-Xyl)	C17side-chain
140	29.41	961.5361	C ₄₈ H ₈₂ O ₁₉	-1.09	289.3505	-H	783.4896, 621.4264, 459.3711	gypenoside XLVI isomer (PPD-2Glc-2Bute-Ace)	PPD
141	29.53	845.4894	C ₄₂ H ₇₂ O ₁₄	-0.63	286.9945	+HCOO	799.4747, 637.4479, 475.3782, 113.0238, 101.0249	notoginsenoside U or its isomer (PPT-2Glc)	PPT
142 ^a	29.74	665.4271	C ₃₆ H ₆₀ O ₈	0.97	247.9503	+HCOO	619.4204, 457.3683, 125.0234, 113.9391	ginsenoside Rk3	C17side-chain
143 ^a	29.88	811.4844	C ₄₂ H ₇₀ O ₁₂	0.00	274.0935	+HCOO	765.4792, 619.4209, 457.3697, 101.4695	ginsenoside F4	C17side-chain
144	29.99	1033.5568	C ₅₀ H ₈₄ O ₁₉	-1.62	309.6836	+HCOO	987.5532, 945.5405, 783.4833, 621.4366, 459.3832, 375.2835, 161.0546, 113.0210, 101.0258	6''-O-acetylginsenoside Rg3 or its isomer (PPD-3Glc-Ace)	PPD
145 ^b	30.39	1033.5575	C ₅₁ H ₈₆ O ₂₁	-0.82	304.9686	-H	945.5267, 783.4871, 621.4304, 459.3854	PPD-3Glc-2CO ₂	PPD

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
146 ^a	30.59	665.4276	C ₃₆ H ₆₀ O ₈	1.78	252.5760	+HCOO	619.4218, 457.3683, 113.9406, 101.9349	ginsenoside Rh4	C17side-chain
147	30.69	929.6381	C ₅₄ H ₉₀ O ₁₂	2.90	298.8051	-H	783.4749, 621.4393, 459.3735	notoginsenosides NL-C1 isomer (PPD-2Glc-Rha)	PPD
148	30.90	975.5530	C ₄₈ H ₈₂ O ₁₇	0.11	291.0070	+HCOO	929.5544, 783.4753, 621.4374, 459.3850, 375.2943, 161.0418, 101.0240	notoginsenosides NL-C1 isomer (PPD-2Glc-Rha)	PPD
149	31.21	827.4782	C ₄₂ H ₇₀ O ₁₃	-1.41	264.7627	+HCOO	781.4713, 619.4088, 375.2918, 113.0241	sanchirrhinoside B isomer (PPD-Xyl-Glc-Bute-CO ₂)	PPD
150 ^b	31.47	1003.5481	C ₄₉ H ₈₂ O ₁₈	0.31	301.9478	+HCOO	957.5555, 915.5203, 783.4829, 621.4448, 459.3820, 375.2862, 161.0467, 113.0245, 101.0237	PPD-2Glc-Xyl-Ace	PPD
151	31.81	961.5368	C ₄₇ H ₈₀ O ₁₇	-0.44	293.0650	+HCOO	915.5368, 783.4905, 621.4393, 459.3856, 375.2903, 161.0434, 113.0225, 101.0260	notoginsenoside Fe isomer (PPD-2Glc-Xyl)	PPD
152	31.87	959.5587	C ₄₉ H ₈₄ O ₁₈	0.86	293.7433	-H	783.4910, 621.4376, 459.3845	notoginsenoside G isomer (PPD-2Glc-GlurA)	PPD
153 ^a	32.06	961.5366	C ₄₇ H ₈₀ O ₁₇	-0.66	292.8520	+HCOO	915.5298, 783.4905, 621.4375, 375.2953	notoginsenoside Ft1	PPD
154	32.41	827.4796	C ₄₂ H ₇₀ O ₁₃	0.38	272.1957	+HCOO	781.4672, 619.4124, 459.3786, 457.3673, 161.0427, 101.0250	sanchirrhinoside B or its isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	C17side-chain
155	32.86	827.4801	C ₄₂ H ₇₀ O ₁₃	1.02	265.6269	+HCOO	781.4522, 619.4282, 457.3701, 113.0246, 101.0243	sanchirrhinoside B or its isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	C17side-chain
156 ^a	33.15	783.4907	C ₄₂ H ₇₂ O ₁₃	0.89	274.0494	-H	621.4376, 459.3847, 443.3499, 331.2606	Ginsenoside Rg3	PPD
157 ^b	33.35	881.4082	C ₄₀ H ₆₆ O ₂₁	7.22	264.8362	-H	675.3726, 627.2632, 475.3863	PPT-Xyl-Glc-Bute-CO ₂	PPT
158 ^a	33.52	829.4959	C ₄₂ H ₇₂ O ₁₃	1.15	267.8248	+HCOO	783.4906, 621.4369, 459.3847	20(R)-ginsenoside Rg3	PPD
159	33.57	925.4801	C ₄₇ H ₇₄ O ₁₈	-0.11	300.9658	-H	819.4666, 707.3689, 459.3847, 293.2176, 161.0455	elatoside A isomer (PPD-Glc-Xyl-Dimal)	PPD
160	33.80	799.4863	C ₄₂ H ₇₂ O ₁₄	1.75	266.6978	-H	731.4279, 613.3790, 569.3814, 375.2811, 279.2336, 113.0227	majoroside F2 isomer (PPD-GlurA-Glc-H ₂ O-Bute)	PPD
161 ^b	33.91	813.4996	C ₄₂ H ₇₂ O ₁₂	-0.65	273.8596	+HCOO	767.4938, 569.3814, 457.3709	C ₃₀ H ₅₀ O ₃ -Glc-Bute-CO ₂ -2H ₂ O	Others

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
162	34.01	825.4998	C ₄₄ H ₇₄ O ₁₄	-0.97	275.1118	-H	621.4302, 459.3834, 441.3809, 161.0476	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
163	34.31	809.4680	C ₄₂ H ₆₈ O ₁₂	-1.05	285.6418	+HCOO	763.4670, 475.3787	pseudoginsenoside RP1 isomer (PPT-GlurA-Bute-CO ₂)	PPT
164	34.40	825.5030	C ₄₄ H ₇₄ O ₁₄	2.91	276.4981	-H	783.4940, 621.4424, 459.3790, 311.2294	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
165	34.62	827.4803	C ₄₂ H ₇₀ O ₁₃	1.28	268.4434	+HCOO	781.4557, 619.4400, 459.3851, 457.3640, 161.0445	sanchirrhinoside B or its isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	C17side-chain
166	34.95	829.4963	C ₄₂ H ₇₂ O ₁₃	1.66	269.8561	+HCOO	783.4952, 621.4428, 459.3792	20(R)-ginsenoside Rg3 isomer (PPD-2Glc)	PPD
167	35.03	925.4786	C ₄₇ H ₇₄ O ₁₈	-1.73	301.2136	-H	749.4457, 569.3832, 455.3526, 161.0473, 113.0285, 101.0257	elatoside A or its isomer (OA-Glc-Xyl-GlurA)	OA
168	35.13	799.4840	C ₄₁ H ₇₀ O ₁₂	-0.53	268.8044	+HCOO	753.4771, 621.4402, 459.3870, 281.2479, 161.0487	gypenoside XIII or its isomer (PPD-Glc-Xyl)	PPD
169 ^b	35.20	923.4629	C ₄₇ H ₇₂ O ₁₈	-1.18	302.9162	-H	731.4364, 551.3696, 551.3696, 455.3577	OA-Rha-Mal-CO ₂	OA
170	35.48	871.5056	C ₄₄ H ₇₄ O ₁₄	0.12	282.2841	+HCOO	825.4403, 783.5090, 621.4521, 459.3826, 375.2951, 161.0439, 113.0229, 101.0221	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
171	35.77	871.5040	C ₄₄ H ₇₄ O ₁₄	-1.82	282.9557	+HCOO	825.5003, 783.4924, 621.4337, 459.3830	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
172	35.78	943.5262	C ₄₇ H ₇₈ O ₁₆	-0.56	304.3458	+HCOO	897.4924, 765.4798, 603.4220, 441.3844, 221.0668, 161.0432, 113.0279, 101.0245	gypenoside A isomer (C ₃₀ H ₅₀ O ₂ -2Glc-Xyl)	Others
173	35.81	793.4375	C ₄₂ H ₆₆ O ₁₄	-0.63	281.1770	-H	621.4337, 551.3757, 459.3830, 293.2184, 113.0239	zingibroside R1 isomer (PPD-Glc-Dimal)	PPD
174	36.15	871.5054	C ₄₄ H ₇₄ O ₁₄	-0.12	279.3517	+HCOO	825.4990, 783.4996, 621.4460, 459.3879, 375.2925, 113.0234, 101.0273	ginsenoside Rs3 or its isomer (PPD-2Glc-Ace)	PPD
175	36.15	943.5264	C ₄₇ H ₇₈ O ₁₆	-0.33	310.2702	+HCOO	897.5142, 765.4798, 603.4265, 491.0407	gypenoside A isomer (OT-Glc-Xyl-CO ₂ -Bute)	OT
176	36.57	807.4888	C ₄₄ H ₇₂ O ₁₃	-1.61	297.3134	-H	765.4689, 637.4213, 475.3814, 279.2322	ginsenoside Rs4 isomer (PPT-Glc-Mal-2Ace)	PPT
177	36.90	871.5030	C ₅₂ H ₇₂ O ₁₁	3.93	281.7834	-H	783.4791, 621.4215, 459.3744	notoginsenosides NL-A4 isomer (PPD-2Glc-2CO ₂)	PPD
178	37.17	517.3908	C ₃₂ H ₅₄ O ₅	1.93	228.2589	-H	475.3789, 391.2827, 101.9331	6 α -acetoxy-3 β ,12 β ,20R-trihydroxydammar-24-ene or its isomer (PPT-Ace)	PPT

No.	t_R (min)	m/z	Formula	Masserror (ppm)	CCS (\AA^2)	Adduct	ESI-MS ²	Identification	Subclass
179^a	37.37	811.4847	C ₄₂ H ₇₀ O ₁₂	0.39	283.6558	+HCOO	765.4794, 603.4269, 527.3040, 441.3726, 113.9438	ginsenoside Rk1	C17side-chain
180^a	37.53	621.4376	C ₃₆ H ₆₂ O ₈	0.64	242.4044	-H	573.3073, 459.3804, 341.7170, 281.2431	compound K	PPD
181^a	37.78	811.4847	C ₄₂ H ₇₀ O ₁₂	0.39	287.5967	+HCOO	765.4796, 689.3535, 527.3024, 441.3736, 341.1687, 101.9253	ginsenoside Rg5	C17side-chain
182	39.96	807.4888	C ₄₄ H ₇₂ O ₁₃	-1.49	293.3270	-H	765.4913, 475.3898	ginsenoside Rs4 isomer (PPT-Glc-Mal-2Ace)	PPT

^a Identified by comparison with the reference standards; ^b Ingredients not found in the "in-house ginsenoside library".

Table S11 Information of the potential steaming associated ginsenoside markers for PG.

No.	VIP	t_R (min)	m/z	Formula	CCS (\AA^2)	ESI-MS ² fragments	Identification	Subclass
M1	16.69	14.04	1193.5927	C ₅₇ H ₉₄ O ₂₆	262.9355	1149.6083, 1107.5957, 1089.5857, 945.5440, 783.4908, 621.4377, 459.3845	malonylginsenoside Rb1 or isomer (PPD-4Glc-Mal)	PPD
M2 ^a	13.62	6.44	945.5456	C ₄₈ H ₈₂ O ₁₈	281.2531	783.4894, 637.4313, 475.3791, 391.2851	ginsenoside Re	PPT
M3	6.47	36.03	825.5024	C ₄₄ H ₇₄ O ₁₄	311.0527	783.4901, 621.4373, 459.3844	ginsenoside Rs3 or isomer (PPD-2Glc-Ace)	PPD
M4	5.93	28.58	1031.5404	C ₅₁ H ₈₄ O ₂₁	338.5213	945.5431, 783.4892, 621.4384, 459.3836	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	PPD
M5	5.21	28.26	1033.5560	C ₅₀ H ₈₄ O ₁₉	327.8051	987.5452, 945.5348, 783.4897, 621.4569, 459.3839	quinquenoside III or isomer (PPD-3Glc-Ace)	PPD
M6 ^a	4.67	18.28	1163.5821	C ₅₆ H ₉₂ O ₂₅	351.2392	1077.5837, 945.5430, 783.4899, 765.4789, 621.4372, 459.3844	malonyl ginsenoside Rb2	PPD
M7	4.16	33.70	825.5028	C ₄₄ H ₇₄ O ₁₄	305.7448	783.4908, 621.4359, 459.3844	ginsenoside Rs3 or isomer (PPD-2Glc-Ace)	PPD
M8	4.03	17.87	1149.6009	C ₅₆ H ₉₄ O ₂₄	359.3736	1107.5948, 1089.5844, 945.5400, 783.4918, 621.4395, 459.3868	quinquenoside R1 or isomer (PPD-4Glc-Ace)	PPD
M9	3.99	27.46	1031.5401	C ₅₁ H ₈₄ O ₂₁	334.3142	987.5542, 945.5428, 783.4915, 621.4367, 459.3848	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	PPD
M10 ^a	3.69	38.45	667.4410	C ₃₆ H ₆₂ O ₈	289.1120	585.3758, 393.5552, 279.2332, 191.8451	20(<i>S</i>)-ginsenoside Rh2	PPD
M11 ^a	3.67	29.14	915.5329	C ₄₇ H ₈₀ O ₁₇	318.1113	915.5293, 783.4923, 621.4392, 459.3853	ginsenoside Rd2	PPD
M12 ^a	3.10	12.88	683.4345	C ₃₆ H ₆₂ O ₉	240.9517	637.4301, 621.4369, 475.3793	20(<i>S</i>)-ginsenoside Rh1	PPT
M13 ^a	2.97	38.74	667.4409	C ₃₆ H ₆₂ O ₈	289.8215	615.3587, 559.5748, 459.3857, 125.8741	20(<i>R</i>)-ginsenoside Rh2	PPD
M14	2.73	29.81	987.5556	C ₅₀ H ₈₄ O ₁₉	337.4006	945.5421, 783.4893, 621.4372, 459.3840	quinquenoside III or isomer (PPD-3Glc-Ace)	PPD

No.	VIP	t_R (min)	m/z	Formula	CCS (\AA^2)	ESI-MS ² fragments	Identification	Subclass
M15	2.63	2.27	961.5392	C ₄₈ H ₈₂ O ₁₉	325.4650	799.4825, 781.4757, 475.4796	ginsenoside Re7 isomer (PPT-3Glc)	PPT
M16	2.18	8.54	1033.5539	C ₅₀ H ₈₄ O ₁₉	338.3757	987.5557, 945.5413, 783.5039, 637.4416, 475.3765	pseudoginsenoside Rs1 or isomer (PPT-2Glc-Rha-Ace)	PPT
M17	2.14	12.97	1107.5921	C ₅₄ H ₉₂ O ₂₃	351.4823	945.5432, 783.4904, 621.4369, 459.3835	ginsenoside Rb1 isomer (PPD-4Glc)	PPD
M18 ^a	2.05	11.08	799.4822	C ₄₂ H ₇₂ O ₁₄	298.6028	621.4304, 553.3371, 475.3796, 391.2859	ginsenoside Rf	PPT
M19	1.94	7.90	1031.5407	C ₅₁ H ₈₄ O ₂₁	318.9505	987.5515, 945.5415, 637.4311, 475.3795	malonyl ginsenoside Rd isomer (PPT- 2Glc-Rha-Mal)	PPT
M20	1.90	37.36	801.4522	C ₄₈ H ₆₆ O ₁₀	300.7692	783.4826, 621.4439, 459.3865	20(<i>S</i>)-ginsenoside Rf2 isomer (PPT- 2Glc-H ₂ O)	PPD
M21 ^a	1.79	14.38	1193.5918	C ₅₇ H ₉₄ O ₂₆	344.9657	1149.6042, 1107.5945, 945.5419, 783.4906, 621.4376, 459.3842	malonyl ginsenoside Rb1	PPD
M22 ^a	1.67	16.03	1077.5815	C ₅₃ H ₉₀ O ₂₂	343.8785	945.5421, 915.5282, 783.4896, 459.3847	ginsenoside Rb3	PPD
M23	1.55	18.17	1149.6052	C ₅₆ H ₉₄ O ₂₄	325.0721	1107.5970, 1089.5866, 945.5462, 783.4902, 621.4383, 459.3827	quinquenoside R1 or isomer (PPD- 4Glc-Ace)	PPD
M24	1.54	8.81	1139.5897	C ₅₃ H ₉₀ O ₂₃	360.0067	1093.5828, 963.5489, 781.4769, 475.3786	floralginsenoside P or isomer (PPT- 3Glc-Xyl)	PPT
M25	1.53	9.04	887.4988	C ₄₄ H ₇₄ O ₁₅	307.8758	841.4846, 637.4323, 475.3791, 391.2840	ginsenoside Rs3 or isomer (PPD- 2Glc-Ace)	PPT
M26	1.51	24.79	1165.6024	C ₅₅ H ₉₂ O ₂₃	357.4083	1119.5904, 1077.5904, 945.5573, 783.4837, 621.4359, 459.3761	ginsenoside Rs11 or isomer (PPD- 3Glc-Xyl-Ace)	PPD

^a Identified by comparison with the reference standards.

Table S12 Information of the potential steaming associated ginsenoside markers for PQ.

No.	VIP	t_R (min)	m/z	Formula	CCS (\AA^2)	ESI-MS ² fragments	Identification	Subclass
M1^a	16.69	14.04	1193.5927	C ₅₇ H ₉₄ O ₂₆	265.7289	1149.6064, 1107.5953, 947.5504, 799.4887, 687.4475, 459.3863, 391.5509	malonyl ginsenoside Rb1	PPD
M2^a	15.24	37.73	765.4796	C ₄₂ H ₇₀ O ₁₂	320.6144	765.4791, 603.4271, 441.3729	ginsenoside Rg5	OT
M3^a	13.62	6.44	945.5421	C ₄₈ H ₈₂ O ₁₈	291.4523	945.5421, 783.4892, 637.4314, 475.3792, 391.2853	ginsenoside Re	PPT
M4^a	11.04	12.86	1107.5923	C ₅₄ H ₉₂ O ₂₃	313.9499	945.5435, 783.4907, 621.4370, 459.3834, 179.0560	ginsenoside Rb1	PPD
M5	7.25	35.67	825.5013	C ₄₄ H ₇₄ O ₁₄	316.2209	783.4902, 621.4363, 459.3845, 375.2914	ginsenoside Rs3 or isomer (PPD-2Glc-Ace)	PPD
M6	6.52	27.57	961.5354	C ₄₇ H ₈₀ O ₁₇	252.6918	915.5331, 821.3955, 621.4373, 459.3845	ginsenoside Rd2 isomer (PPD-2Glc-Xyl)	PPD
M7	6.47	36.03	825.5041	C ₄₄ H ₇₄ O ₁₄	314.8504	783.4895, 621.4379, 459.3844, 375.2895	ginsenoside Rs3 or isomer (PPD-2Glc-Ace)	PPD
M8	5.93	28.58	1031.5404	C ₅₁ H ₈₄ O ₂₁	340.4254	987.5550, 945.5429, 783.4911, 621.4372, 459.3862	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	PPD
M9	5.21	28.26	987.5523	C ₅₀ H ₈₄ O ₁₉	344.6162	987.5523, 945.5415, 783.4902, 621.4371, 459.3842	quinquenoside III or isomer (PPD-3Glc-Ace)	PPD
M10	4.67	18.28	1163.5821	C ₅₆ H ₉₂ O ₂₅	354.4115	1077.5839, 915.5321, 783.4890, 621.4382, 459.3846	malonyl ginsenoside Rb2 isomer (PPD-3Glc-Xyl-Mal)	PPD
M11	4.51	24.83	945.5396	C ₄₈ H ₈₂ O ₁₈	293.8867	783.4893, 621.4371, 459.3849	ginsenoside Rd isomer (PPD-3Glc)	PPD
M12	3.99	27.46	1031.5401	C ₅₁ H ₈₄ O ₂₁	339.3513	987.5525, 783.4887, 621.4366, 459.3846	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	PPD
M13^a	3.96	16.54	955.4886	C ₄₈ H ₇₆ O ₁₉	262.9421	793.4379, 569.3846, 455.3529	ginsenoside Ro	OA
M14^a	3.84	13.92	1077.5814	C ₅₃ H ₉₀ O ₂₂	347.5792	915.5338, 783.4904, 765.4803, 621.3848, 459.3848	ginsenoside Rc	PPD

No.	VIP	t_R (min)	m/z	Formula	CCS (\AA^2)	ESI-MS ² fragments	Identification	Subclass
M15	3.41	11.23	1117.5409	C ₅₄ H ₈₆ O ₂₄	355.3801	793.4376, 613.3735, 523.3804, 455.3534	ginsenoside Rb1 isomer (OA-GlurA-3Glc)	OA
M16	3.07	17.14	1107.5968	C ₅₄ H ₉₂ O ₂₃	315.9357	1107.5962, 945.5429, 783.4903, 621.4383, 459.3520	ginsenoside Rb1 isomer (PPD-4Glc)	PPD
M17	2.88	34.08	825.5021	C ₄₄ H ₇₄ O ₁₄	307.3350	783.4889, 621.4370, 459.3844, 375.2896	ginsenoside Rs3 or isomer (PPD-2Glc-Ace)	PPD
M18	2.67	19.31	1163.5814	C ₅₆ H ₉₂ O ₂₅	358.2478	1077.5855, 1059.5742, 765.47498, 621.4364, 459.3850	malonyl ginsenoside Rb2 isomer (PPD-3Glc-Xyl-Mal)	PPD
M19	2.24	36.76	825.5027	C ₄₄ H ₇₄ O ₁₄	318.6220	783.4885, 621.4365, 459.3839	ginsenoside Rs3 or isomer (PPD-2Glc-Ace)	PPD
M20^a	2.12	23.06	1031.5395	C ₅₁ H ₈₄ O ₂₁	341.0989	987.5546, 945.5426, 783.4908, 621.4376, 459.3853	malonyl ginsenoside Rd	PPD
M21	2.05	11.08	799.4822	C ₄₂ H ₇₂ O ₁₄	306.2527	653.4269, 637.4309, 475.3791, 391.4845	ginsenoside Rf isomer (PPT-2Glc)	PPT
M22	1.94	7.90	1031.5407	C ₅₁ H ₈₄ O ₂₁	324.1783	987.5535, 945.5414, 783.4880, 637.4337, 475.3794	malonyl ginsenoside Rd isomer (PPT-Rha-2Glc-Mal)	PPT
M23	1.82	8.54	1031.5402	C ₅₁ H ₈₄ O ₂₁	326.8279	987.5540, 945.5434, 783.4882, 637.4305, 475.3783	malonyl ginsenoside Rd isomer (PPT-Rha-2Glc-Mal)	PPT
M24^a	1.81	9.76	961.5379	C ₄₇ H ₈₀ O ₁₇	333.2298	961.5373, 799.4862, 637.4333, 475.3804	vinaginsenoside R8	PPT
M25	1.67	19.78	991.5440	C ₄₈ H ₈₂ O ₁₈	332.1383	945.5407, 783.4886, 621.4362, 459.3843, 375.2920	ginsenoside Rd isomer (PPD-3Glc)	PPD
M26	1.65	33.64	827.4775	C ₄₃ H ₇₂ O ₁₅	302.1386	781.4790, 621.4375, 375.2898	12-O-glucoginsenoside Rh4 isomer (PPD-GlurA-Glc-Bute)	PPD
M27	1.56	30.95	827.4774	C ₄₃ H ₇₂ O ₁₅	301.2152	827.4796, 781.4747, 619.4196, 457.3677	12-O-glucoginsenoside Rh4 or isomer (C ₃₀ H ₅₀ O ₃ -2Glc)	Others
M28^b	1.53	9.04	887.4988	C ₄₅ H ₇₆ O ₁₇	305.8177	845.2942, 637.4311, 475.3802	PPT-2Glc-2CO ₂	PPT

Note: ^a Identification of reference substances; ^b Ingredients not found in "self-built ginsenoside library".

Table S13 Information of the potential steaming associated ginsenoside markers for PN.

No.	VIP	t_R (min)	m/z	Formula	CCS (\AA^2)	ESI-MS ² fragments	Identification	Subclass
M1	14.38	20.01	991.5464	C ₄₈ H ₈₂ O ₁₈	331.4052	945.5423, 783.4894, 621.4369, 459.3843	ginsenoside Rd isomer (PPD-3Glc)	PPD
M2^a	11.99	6.51	991.5465	C ₄₈ H ₈₂ O ₁₈	256.2549	945.5440, 783.4899, 637.4324, 475.3793, 161.0449	ginsenoside Re	PPT
M3^a	11.93	12.97	1107.5928	C ₅₄ H ₉₂ O ₂₃	273.1015	945.5439, 783.4901, 621.4376, 459.3833	ginsenoside Rb1	PPD
M4^a	5.13	11.22	1239.6333	C ₅₉ H ₁₀₀ O ₂₇	228.5816	1107.5963, 1077.5852, 945.5433, 783.4908, 621.4380, 459.3847	notoginsenoside R4	PPD
M5	4.96	3.75	961.5376	C ₄₈ H ₈₂ O ₁₉	316.1389	961.5373, 799.4858, 637.4323, 475.3798	notoginsenoside R3 or isomer (PPT-3Glc)	PPT
M6^a	4.87	28.22	961.5359	C ₄₇ H ₈₀ O ₁₇	325.2795	915.5321, 783.4886, 621.4366, 459.3845	notoginsenoside Fd	PPD
M7^a	4.35	16.15	637.4323	C ₃₆ H ₆₂ O ₉	271.8901	503.2468, 391.2846	20(<i>S</i>)-ginsenoside F1	PPT
M8	4.23	33.21	881.4069	C ₄₀ H ₆₆ O ₂₁	291.5900	837.3847, 621.2215, 475.3813	PPT-Xyl-Glc-Bute-CO ₂	PPT
M9^a	4.02	11.83	1239.6333	C ₅₉ H ₁₀₀ O ₂₇	232.4833	1107.5959, 945.5422, 783.4910, 621.4339, 459.3484	notoginsenoside Fa	PPD
M10	3.87	9.04	815.4781	C ₄₂ H ₇₂ O ₁₅	284.7303	769.4837, 637.4325, 475.3779, 391.2926	ginsenoside F3 isomer (PPT-Glc-Xyl)	PPT
M11	3.85	16.29	1087.5309	C ₅₃ H ₈₄ O ₂₃	364.5227	925.4803, 793.4366, 731.4379, 551.3734, 455.3527	stipuleanoside R2 isomer (OA-3Glc-Rha)	OA
M12	3.18	10.65	1371.6761	C ₆₄ H ₁₀₈ O ₃₁	393.4504	1325.5802, 1107.5939, 945.5431, 783.4920, 621.4368, 459.3864	malonyl ginsenoside Ra3 or isomer (PPD-4Glc-Xyl-Mal)	PPD
M13^a	3.12	14.72	1193.5951	C ₅₇ H ₉₄ O ₂₆	339.2707	1107.5963, 1089.5866, 945.5457, 783.4918, 621.4376, 459.3841	malonyl ginsenoside Rb1	PPD
M14	2.64	11.14	845.4878	C ₄₂ H ₇₂ O ₁₄	307.6257	799.4846, 637.4318, 475.3796	notoginsenoside U or isomer (PPT-2Glc)	PPT
M15	2.58	4.15	1007.5411	C ₄₈ H ₈₂ O ₁₉	317.5184	961.5376, 637.4337, 475.3799, 221.0660	notoginsenoside R3 or isomer (PPT-3Glc)	PPT

No.	VIP	t_R (min)	m/z	Formula	CCS (\AA^2)	ESI-MS ² fragments	Identification	Subclass
M16	2.54	24.81	1031.5406	C ₅₁ H ₈₄ O ₂₁	342.8548	987.5539, 825.5009, 783.4895, 459.3842	malonyl ginsenoside Rd isomer (PPD-3Glc-Mal)	PPD
M17^a	2.47	14.11	1209.6306	C ₅₈ H ₉₈ O ₂₆	354.9639	1077.5859, 915.5341, 629.1090, 459.3451	ginsenoside Ra1	PPD
M18	1.72	17.44	1077.5868	C ₅₃ H ₉₀ O ₂₂	340.6942	1077.5872, 825.5032, 459.3863	chikusetsusaponin FK6 or its isomer (PPD-3Glc-Xyl)	PPD

^a Identified by comparison with the reference standards.

Table S14 Optimization of the freezing temperature and time in the DESI-MSI experiments.

Temperature	Time	Results
Optimization of freezing temperature		
-20°C	10 min	Insufficient hardness and difficulty in slicing
-80°C		Better hardness and easier slicing
Optimization of freezing time		
-80°C	1 min	Insufficient hardness and wrinkled tissue slice
	2 min	Insufficient hardness and wrinkled tissue slice
	5 min	Insufficient hardness and wrinkled tissue slice
	8 min	Insufficient hardness and wrinkled tissue slice
	10 min	Incomplete tissue slice
	15 min	complete tissue slice and easier slicing
	20 min	Incomplete tissue slice and difficulty in slicing