

# Multicomponent Characterization of the Flower Bud of *Panax notoginseng* and Its Metabolites in Rat Plasma by Ultra-High Performance Liquid Chromatography/Ion Mobility Quadrupole Time-of-Flight Mass Spectrometry

Xiaonan Yang <sup>1,2,†</sup>, Ying Xiong <sup>1,2,†</sup>, Hongda Wang <sup>1,2,†</sup>, Meiting Jiang <sup>1,2</sup>, Xiaoyan Xu <sup>1,2</sup>, Yueguang Mi <sup>1,2</sup>, Jia Lou <sup>1,2</sup>, Xiaohang Li <sup>1,2</sup>, He Sun <sup>1,2</sup>, Yuying Zhao <sup>1,2</sup>, Xue Li <sup>1,2,\*</sup> and Wenzhi Yang <sup>1,2,\*</sup>

<sup>1</sup> State Key Laboratory of Component-based Chinese Medicine, Tianjin University of Traditional Chinese Medicine, 10 Poyanghu Road, , Tianjin 301617, China

<sup>2</sup> Haihe Laboratory of Modern Chinese Medicine, Tianjin University of Traditional Chinese Medicine, 10 Poyanghu Road, Tianjin 301617, China

\* Correspondence: tjdxsyzx@163.com (X.L.); wzyang0504@tjutc.edu.cn (W.Y.); Tel.: +86-022-5979-1833 (W.Y.)

† These authors contributed equally to this work.

## Contents

Figure S1 Stationary phase screening for the establishment of UPHLC/IM-QTOF-MS by showing the base peak chromatogram (BPCs) of PNF extract on 20 candidate reversed-phase chromatographic columns.

Figure S2 Histograms of the numbers of detected components under three different top N settings. The data were obtained by processing the negative HDMS<sup>E</sup> data using UNIFI, generating the lists of “Identified Components” and “Unknown Components”.

Figure S3 MS/MS spectra of 18 prototype components of PNF-administrated rat plasma.

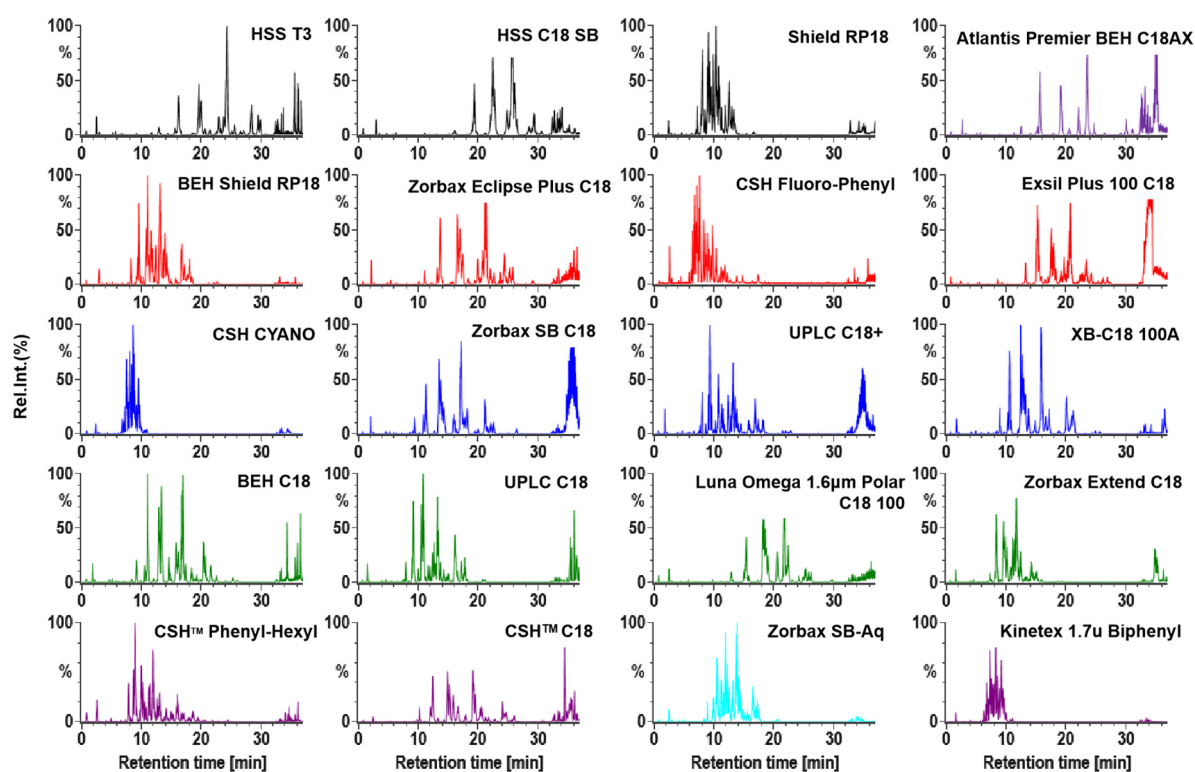
Table S1 Information for 51 ginsenoside reference compounds used in this work.

Table S2 Information for the 219 saponins characterized from the flower bud of *Panax notoginseng*.

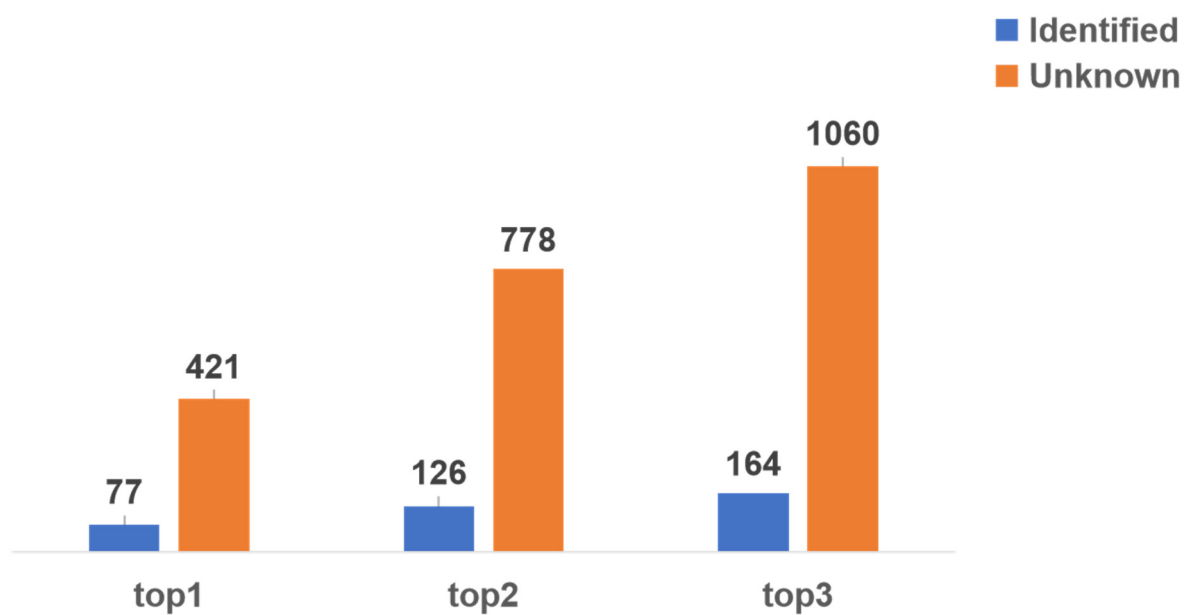
Table S3 Information for the 40 prototype components characterized from rat plasma.

Table S4 Information for 11 metabolites identified from rat plasma.

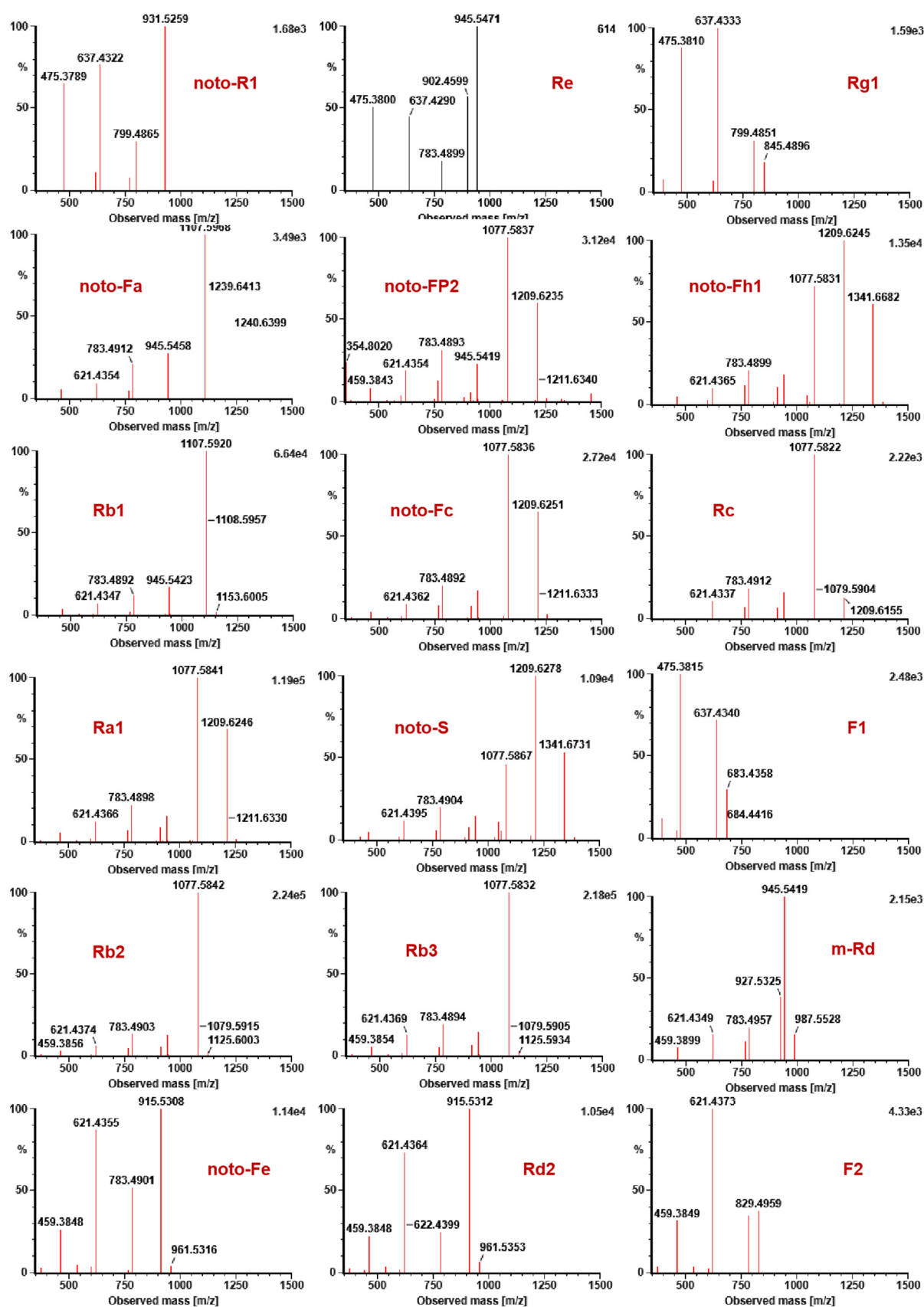
Table S5 CCS prediction of isomers in rat plasma based on ALLCCS and CCSbase.



**Figure S1.** Stationary phase screening for the establishment of UPHLC/IM-QTOF-MS by showing the base peak chromatogram (BPCs) of PNF extract on 20 candidate reversed-phase chromatographic columns.



**Figure S2.** Histograms of the numbers of detected components under three different top N settings. The data were obtained by processing the negative HDMS<sup>E</sup> data using UNIFI, generating the lists of “Identified Components” and “Unknown Components”.



**Figure S3.** MS/MS spectra of 18 prototype components of PNF-administrated rat plasma. (Noto-R4, Ro, and m-Rb1 failed to provide MS/MS spectra due to low response).

**Table S1.** Information for 51 ginsenoside reference compounds used in this work.

No.	Trivial name	M.F.	Exact Mass	Subclass
1	ginsenoside F2	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	784.4901	PPD
2	ginsenoside Rb2	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	1078.5924	
3	ginsenoside Rb1	C <sub>54</sub> H <sub>92</sub> O <sub>23</sub>	1108.6029	
4	ginsenoside Ra1	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	1210.6346	
5	ginsenoside Rd	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	946.5501	
6	20(S)-ginsenoside Rh2	C <sub>36</sub> H <sub>62</sub> O <sub>8</sub>	622.4445	
7	20(R)-ginsenoside Rh2	C <sub>36</sub> H <sub>62</sub> O <sub>8</sub>	622.4445	
8	notoginsenoside Fc	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	1210.4346	
9	notoginsenoside R4	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	1240.6452	
10	notoginsenoside Ft1	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	916.5396	
11	ginsenoside Rb3	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	1078.5924	
12	ginsenoside Ra2	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	1210.6346	
13	20(S)-ginsenoside Rg3	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	784.4973	
14	20(R)-ginsenoside Rg3	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	784.4973	
15	notoginsenoside Fe	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	916.5396	
16	notoginsenoside Fa	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	1240.6452	
17	ginsenoside Rs3	C <sub>44</sub> H <sub>74</sub> O <sub>14</sub>	826.5079	
18	ginsenoside Rc	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	1078.5924	
19	compound K	C <sub>36</sub> H <sub>62</sub> O <sub>8</sub>	622.4445	
20	notoginsenoside FP2	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	1210.6346	
21	notoginsenoside Fd	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	916.5396	
22	notoginsenoside S	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	1342.6769	
23	notoginsenoside Fh1	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	1342.6769	
24	ginsenoside Ra3	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	1240.6452	
25	gypenoside XVII	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	946.5501	
26	ginsenoside Rd2	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	916.5396	
27	ginsenoside F3	C <sub>41</sub> H <sub>70</sub> O <sub>13</sub>	770.4816	PPT
28	notoginsenoside R1	C <sub>47</sub> H <sub>80</sub> O <sub>18</sub>	932.5345	
29	20(R)-notoginsenoside R2	C <sub>41</sub> H <sub>70</sub> O <sub>13</sub>	770.4816	
30	20(S)-notoginsenoside R2	C <sub>41</sub> H <sub>70</sub> O <sub>13</sub>	770.4816	
31	20(R)-ginsenoside Rh1	C <sub>36</sub> H <sub>62</sub> O <sub>9</sub>	638.4394	
32	20(S)-ginsenoside Rh1	C <sub>36</sub> H <sub>62</sub> O <sub>9</sub>	638.4394	
33	20(R)-ginsenoside Rg2	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	784.4973	
34	20(S)-ginsenoside Rg2	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	784.4973	
35	ginsenoside Rg1	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	800.4922	
36	vinaginsenoside R4	C <sub>48</sub> H <sub>82</sub> O <sub>19</sub>	962.5450	
37	ginsenoside F5	C <sub>41</sub> H <sub>70</sub> O <sub>13</sub>	770.4816	

38	ginsenoside Rf	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	800.4922	
39	ginsenoside Re	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	946.5501	
40	chikusetsusaponin L5	C <sub>46</sub> H <sub>78</sub> O <sub>17</sub>	902.5239	
41	20(S)-ginsenoside F1	C <sub>36</sub> H <sub>62</sub> O <sub>9</sub>	638.4394	
42	ginsenoside F4	C <sub>42</sub> H <sub>70</sub> O <sub>12</sub>	766.4867	Other
43	ginsenoside Rh3	C <sub>36</sub> H <sub>60</sub> O <sub>7</sub>	604.4339	
44	ginsenoside Rk1	C <sub>42</sub> H <sub>70</sub> O <sub>12</sub>	766.4867	
45	ginsenoside Rk3	C <sub>36</sub> H <sub>60</sub> O <sub>8</sub>	620.4288	
46	malonyl-ginsenoside Rb1	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	1194.6033	Mal
47	malonyl-ginsenoside Rb2	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	1164.5928	
48	malonyl-ginsenoside Rd	C <sub>51</sub> H <sub>84</sub> O <sub>21</sub>	1032.5505	
49	malonyl-ginsenoside Rc	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	1164.5928	OA
50	ginsenoside Ro	C <sub>48</sub> H <sub>76</sub> O <sub>19</sub>	956.4981	
51	chikusetsusaponin IVa	C <sub>42</sub> H <sub>66</sub> O <sub>14</sub>	794.4453	

**Table S2.** Information for the 219 saponins characterized from the flower bud of *Panax notoginseng*.

No.	Observed RT (min)	Observed m/z	Formula	Mass error (ppm)	CCA(Å <sup>2</sup> )	Adducts	ESI-MS <sup>2</sup>	Identification
1	4.95	977.5347 <sup>d/f</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>18</sub>	2.09	314.48	+HCOO	931.5317, 799.4833, 637.4327, 475.3777	quinquenoside L17 or isomer
2	4.99	1109.5779 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>24</sub>	2.66	331.14	+HCOO	1063.5673, 931.5302, 637.4337, 475.3743	PPT-xyl-2rha-glc
3	5.04	1007.5459 <sup>d/f</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>19</sub>	−2.34	324.85	+HCOO	961.5355, 799.4810, 637.4307, 475.3768	chikusetsusaponin LM4 or isomer
4	5.28	977.5315 <sup>a</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>18</sub>	−1.15	322.41	+HCOO	931.5263, 799.4839, 637.4322, 475.3793, 391.2845	notoginsenoside R1
5	5.67	945.5432 <sup>c/f</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	0.38	324.43	−H	799.4837, 637.4319, 475.3791, 391.2850	ginsenoside Rg18 or isomer
6	5.68	991.5484 <sup>a</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	0.06	327.00	+HCOO	945.5429, 783.4936, 637.4319, 619.4202, 475.3887, 391.2848	ginsenoside Re
7	5.73	845.4997 <sup>a</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	0.21	297.89	+HCOO	799.4851, 637.4321, 475.3798, 391.2867	ginsenoside Rg1
8	6.01	1025.5559 <sup>d/f</sup>	C <sub>48</sub> H <sub>84</sub> O <sub>20</sub>	1.00	334.87	+HCOO	979.5493, 817.4986, 655.4431, 493.3887, 475.3794	ginsengenin-S3 or isomer
9	6.10	885.4862 <sup>b/e/f</sup>	C <sub>48</sub> H <sub>72</sub> O <sub>13</sub>	−4.46	303.56	−H	885.4840, 799.4862, 637.4324, 475.3806, 391.2857	PPT-mal-2glc
10	6.32	1139.5858 <sup>b/e/f</sup>	C <sub>54</sub> H <sub>92</sub> O <sub>25</sub>	0.26	359.88	+HCOO	1093.5788, 961.5443, 799.4830, 637.4346, 475.3806	PPT-xyl-3glc
11	6.42	1271.6292 <sup>d/f</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>27</sub>	2.06	359.99	+HCOO	1225.6248, 1093.5824, 961.5395, 799.4849, 637.4314, 475.3782	notoginsenosides NL-B3 or isomer
12	6.48	1169.5967 <sup>d/f</sup>	C <sub>54</sub> H <sub>92</sub> O <sub>24</sub>	2.87	356.15	+HCOO	1123.5938, 961.5368, 799.4857, 637.4347, 475.3740	6-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl]-20-O-[β-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl]-20(S)-protopanaxatriol or isomer
13	6.72	1139.5865 <sup>b/f</sup>	C <sub>54</sub> H <sub>92</sub> O <sub>25</sub>	0.88	365.09	+HCOO	1093.5801, 961.5363, 799.4864, 781.4749, 637.4324, 475.3803	PPT-xyl-3glc
14	6.99	1209.6048 <sup>b/e/f</sup>	C <sub>61</sub> H <sub>94</sub> O <sub>24</sub>	−1.18	342.71	−H	1123.5899, 961.5276, 799.4836, 637.4332, 475.3776	PPT-mal-4glc
15	7.13	1139.5868 <sup>b/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>23</sub>	1.17	355.51	+HCOO	1093.5806, 961.5403, 799.4856, 637.4334, 475.3791	PPT-xyl-3glc
16	7.37	1179.5825 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>26</sub>	1.77	347.77	−H	1093.5811, 961.5401, 799.4880, 637.4314, 475.3809	PPT-mal-xyl-3glc
17	7.67	1155.5809 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>24</sub>	−2.73	352.66	+HCOO	1109.5719, 1091.5697, 797.4728, 635.4145, 473.3642, 455.3563	C <sub>30</sub> H <sub>48</sub> O <sub>3</sub> -H <sub>2</sub> O-xyl-3glc
18	7.70	1139.5885 <sup>b/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>23</sub>	2.82	360.70	+HCOO	1093.5831, 961.5359, 799.4851, 637.4339, 475.3794	PPT-xyl-3glc
19	7.81	1179.5829 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>26</sub>	2.11	343.99	−H	1093.5828, 961.5361, 799.4853, 781.4738, 637.4317, 475.3796	PPT-mal-xyl-3glc

20	7.93	1007.5573 <sup>a</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>19</sub>	0.26	332.65	+HCOO	961.5380, 799.4842, 637.4299, 475.3807	vina ginsenoside R <sub>4</sub>
21	8.21	1179.5815 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>26</sub>	0.93	348.65	−H	1093.5801, 961.5381, 799.4886, 781.4746, 637.4322, 475.3796	PPT-mal-xyl-3glc
22	8.62	1179.5824 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>26</sub>	1.69	346.23	−H	1093.5826, 961.5357, 799.4850, 781.4749, 637.4304, 475.3789	PPT-mal-xyl-3glc
23	8.94	1195.5739 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>27</sub>	−1.19	350.69	−H	1109.5717, 1091.5532, 797.4655, 635.4175, 617.4071, 455.3482	C <sub>30</sub> H <sub>48</sub> O <sub>3</sub> -mal-2H <sub>2</sub> O-xyl-3glc
24	9.04	1137.5712 <sup>b/f</sup>	C <sub>53</sub> H <sub>88</sub> O <sub>23</sub>	0.77	355.38	+HCOO	1091.5652, 959.5242, 797.4716, 635.4144, 617.4066, 455.3552	C <sub>30</sub> H <sub>48</sub> O <sub>3</sub> -xyl-3glc
25	9.14	1417.6852 <sup>b/f</sup>	C <sub>64</sub> H <sub>108</sub> O <sub>31</sub>	−0.50	396.96	+HCOO	1371.6795, 1239.6379, 1107.5963, 945.5434, 783.4911, 621.4374, 459.3847, 353.1078	PPD-2xyl-4glc
26	9.28	1049.5527 <sup>d/f</sup>	C <sub>50</sub> H <sub>84</sub> O <sub>20</sub>	−3.20	344.20	+HCOO	1003.5451, 961.5396, 799.4855, 637.4335, 475.3800, 391.2832	6-acetyl ginsenoside Rg3 or isomer
27	10.03	947.5243 <sup>d/f</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>19</sub>	2.36	311.48	+HCOO	901.5179, 769.4735, 637.4312, 475.3807	notoginsenoside Rw1 or isomer
28	10.18	845.4899 <sup>d/f</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	0.09	301.66	+HCOO	799.4850, 637.4345, 491.3763	20(R)-pseudoginsenoside F11 or isomer
29	10.43	947.5235 <sup>d/f</sup>	C <sub>46</sub> H <sub>78</sub> O <sub>17</sub>	3.30	308.38	+HCOO	901.5196, 769.4787, 475.3762	chikusetsusaponin LM2 or isomer
30	10.69	845.4912 <sup>d/f</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	0.84	300.20	+HCOO	799.4856, 637.4346, 475.3800, 391.2863	20(S)-ginsenoside Rf or isomer
31	10.86	1285.6450 <sup>a</sup>	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	0.95	372.56	+HCOO	1239.6391, 1107.5986, 945.5443, 783.4914, 621.4364, 459.3857, 353.1086	notoginsenosides R4
32	11.39	815.4801 <sup>a</sup>	C <sub>41</sub> H <sub>70</sub> O <sub>13</sub>	0.26	298.98	+HCOO	769.4732, 637.4328, 475.3802, 391.2842	20(S)-notoginsenoside R2
33	11.67	1387.6756 <sup>b/e/f</sup>	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	−0.16	383.00	+HCOO	1341.6694, 1209.6275, 1077.5866, 945.5441, 783.4914, 621.4379, 459.3848	notoginsenoside Q or Fh1 (PPD-3xyl-3glc)
34	11.70	947.5218 <sup>a</sup>	C <sub>46</sub> H <sub>78</sub> O <sub>17</sub>	−0.34	321.67	+HCOO	901.5168, 769.4745, 637.4331, 475.3796, 391.2849	chikusetsusaponin L5
35	11.88	1315.6529 <sup>d/f</sup>	C <sub>60</sub> H <sub>102</sub> O <sub>28</sub>	0.48	375.87	+HCOO	1269.6491, 1107.5946, 945.5464, 783.4926, 621.4363, 459.3794	ginsenoside Rb5 or isomer
36	12.02	1417.6849 <sup>b/f</sup>	C <sub>64</sub> H <sub>108</sub> O <sub>31</sub>	0.23	391.45	+HCOO	1371.6805, 1209.6280, 1077.5863, 945.5479, 783.4892, 621.4388, 459.3838	PPD-4glc-2xyl
37	12.26	1387.6772 <sup>b/e/f</sup>	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	−0.16	382.62	+HCOO	1341.6694, 1209.6283, 1077.5849, 945.5443, 783.4888, 621.4370, 459.3837	PPD-3xyl-3glc
38	12.92	1285.6412 <sup>a</sup>	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	−0.53	372.92	+HCOO	1239.6357, 1107.5938, 945.5416, 783.4887, 621.4366, 459.3876	notoginsenoside Fa
39	13.14	1341.6665 <sup>c/f</sup>	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	−2.32	384.79	−H	1341.6664, 1209.6253, 1077.5841, 945.5425, 783.4892, 621.4363, 459.3841	PPD-3xyl-2glc
40	13.31	829.4945 <sup>a</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	−1.21	302.67	+HCOO	783.4869, 637.4288, 475.3795	20(S)-ginsenoside Rg2
41	13.69	683.4361 <sup>a</sup>	C <sub>36</sub> H <sub>62</sub> O <sub>9</sub>	−1.42	−	+HCOO	637.4312, 475.3790, 391.2845	20(S)-ginsenoside Rh1
42	14.17	1285.6450 <sup>d/f</sup>	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	0.47	367.32	+HCOO	1239.6385, 1077.5860, 945.5416, 783.4900, 621.4380, 459.3840	chikusetsusaponin VI or isomer



43	14.34	1255.6334 <sup>d/f</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	0.45	357.40	+HCOO	1209.6279, 1077.5879, 945.5448, 783.4903, 621.4365, 459.3855	notoginsenoside-FZ or isomer
44	14.50	815.4802 <sup>a</sup>	C <sub>41</sub> H <sub>70</sub> O <sub>13</sub>	0.38	300.73	+HCOO	769.4739, 637.4308, 475.3801, 391.2863	ginsenoside F3
45	14.90	1355.6619 <sup>b/e/f</sup>	C <sub>67</sub> H <sub>104</sub> O <sub>28</sub>	−1.65	380.71	−H	1269.6495, 1107.5961, 945.5439, 783.4899, 621.4364, 459.3872	PPD-mal-5glc
46	15.03	1325.6562 <sup>b/f</sup>	C <sub>66</sub> H <sub>102</sub> O <sub>27</sub>	0.50	370.80	−H	1239.6386, 1107.5980, 945.5439, 783.4889, 621.4364, 459.3835	PPD-mal-xyl-4glc
47	15.18	1427.6713 <sup>b/e/f</sup>	C <sub>66</sub> H <sub>108</sub> O <sub>33</sub>	0.90	399.08	−H	1341.6725, 1209.6271, 1077.5861, 945.5463, 783.4899, 621.4379, 459.3838	PPD-mal-3xyl-3glc
48	15.56	1255.6315 <sup>a</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	0.67	365.25	+HCOO	1209.6261, 1077.5841, 945.5425, 783.4896, 621.4359, 459.3872	notoginsenoside FP2
49	15.84	1387.6914 <sup>a</sup>	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	−0.53	302.07	+HCOO	1341.6689, 1209.6272, 1077.5856, 945.5442, 783.4902, 765.4810, 621.4379, 459.3851	notoginsenoside Fh1
50	16.18	1153.6010 <sup>a</sup>	C <sub>54</sub> H <sub>92</sub> O <sub>23</sub>	−0.60	355.55	+HCOO	1107.5950, 1089.5862, 945.5424, 783.4899, 621.4378, 459.3842	ginsenoside Rb1
51	16.47	1325.6375 <sup>b/f</sup>	C <sub>62</sub> H <sub>102</sub> O <sub>30</sub>	−0.58	373.85	−H	1239.6383, 1107.5957, 945.5436, 783.4907, 621.4373, 459.3849	PPD- mal-xyl-4glc
52	16.58	1255.6320 <sup>d/f</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	0.12	361.25	+HCOO	1209.6275, 1077.5861, 945.5440, 783.4904, 621.4373, 459.3847	notoginsenoside-FZ or isomer
53	17.01	1285.6456 <sup>d/f</sup>	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	2.56	378.02	+HCOO	1239.6411, 1077.5892, 945.5443, 783.4880, 621.4335, 459.3828	ginsenoside Ra3 or isomer
54	17.38	1427.6714 <sup>b/e/f</sup>	C <sub>66</sub> H <sub>108</sub> O <sub>33</sub>	0.97	394.31	−H	1341.6744, 1323.6604, 1209.6280, 1077.5861, 915.5334, 783.4920, 621.4379, 459.3842	PPD-mal-3xyl-3glc
55	17.77	1295.6294 <sup>b/e/f</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	1.27	364.76	−H	1209.6284, 1077.5880, 945.5444, 783.4899, 621.4377, 459.3847	PPD-mal-2xyl-3glc
56	17.83	955.4923 <sup>a</sup>	C <sub>48</sub> H <sub>76</sub> O <sub>19</sub>	1.54	200.20	−H	955.4915, 793.4887, 613.3763, 569.3852, 523.3783, 497.3650, 455.3536	ginsenoside Ro
57	17.93	855.4841 <sup>b/f</sup>	C <sub>48</sub> H <sub>72</sub> O <sub>13</sub>	−6.91	294.69	−H	769.4763, 475.3796	PPT-mal-xyl-glc
58	18.14	1285.6434 <sup>d/f</sup>	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	−0.10	376.64	+HCOO	1239.6378, 1077.5868, 945.5436, 783.4904, 621.4361, 459.3836	chikusetsusaponin VI or isomer
59	18.31	1193.5966 <sup>a</sup>	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	0.49	265.46	−H	1107.5965, 945.5437, 783.4904, 621.4378, 459.3853	malonyl-ginsenoside Rb1
60	18.50	1295.6264 <sup>b/e/f</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	−1.04	368.16	−H	1209.6282, 1077.5860, 945.5454, 783.4882, 621.4351, 459.3817	PPD-mal-2xyl-3glc
61	18.72	1255.6323 <sup>a</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	0.80	368.97	+HCOO	1209.6268, 1077.5853, 945.5437, 783.4903, 621.4368, 459.3845	notoginsenoside Fc
62	18.87	1193.5969 <sup>b/f</sup>	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	0.72	355.53	−H	1107.5960, 945.5431, 783.4903, 621.4369, 459.3849	PPD-mal-4glc
63	18.93	855.4754 <sup>b/e/f</sup>	C <sub>44</sub> H <sub>72</sub> O <sub>16</sub>	0.75	302.22	−H	769.4748, 475.3794	PPT-mal-xyl-glc
64	19.43	1123.5893 <sup>a</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	0.37	275.15	+HCOO	1077.5830, 945.5417, 783.4889, 653.4628, 537.3445, 459.3856	ginsenoside Rc
65	19.80	1193.5956 <sup>b/f</sup>	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	−0.38	214.50	−H	1149.6067, 1107.5959, 945.5434, 783.4903, 621.4369, 459.3848	PPD-mal-4glc
66	19.86	1255.6317 <sup>a</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	0.32	363.00	+HCOO	1209.6260, 1077.5844, 945.5436, 783.4892, 621.4370, 459.3845	ginsenoside Ra1
67	20.19	1295.6268 <sup>b/e/f</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	−0.73	366.26	−H	1209.6269, 1077.5858, 945.5431, 783.4894, 621.4375, 459.3847	PPD-mal-2xyl-3glc
68	20.25	1193.5952 <sup>b/e/f</sup>	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	−0.68	—	−H	1149.6070, 1107.5955, 945.5430, 783.4901, 621.4373, 459.3847	PPD-mal-4glc

69	20.43	1193.5946 <sup>c/e/f</sup> <sub>f</sub>	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	−1.22	350.45	−H	1149.6064, 1107.5957, 945.5432, 783.4893, 621.4378, 459.3828	PPD-mal-4glc
70	20.67	1193.5948 <sup>b/e/f</sup>	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	−1.07	–	−H	1107.5958, 945.5429, 783.4896, 621.4370, 459.3839	PPD-mal-4glc
71	21.11	1387.6721 <sup>a</sup>	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	−1.5	381.91	+HCOO	1341.6676, 1209.6257, 1077.5843, 945.5428, 783.4897, 621.4367, 459.3850	notoginsenoside S
72	21.42	1163.5851 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−0.34	–	−H	1077.5927, 945.5433, 783.4911, 621.4375, 459.3808	PPD-mal-xyl-3glc
73	21.55	683.4455 <sup>a</sup>	C <sub>36</sub> H <sub>62</sub> O <sub>9</sub>	−0.48	275.30	+HCOO	637.4327, 621.4337, 475.3801, 391.2873	ginsenoside F1
74	21.68	1163.5860 <sup>a</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	0.44	348.79	−H	1077.5850, 1059.5755, 945.5441, 783.4900, 621.4362, 459.3845	malonyl-ginsenoside Rc
75	21.77	1295.6272 <sup>b/e/f</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	−0.42	374.67	−H	1209.6284, 1077.5854, 945.5435, 783.4897, 621.4372, 459.3849	PPD-mal-2xyl-3glc
76	21.85	1195.6267 <sup>d/f</sup>	C <sub>56</sub> H <sub>94</sub> O <sub>24</sub>	−0.28	370.43	+HCOO	1149.6059, 1107.5978, 945.5462, 783.4859, 621.4365, 459.3841	quinquenoside R1 or isomer
77	21.97	1163.5860 <sup>b/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	0.44	–	−H	1077.5853, 945.5437, 783.4878, 621.4337, 459.3830	PPD-mal-xyl-3glc
78	22.04	1165.6157 <sup>b/f</sup>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	−3.54	359.82	+HCOO	1119.5917, 1077.5852, 945.5415, 783.4886, 621.4348, 459.3859	PPD-Ace-xyl-3glc
79	22.07	1279.6151 <sup>b/e/f</sup>	C <sub>57</sub> H <sub>100</sub> O <sub>31</sub>	−1.94	282.37	−H	1107.5958, 945.5442, 783.4866, 621.4349, 459.3873	PPD-Dimal-4glc
80	22.09	1295.6435 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>104</sub> O <sub>31</sub>	−4.15	370.92	−H	1209.6264, 1077.5845, 945.5424, 783.4903, 621.4374, 459.3841	PPD-mal-2xyl-3glc
81	22.21	1163.5852 <sup>b/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−0.22	342.77	−H	1077.5854, 945.5439, 783.4902, 621.4365, 459.3849	PPD-mal-xyl-3glc
82	22.23	1279.6135 <sup>b/e/f</sup>	C <sub>57</sub> H <sub>100</sub> O <sub>31</sub>	−3.19	282.37	−H	1107.5959, 945.5433, 783.4897, 621.4363, 459.3831	PPD-Dimal-4glc
83	22.24	1119.5961 <sup>c/f</sup>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	0.39	353.83	−H	1077.5854, 783.4904, 621.4381, 459.3856	PPD-Ace-xyl-3glc
84	22.59	1123.5885 <sup>a</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	0.04	359.67	+HCOO	1077.5821, 945.5406, 783.4878, 621.4378, 459.3845	ginsenoside Rb2
85	22.86	1295.6253 <sup>b/e/f</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	−1.89	362.70	−H	1209.6273, 1077.5848, 945.5426, 783.4900, 621.4372, 459.3836	PPD-mal-2xyl-3glc
86	22.87	1119.5961 <sup>c/e/f</sup> <sub>f</sub>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	0.39	353.17	−H	1077.5853, 945.5441, 783.4903, 621.4367, 459.3849	PPD-Ace-xyl-3glc
87	23.04	1163.5846 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−0.77	–	−H	1077.5843, 945.5442, 783.4853, 621.4353, 459.3890	PPD-mal-xyl-3glc
88	23.31	1163.5840 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−1.31	351.16	−H	1077.5836, 945.5427, 783.4899, 621.4361, 459.3848	PPD-mal-xyl-3glc
89	23.66	1295.6442 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>104</sub> O <sub>31</sub>	−3.61	369.48	−H	1209.6276, 1077.5843, 945.5437, 783.4896, 621.4360, 459.3852	PPD-mal-2xyl-3glc
90	23.69	1123.5891 <sup>a</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	−1.29	347.37	+HCOO	1077.5834, 945.5422, 783.4891, 621.4364, 459.3842	ginsenoside Rb3
91	23.93	1279.5942 <sup>b/e/f</sup>	C <sub>60</sub> H <sub>96</sub> O <sub>29</sub>	−1.76	278.92	−H	1107.5952, 945.5413, 783.4886, 621.4369, 459.3841	PPD-Dimal-4glc
92	23.97	1123.5891 <sup>d/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	−1.36	357.13	+HCOO	1077.5840, 945.5433, 783.4892, 621.4366, 459.3841	ginsenoside Rc or isomer
93	23.99	1295.6437 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>104</sub> O <sub>31</sub>	−4.00	374.68	−H	1209.6282, 1077.5855, 945.5428, 783.4889, 621.4371, 459.3855	PPD-mal-2xyl-3glc
94	24.27	1295.6269 <sup>b/e/f</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	−0.66	–	−H	1209.6274, 1077.5854, 945.5438, 783.4898, 621.4371, 459.3848	PPD-mal-2xyl-3glc

95	24.64	1295.6260 <sup>b/e/f</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	−1.35	365.66	−H	1209.6266, 1077.5850, 945.5430, 783.4895, 621.4371, 459.3844	PPD-mal-2xyl-3glc
96	24.67	1163.5858 <sup>a</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	0.26	354.92	−H	1077.5860, 1059.5721, 945.5433, 783.4896, 621.4357, 459.3852	malonylginsenoside Rb2
97	24.81	1123.6076 <sup>d/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	1.30	357.12	+HCOO	1077.5865, 945.5421, 783.4893, 621.4356, 459.3807	notoginsenoside L or isomer
98	24.85	1255.6309 <sup>d/f</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	−1.45	284.63	+HCOO	1209.6256, 1077.5844, 945.5424, 783.4896, 621.4362, 459.3839	notoginsenoside-FZ or isomer
99	25.41	1165.5999 <sup>b/e/f</sup>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	−2.64	364.03	+HCOO	1119.5927, 1077.5849, 945.5417, 783.4885, 621.4369, 459.3845	PPD-Ace-xyl-3glc
100	25.43	1137.6066 <sup>d/f</sup>	C <sub>54</sub> H <sub>92</sub> O <sub>22</sub>	2.06	349.98	+HCOO	1091.6030, 945.5491, 783.4910, 621.4379, 459.3836	gypenoside V or isomer
101	25.63	1249.5844 <sup>b/e/f</sup>	C <sub>59</sub> H <sub>94</sub> O <sub>28</sub>	−1.19	358.25	−H	1077.5835, 945.5442, 783.4898, 621.4364, 459.3829	PPD-Dimal-xyl-3glc
102	25.68	1163.5844 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−0.90	346.28	−H	1077.5844, 945.5423, 783.4899, 621.4364, 459.3845	PPD-mal-xyl-3glc
103	25.83	1119.5956 <sup>c/e/f</sup>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	−0.05	278.92	−H	1077.5846, 945.5440, 783.4895, 621.4361, 459.3856	PPD-Ace-xyl-3glc
104	25.95	1163.5842 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−1.11	279.06	−H	1077.5843, 945.5430, 783.4901, 621.4371, 459.3841	PPD-mal-xyl-3glc
105	26.03	1205.5949 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	−0.96	347.64	−H	1119.5936, 1077.5877, 945.5422, 783.4886, 621.4379, 459.3833	PPD-mal-Ace-xyl-3glc
106	26.24	1163.5833 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−1.92	343.52	−H	1077.5840, 945.5425, 783.4895, 621.4366, 459.3842	PPD-mal-xyl-3glc
107	26.97	1119.5969 <sup>c/f</sup>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	1.11	365.10	−H	1077.5856, 945.5439, 783.4910, 459.3843	PPD-Ace-xyl-3glc
108	27.13	1163.5837 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−1.50	267.37	−H	1077.5833, 945.5418, 783.4889, 621.4364, 459.3841	PPD-mal-xyl-3glc
109	27.34	1119.5975 <sup>c/f</sup>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	1.64	334.07	−H	1077.5852, 945.5430, 783.4901, 621.4375, 459.3837	PPD-Ace-xyl-3glc
110	27.35	1163.5827 <sup>c/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−2.40	342.82	−H	1077.5852, 945.5430, 783.4901, 621.4375, 459.3837	PPD-mal-xyl-3glc
111	27.67	1163.5836 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−1.66	349.64	−H	1077.5842, 945.5424, 783.4889, 621.4363, 459.3842	PPD-mal-xyl-3glc
112	27.75	1249.5840 <sup>c/e/f</sup>	C <sub>59</sub> H <sub>94</sub> O <sub>28</sub>	−1.51	358.93	−H	1077.5847, 945.5433, 621.4371, 459.3852	PPD-Dimal-xyl-3glc
113	27.95	1163.5853 <sup>b/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−0.16	278.78	−H	1077.5831, 945.5420, 783.4892, 621.4264, 459.3834	PPD-mal-xyl-3glc
114	28.24	1163.5837 <sup>b/e/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	−1.53	287.08	−H	1077.5835, 945.5424, 783.4891, 621.4364, 459.3843	PPD-mal-xyl-3glc
115	28.40	1295.6251 <sup>b/e/f</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	−2.04	359.27	−H	1209.6257, 1077.5825, 945.5415, 783.4886, 621.4358, 459.3844	PPD-mal-2xyl-3glc
116	28.71	991.5467 <sup>a</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	−1.20	331.74	+HCOO	945.5414, 783.4889, 621.4363, 459.3844	ginsenoside Rd
117	28.94	1163.5860 <sup>b/f</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	0.44	362.64	−H	1077.5866, 945.5359, 783.4867, 621.4315, 459.3817	PPD-mal-xyl-3glc
118	29.19	1249.5853 <sup>b/e/f</sup>	C <sub>59</sub> H <sub>94</sub> O <sub>28</sub>	−0.47	356.61	−H	1077.5860, 945.5427, 783.4894, 621.4360, 459.3845	PPD-Dimal-xyl-3glc
119	29.49	1205.5971 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	0.86	346.54	−H	1119.5960, 1077.5864, 945.5445, 783.4911, 621.4378, 459.3840	PPD-mal-Ace-xyl-3glc
120	29.76	1093.5802 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>23</sub>	0.17	351.04	−H	1047.5738, 915.5288, 753.4805, 621.4349, 459.3830	PPD-2xyl-2glc

121	29.95	1249.5857 <sup>b/e/f</sup>	C <sub>59</sub> H <sub>94</sub> O <sub>28</sub>	−0.15	359.08	−H	1077.5859, 945.5401, 783.4889, 621.4357, 459.3859	PPD-Dimal-xyl-3glc
122	29.99	1205.5949 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	−0.96	368.19	−H	1119.5939, 1077.5868, 945.5465, 783.4856, 621.4373, 459.3851	PPD-mal-Ace-xyl-3glc
123	30.26	1249.5862 <sup>b/e/f</sup>	C <sub>59</sub> H <sub>94</sub> O <sub>28</sub>	0.25	–	−H	1077.5860, 945.5461, 783.4899, 621.4377, 459.3850	PPD-Dimal-xyl-3glc
124	30.40	1205.5978 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	1.44	357.28	−H	1119.5965, 1077.5849, 945.5417, 783.4902, 621.4393, 459.3855	PPD-mal-Ace-xyl-3glc
125	30.51	1207.6108 <sup>b/e/f</sup>	C <sub>57</sub> H <sub>94</sub> O <sub>24</sub>	2.04	389.96	+HCOO	1161.6086, 1119.5955, 1077.5862, 783.4927, 621.4374, 459.3842	PPD-2Ace-xyl-3glc
126	30.63	1249.5826 <sup>b/e/f</sup>	C <sub>59</sub> H <sub>94</sub> O <sub>28</sub>	−2.63	363.75	−H	1077.5864, 945.5442, 783.4905, 621.4372, 459.3839	PPD-Dimal-xyl-3glc
127	30.81	1031.5443 <sup>a</sup>	C <sub>51</sub> H <sub>84</sub> O <sub>21</sub>	1.00	340.41	−H	945.5435, 783.4904, 621.4387, 459.3845	malonylginsenoside Rd
128	30.91	1093.5811 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>23</sub>	1.00	347.43	−H	1047.5737, 915.5361, 753.4784, 621.4368, 459.3859	PPD-2xyl-2glc
129	30.98	1249.5873 <sup>b/e/f</sup>	C <sub>59</sub> H <sub>94</sub> O <sub>28</sub>	1.13	–	−H	1077.5864, 945.5387, 783.4928, 621.4345, 459.3815	PPD-Dimal-xyl-3glc
130	31.04	1093.5818 <sup>b/f</sup>	C <sub>52</sub> H <sub>88</sub> O <sub>21</sub>	−1.75	347.43	+HCOO	1047.5727, 915.5441, 753.4770, 621.4371, 459.3876	notoginsenoside O or isomer
131	31.10	1205.5955 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	−0.46	351.34	−H	1119.5958, 1077.5868, 945.5441, 783.4876, 621.4343, 459.3878	PPD-mal-Ace-xyl-3glc
132	31.25	1249.5855 <sup>b/e/f</sup>	C <sub>59</sub> H <sub>94</sub> O <sub>28</sub>	−0.31	363.76	−H	1077.5858, 945.5440, 783.4906, 621.4361, 459.3842	PPD-Dimal-xyl-3glc
133	31.35	1205.5974 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	1.11	351.34	−H	1119.5970, 1077.5855, 945.5436, 783.4907, 621.4373, 459.3851	PPD-mal-Ace-xyl-3glc
134	31.55	1165.6015 <sup>b/e/f</sup>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	−1.22	363.62	+HCOO	1119.5943, 1077.5847, 945.5485, 783.4889, 621.4335, 459.3856	PPD-Ace-xyl-3glc
135	31.66	1249.5846 <sup>b/e/f</sup>	C <sub>59</sub> H <sub>94</sub> O <sub>28</sub>	−1.03	357.75	−H	1077.5854, 945.5431, 783.4903, 621.4370, 459.3844	PPD-Dimal-xyl-3glc
136	31.67	1205.5964 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	0.28	346.77	−H	1119.5955, 1077.5848, 945.5429, 783.4906, 621.4368, 459.3847	PPD-mal-Ace-xyl-3glc
137	31.90	1031.5420 <sup>d/f</sup>	C <sub>51</sub> H <sub>84</sub> O <sub>21</sub>	−1.20	323.41	−H	945.5417, 783.4897, 621.4367, 459.3845	malonylfloralginsenoside Rd4 or isomer
138	31.94	1121.4425 <sup>c/e/f</sup>	C <sub>43</sub> H <sub>78</sub> O <sub>33</sub>	6.46	330.93	−H	945.5424, 783.4906, 459.3844	PPD-glurA-3glc
139	31.94	991.5484 <sup>c/f</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	−0.46	332.37	+HCOO	945.5424, 783.4906, 621.4371, 459.3844	chikusetsusaponin FK7 or isomer
140	32.17	1033.5569 <sup>b/e/f</sup>	C <sub>50</sub> H <sub>84</sub> O <sub>19</sub>	1.01	213.18	+HCOO	987.5544, 945.5428, 783.4905, 621.4370, 459.3838	PPD-Ace-3glc
141	32.44	1265.6203 <sup>b/e/f</sup>	C <sub>60</sub> H <sub>98</sub> O <sub>28</sub>	2.46	362.88	−H	1179.6118, 1047.5701, 915.5317, 783.4894, 621.4398, 459.3867	PPD-mal-3xyl-2glc
142	32.55	987.5539 <sup>c/f</sup>	C <sub>50</sub> H <sub>84</sub> O <sub>19</sub>	0.50	340.81	−H	945.5423, 783.4894, 621.4376, 459.3848	PPD-Ace-3glc
143	32.65	1205.5984 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	1.94	349.93	−H	1119.6081, 1077.5871, 945.5346, 783.4859, 621.4466, 459.3820	PPD-mal-Ace-xyl-3glc
144	32.92	769.4389 <sup>d/f</sup>	C <sub>40</sub> H <sub>66</sub> O <sub>14</sub>	1.20	284.23	−H	769.4389, 637.4305, 475.3798, 391.2861	20(S)-sanchirrhinoside A3 or isomer
145	33.07	1165.6027 <sup>b/e/f</sup>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	0.21	372.42	+HCOO	1119.5959, 1077.5866, 945.5435, 783.4903, 621.4378, 459.3818	PPD-Ace-xyl-3glc

146	33.16	1205.5956 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	−0.38	360.77	−H	1119.6002, 1077.5904, 945.5433, 783.4878, 621.4329, 459.3829	PPD-mal-Ace-xyl-3glc
147	33.25	1033.5594 <sup>c/e/f</sup>	C <sub>50</sub> H <sub>84</sub> O <sub>19</sub>	−0.41	344.24	+HCOO	987.5530, 945.5432, 783.4897, 621.4373, 459.3846	PPD-Ace-3glc
148	33.27	1073.5543 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>86</sub> O <sub>22</sub>	0.47	352.29	−H	987.5548, 945.5431, 783.4909, 621.4364, 459.3853	PPD-mal-Ace-3glc
149	33.31	1117.5441 <sup>b/e/f</sup>	C <sub>54</sub> H <sub>86</sub> O <sub>24</sub>	0.44	337.86	−H	945.5423, 783.4903, 621.4373, 459.3848	PPD-Dimal-3glc
150	33.36	1075.5705 <sup>b/e/f</sup>	C <sub>52</sub> H <sub>86</sub> O <sub>20</sub>	0.94	353.87	+HCOO	1029.5621, 987.5532, 945.5446, 783.4933, 621.4358, 459.3846	PPD-2Ace-3glc
151	33.42	1093.5821 <sup>d/f</sup>	C <sub>52</sub> H <sub>88</sub> O <sub>21</sub>	1.95	338.31	+HCOO	1047.5744, 915.5307, 783.4891, 621.4413, 459.3842	notoginsenoside P or isomer
152	33.57	991.5488 <sup>a</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	−0.15	321.69	+HCOO	945.5427, 927.5316, 783.4927, 621.4397, 459.3835	gypenoside XV II
153	33.59	1117.5444 <sup>b/e/f</sup>	C <sub>54</sub> H <sub>86</sub> O <sub>24</sub>	0.66	342.21	−H	945.5448, 621.4384, 459.3850	PPD-Dimal-3glc
154	33.62	1033.5746 <sup>b/f</sup>	C <sub>50</sub> H <sub>84</sub> O <sub>19</sub>	0.50	341.25	+HCOO	987.5539, 945.5434, 783.4908, 621.4373, 459.3844	PPD-Ace-3glc
155	33.64	1031.5442 <sup>d/f</sup>	C <sub>51</sub> H <sub>84</sub> O <sub>21</sub>	0.90	331.98	−H	945.5425, 783.4914, 621.4372, 459.3853	malonylfloralginsenoside Rd3 or isomer
156	33.68	1047.5745 <sup>c/f</sup>	C <sub>52</sub> H <sub>88</sub> O <sub>21</sub>	−0.03	348.56	−H	915.5324, 783.4896, 621.4372, 459.3845	notoginsenoside P or isomer
157	33.73	1133.5780 <sup>b/e/f</sup>	C <sub>55</sub> H <sub>90</sub> O <sub>24</sub>	2.71	339.22	−H	1047.5774, 915.5325, 783.4870, 621.4406, 459.3867	PPD-mal-2xyl-2glc
158	33.74	1093.5808 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>23</sub>	0.68	350.95	−H	1047.5753, 915.5323, 783.4909, 621.4373, 459.3840	PPD-2xyl-2glc
159	33.76	1165.6014 <sup>b/e/f</sup>	C <sub>55</sub> H <sub>92</sub> O <sub>23</sub>	1.91	372.70	+HCOO	1119.5978, 1077.5856, 945.5436, 783.4907, 621.4372, 459.3863	PPD-Ace-xyl-3glc
160	33.87	1075.5682 <sup>b/e/f</sup>	C <sub>52</sub> H <sub>86</sub> O <sub>20</sub>	−1.17	359.94	+HCOO	1029.5632, 987.5533, 945.5435, 621.4370, 459.3854	PPD-2Ace-3glc
161	33.94	1117.5432 <sup>b/e/f</sup>	C <sub>54</sub> H <sub>86</sub> O <sub>24</sub>	−0.39	337.74	−H	945.5437, 783.4904, 621.4372, 459.3847	PPD-Dimal-3glc
162	33.94	1073.5715 <sup>b/e/f</sup>	C <sub>57</sub> H <sub>86</sub> O <sub>19</sub>	2.28	207.00	−H	987.5531, 945.5425, 783.4890, 621.4369, 459.3849	PPD-mal-Ace-3glc
163	34.06	1075.5842 <sup>b/e/f</sup>	C <sub>52</sub> H <sub>86</sub> O <sub>20</sub>	5.86	359.94	+HCOO	1029.5700, 987.5529, 945.5418, 783.4983, 621.4390, 459.3864	PPD-2Ace-3glc
164	34.08	1031.5460 <sup>d/f</sup>	C <sub>51</sub> H <sub>84</sub> O <sub>21</sub>	2.68	338.12	−H	945.5442, 783.4894, 621.4401, 459.3868	malonylfloralginsenoside Rd1 or isomer
165	34.14	961.5397 <sup>d/f</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	2.00	325.41	+HCOO	915.5298, 783.4868, 621.4379, 459.3836	vinaginsenoside R17 or isomer
166	34.17	1117.5445 <sup>b/e/f</sup>	C <sub>54</sub> H <sub>86</sub> O <sub>24</sub>	0.81	338.33	−H	945.5438, 765.4731, 621.4294, 459.3874	PPD-Dimal-3glc
167	34.18	1073.5557 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>86</sub> O <sub>22</sub>	1.77	351.78	−H	987.5534, 945.5453, 783.4893, 621.4348, 459.3862	PPD-mal-Ace-3glc
168	34.23	1093.5818 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>23</sub>	1.61	337.32	−H	1047.5712, 915.5339, 783.5080, 621.4369, 459.3815	PPD-2xyl-2glc
169	34.26	1205.5983 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	1.86	349.05	−H	1119.5945, 1077.5852, 915.5349, 783.4860, 621.4381, 459.3853	PPD-mal-Ace-3glc-xyl
170	34.47	1115.5664 <sup>b/e/f</sup>	C <sub>55</sub> H <sub>88</sub> O <sub>23</sub>	1.83	362.71	−H	1029.5652, 987.5533, 945.5428, 783.4873, 621.4390, 459.3847	PPD-mal-2Ace-3glc
171	34.47	1159.5549 <sup>c/e/f</sup>	C <sub>56</sub> H <sub>88</sub> O <sub>25</sub>	0.61	352.77	−H	987.5538, 945.5429, 783.4900, 621.4362, 459.3837	PPD-Dimal-Ace-3glc

172	34.48	1119.5673 <sup>c/e/f</sup> <sub>f</sub>	C <sub>58</sub> H <sub>88</sub> O <sub>21</sub>	−6.46	351.45	−H	987.5538, 945.5429, 783.4900, 621.4362, 459.3837	PPD-xyl-Ace-3glc
173	34.50	1117.5581 <sup>b/f</sup>	C <sub>51</sub> H <sub>86</sub> O <sub>21</sub>	−0.70	−	−H	945.5441, 783.4869, 621.4386, 459.3821	PPD-Dimal-3glc
174	34.56	1075.5715 <sup>b/e/f</sup>	C <sub>52</sub> H <sub>86</sub> O <sub>20</sub>	1.94	350.72	+HCOO	1029.5595, 987.5542, 945.5452, 783.4876, 621.4364, 459.3855	PPD-2Ace-3glc
175	34.62	1205.5963 <sup>b/e/f</sup>	C <sub>58</sub> H <sub>94</sub> O <sub>26</sub>	0.20	348.95	−H	1119.5990, 1077.5862, 945.5453, 783.4897, 621.4371, 459.3859	PPD-mal-Ace-xyl-3glc malonylfloralginsenoside Rd2 or isomer
176	34.65	1031.5446 <sup>d/f</sup>	C <sub>51</sub> H <sub>84</sub> O <sub>21</sub>	1.33	328.62	−H	945.5423, 783.489, 621.4371, 459.3829	PPD-Dimal-3glc
177	34.72	1117.5443 <sup>b/e/f</sup>	C <sub>54</sub> H <sub>86</sub> O <sub>24</sub>	0.60	354.91	−H	945.5452, 783.4901, 621.4369, 459.3809	PPD-mal-Ace-3glc
178	34.73	1073.5553 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>86</sub> O <sub>22</sub>	1.40	354.93	−H	987.5546, 945.5414, 783.4906, 621.4337, 459.3851	notoginsenoside Fe
179	34.79	961.5373 <sup>a</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	−2.92	322.31	+HCOO	915.5296, 783.4889, 621.4361, 459.3817	PPD-glurA-Ace-xyl-2glc
180	34.84	1133.5785 <sup>b/e/f</sup>	C <sub>55</sub> H <sub>90</sub> O <sub>24</sub>	3.15	340.64	−H	957.5421, 915.5311, 783.4892, 621.4408, 459.3806	notoginsenoside Fd
181	34.86	961.5378 <sup>a</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	−0.11	325.83	+HCOO	915.5301, 783.4895, 621.4356, 459.3857	PPD-2Ace-2xyl-2glc
182	34.87	1131.4683 <sup>b/e/f</sup>	C <sub>49</sub> H <sub>80</sub> O <sub>29</sub>	−2.61	334.97	−H	1089.5933, 957.5457, 915.5326, 783.4870, 621.4336, 459.3895	PPD-mal-2xyl-2glc
183	35.13	1133.5763 <sup>b/e/f</sup>	C <sub>55</sub> H <sub>90</sub> O <sub>24</sub>	1.21	334.2	−H	1047.5714, 915.5313, 783.4956, 621.4364, 459.3836	PPD-xyl-2glc
184	35.14	957.5456 <sup>c/e/f</sup>	C <sub>49</sub> H <sub>82</sub> O <sub>18</sub>	2.88	332.53	−H	915.5307, 783.4903, 621.4365, 459.3840	ginsenoside Rd2
185	35.29	961.5381 <sup>a</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	0.32	322.73	+HCOO	915.5321, 762.4102, 621.4382, 459.3866	PPD-mal-xyl-2glc
186	35.43	1001.5333 <sup>b/e/f</sup>	C <sub>50</sub> H <sub>82</sub> O <sub>20</sub>	0.63	319.34	−H	915.5328, 783.4955, 621.4380, 459.3850	PPD-Dimal-3glc
187	35.54	1117.5466 <sup>b/e/f</sup>	C <sub>54</sub> H <sub>86</sub> O <sub>24</sub>	2.66	332.19	−H	945.5385, 783.4889, 621.4386, 459.3772	ginsenoside Rb4 or isomer
188	35.56	1107.5993 <sup>d/f</sup>	C <sub>54</sub> H <sub>92</sub> O <sub>23</sub>	3.30	350.34	−H	1061.5912, 929.5502, 783.4905, 621.4363, 459.3829	PPD-2xyl-2glc
189	35.60	1093.5801 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>23</sub>	0.12	338.01	−H	1047.5758, 915.5321, 783.4890, 621.4381, 459.3849	PPD-xyl-Ace-2glc
190	35.62	1003.5460 <sup>c/e/f</sup> <sub>f</sub>	C <sub>49</sub> H <sub>82</sub> O <sub>18</sub>	0.06	339.24	+HCOO	957.5429, 825.5001, 783.4907, 621.4374, 459.3841	PPD-Ace-xyl-2glc
191	35.62	957.5430 <sup>c/e/f</sup>	C <sub>49</sub> H <sub>82</sub> O <sub>18</sub>	0.17	333.21	−H	915.5324, 783.4907, 621.4374, 459.3841	PPD-Ace-3glc
192	35.83	1033.5607 <sup>b/f</sup>	C <sub>50</sub> H <sub>84</sub> O <sub>19</sub>	0.81	344.07	+HCOO	987.5542, 945.5422, 783.4919, 621.4376, 459.3827	PPD-xyl-Ace-2glc
193	35.91	1003.5460 <sup>c/e/f</sup> <sub>f</sub>	C <sub>49</sub> H <sub>82</sub> O <sub>18</sub>	0.17	331.47	+HCOO	957.5430, 825.4987, 783.4922, 621.4386, 459.3854	PPD-Dimal-xyl-2glc
194	35.94	1087.5342 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>84</sub> O <sub>23</sub>	1.06	335.49	−H	915.5337, 783.4925, 621.4376, 459.3854	PPD-Dimal-xyl-2glc
195	36.03	1087.5500 <sup>b/e/f</sup>	C <sub>57</sub> H <sub>84</sub> O <sub>20</sub>	1.55	335.49	−H	915.5311, 783.5023, 621.4356, 459.3858	PPD-mal-xyl-2glc
196	36.14	1001.5326 <sup>b/e/f</sup>	C <sub>50</sub> H <sub>82</sub> O <sub>20</sub>	−0.07	331.19	−H	915.5347, 783.4903, 621.4380, 459.3852	PPD-Dimal-xyl-2glc
197	36.27	1087.5342 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>84</sub> O <sub>23</sub>	1.05	326.23	−H	915.5283, 783.4935, 621.4361, 459.3896	PPD-xyl-2glc
198	36.40	1001.5322 <sup>b/e/f</sup>	C <sub>50</sub> H <sub>82</sub> O <sub>20</sub>	−0.47	317.59	−H	915.5261, 783.4832, 621.4363, 459.3820	PPD-rha-2glc
199	36.43	975.5680 <sup>b/e/f</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>17</sub>	2.77	329.90	+HCOO	929.5505, 783.4911, 621.4366, 459.3833	PPD-mal-Ace-3glc
200	36.51	1073.5566 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>86</sub> O <sub>22</sub>	2.61	354.99	−H	987.5517, 945.5475, 783.4876, 621.4338, 459.3860	PPD-Dimal-xyl-2glc
201	36.74	1087.5351 <sup>b/e/f</sup>	C <sub>53</sub> H <sub>84</sub> O <sub>23</sub>	1.85	329.07	−H	915.5280, 783.4866, 621.4361, 459.3827	

202	36.84	829.4961 <sup>a</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	0.73	306.82	+HCOO	783.4929, 621.4385, 459.3844, 375.2900	ginsenoside F2
203	37.07	1015.5495 <sup>b/e/f</sup>	C <sub>51</sub> H <sub>84</sub> O <sub>20</sub>	1.16	339.42	−H	929.5497, 783.4898, 621.4363, 459.3850	PPD-mal-rha-2glc
204	37.15	1101.5507 <sup>b/e/f</sup>	C <sub>54</sub> H <sub>86</sub> O <sub>23</sub>	1.82	341.83	−H	929.5503, 783.4887, 621.4401, 459.3838	PPD-Dimal-rha-2glc
205	37.18	871.5053 <sup>b/e/f</sup>	C <sub>44</sub> H <sub>74</sub> O <sub>14</sub>	1.96	317.61	+HCOO	825.5022, 783.4867, 763.4077, 621.4384, 459.3845	PPD-Ace-2glc
206	37.28	1015.5488 <sup>b/e/f</sup>	C <sub>51</sub> H <sub>84</sub> O <sub>20</sub>	0.48	336.21	−H	929.5489, 783.4937, 621.4384, 459.3852	PPD-mal-rha-2glc
207	37.43	1059.5769 <sup>d/f</sup>	C <sub>52</sub> H <sub>86</sub> O <sub>19</sub>	−0.94	352.06	+HCOO	1013.5681, 945.5435, 783.4935, 621.4352, 459.3854	quinquenoside I or isomer
208	37.67	869.4914 <sup>b/e/f</sup>	C <sub>45</sub> H <sub>74</sub> O <sub>18</sub>	1.14	310.02	−H	783.4901, 621.4354, 459.3837	PPD-mal-2glc
209	37.75	871.5049 <sup>b/e/f</sup>	C <sub>44</sub> H <sub>74</sub> O <sub>14</sub>	−3.13	318.66	+HCOO	825.4980, 783.4939, 621.4325, 459.3869	PPD-Ace-2glc
210	37.83	829.4954 <sup>a</sup>	C <sub>43</sub> H <sub>74</sub> O <sub>15</sub>	−0.15	305.11	+HCOO	783.4895, 621.4386, 459.3843	20(S)-ginsenoside Rg3
211	37.93	955.4918 <sup>b/e/f</sup>	C <sub>48</sub> H <sub>76</sub> O <sub>19</sub>	1.03	314.77	−H	783.5115, 621.4362, 459.3832	PPD-Dimal-2glc
212	38.16	829.4950 <sup>a</sup>	C <sub>43</sub> H <sub>74</sub> O <sub>15</sub>	−0.64	301.13	+HCOO	783.4913, 621.4358, 459.3842	20(R)-ginsenoside Rg3
213	38.44	871.5056 <sup>b/f</sup>	C <sub>44</sub> H <sub>74</sub> O <sub>14</sub>	−0.95	320.28	+HCOO	825.4998, 783.4899, 621.4381, 459.3847	PPD-Ace-2glc
214	38.54	955.4925 <sup>b/e/f</sup>	C <sub>48</sub> H <sub>76</sub> O <sub>19</sub>	1.76	316.29	−H	783.4930, 621.4353, 459.3849	PPD-Dimal-2glc
215	38.58	869.4916 <sup>b/e/f</sup>	C <sub>45</sub> H <sub>74</sub> O <sub>18</sub>	1.37	306.02	−H	783.4867, 621.4305, 459.3837	PPD-mal-2glc
216	39.05	799.4858 <sup>b/e/f</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	1.11	304.12	−H	753.4762, 621.4373, 459.3840	PPD-xyl-glc
217	39.45	799.4856 <sup>d/f</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	0.88	304.95	+HCOO	753.4789, 621.4361, 459.3843	gypenoside XIII or isomer
218	40.76	811.4987 <sup>a</sup>	C <sub>42</sub> H <sub>70</sub> O <sub>12</sub>	1.76	315.78	+HCOO	765.4808, 603.4288	ginsenoside Rk1
219	41.81	753.4446 <sup>d/f</sup>	C <sub>40</sub> H <sub>66</sub> O <sub>13</sub>	2.04	287.12	−H	621.4371, 459.3814	gypenoside XIII or isomer

a: Identification assisted with reference compounds comparison; b: Components identified in the "Unknown Components" section of the DDA data; c: Components identified in HDMS<sup>E</sup> data; d: Components identified in the "Identified Components" section of the DDA data; e: The reported components may not have been isolated from *Panax ginseng*; f: Tentative characterization by analyzing the high-accuracy MS<sup>2</sup> data.

**Table S3.** Information for the 40 prototype components characterized from rat plasma.

No.	Observed RT (min)	Observed m/z	Formula	Mass error (ppm)	CCA (Å <sup>2</sup> )	Adducts	ESI-MS <sup>2</sup>	Identification
4	5.25	977.5315 <sup>a</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>18</sub>	−1.15	322.41	+HCOO	931.5263, 799.4839, 637.4322, 475.3793, 391.2845	notoginsenoside R1
6	5.65	991.5484 <sup>a</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	0.06	327.00	+HCOO	945.5429, 799.4842, 637.4319, 619.4202, 475.3887, 391.2848	ginsenoside Re
7	5.69	845.4997 <sup>a</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	0.21	297.89	+HCOO	799.4851, 637.4321, 475.3798, 391.2867	ginsenoside Rg1
31	10.81	1285.6450 <sup>a</sup>	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	0.95	372.56	+HCOO	1239.6391, 1107.5986, 945.5443, 783.4914, 621.4364, 459.3857, 353.1086	notoginsenosides R4
38	12.84	1285.6410 <sup>a</sup>	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	−0.53	372.92	+HCOO	1239.6357, 1107.5938, 945.5416, 783.4887, 621.4366, 459.3876	notoginsenoside Fa
39	13.03	1341.6670 <sup>b</sup>	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	−2.32	384.79	−H	1341.6664, 1209.6253, 1077.5841, 945.5425, 783.4892, 621.4363, 459.3841	PPD-3xyl-2glc
48	15.40	1255.6320 <sup>a</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	0.67	365.25	+HCOO	1209.6261, 1077.5841, 945.5425, 783.4896, 621.4359, 459.3872	notoginsenoside FP2
49	15.63	1387.6910 <sup>a</sup>	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	−0.53	302.07	+HCOO	1341.6689, 1209.6272, 1077.5856, 945.5442, 783.4902, 765.4810, 621.4379, 459.3851	notoginsenoside Fh1
50	16.10	1153.6020 <sup>a</sup>	C <sub>54</sub> H <sub>92</sub> O <sub>23</sub>	−0.60	355.55	+HCOO	1107.5950, 1089.5862, 945.5424, 783.4899, 621.4378, 459.3842	ginsenoside Rb1
51	16.26	1325.6380 <sup>b</sup>	C <sub>62</sub> H <sub>102</sub> O <sub>30</sub>	−0.58	373.85	−H	1239.6383, 1107.5957, 945.5436, 783.4907, 621.4373, 459.3849	malonylginsenoside Ra3 or isomer
52	16.38	1255.6320 <sup>b</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	0.12	361.25	+HCOO	1209.6275, 1077.5861, 945.5440, 783.4904, 621.4373, 459.3847	notoginsenoside-FZ or isomer
56	17.58	955.4923 <sup>a</sup>	C <sub>48</sub> H <sub>76</sub> O <sub>19</sub>	1.54	200.20	−H	955.4915, 793.4887, 613.3763, 569.3852, 523.3783, 497.3650, 455.3536	ginsenoside Ro
59	18.13	1193.5970 <sup>a</sup>	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	0.49	265.46	−H	1107.5965, 945.5437, 783.4904, 621.4378, 459.3853	malonylginsenoside Rb1
61	18.40	1255.6320 <sup>a</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	0.80	368.97	+HCOO	1209.6268, 1077.5853, 945.5437, 783.4903, 765.4802, 621.4368, 459.3845	notoginsenoside Fc
64	19.34	1123.5890 <sup>a</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	0.37	275.15	+HCOO	1077.5830, 945.5417, 783.4889, 653.4628, 537.3445, 459.3856	ginsenoside Rc
66	19.80	1255.6320 <sup>a</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	0.32	363.00	+HCOO	1209.6260, 1077.5844, 945.5436, 783.4892, 621.4370, 459.3845	ginsenoside Ra1
68	20.14	1193.5950 <sup>b</sup>	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	−0.68	–	−H	1149.6070, 1107.5955, 945.5430, 783.4901, 621.4373, 459.3847	malonylfloralginsenoside Rb2 or isomer
71	20.92	1387.6720 <sup>a</sup>	C <sub>63</sub> H <sub>106</sub> O <sub>30</sub>	−1.50	381.91	+HCOO	1341.6676, 1209.6257, 1077.5843, 945.5428, 783.4897, 621.4367, 459.3850	notoginsenoside S
73	21.19	683.4455 <sup>a</sup>	C <sub>36</sub> H <sub>62</sub> O <sub>9</sub>	−0.48	275.30	+HCOO	637.4327, 621.4337, 475.3801, 391.2873	ginsenoside F1
75	21.62	1295.6270 <sup>b</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	−0.42	374.67	−H	1209.6284, 1077.5854, 945.5435, 783.4897, 621.4372, 459.3849	PPD-mal-2xyl-3glc



77	21.97	1163.5860 <sup>b</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	0.44	–	–H	1077.5853, 945.5437, 783.4878, 621.4337, 459.3830	malonylginsenoside Rb2 or isomer
84	22.28	1123.5890 <sup>a</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	0.04	359.67	+HCOO	1077.5821, 945.5406, 783.4878, 621.4378, 459.3845	ginsenoside Rb2
85	22.58	1295.6250 <sup>b</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	–1.89	362.70	–H	1209.6273, 1077.5848, 945.5426, 783.4900, 621.4372, 459.3836	PPD-mal-2xyl-3glc
87	23.13	1163.5850 <sup>b</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	–0.77	–	–H	1077.5843, 945.5442, 783.4853, 621.4353, 459.3890	malonylfloralginsenoside Rc3 or isomer
90	23.43	1123.5890 <sup>a</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	–1.29	347.37	+HCOO	1077.5834, 945.5422, 783.4891, 621.4364, 459.3842	ginsenoside Rb3
94	24.24	1295.6270 <sup>b</sup>	C <sub>61</sub> H <sub>100</sub> O <sub>29</sub>	–0.66	–	–H	1209.6274, 1077.5854, 945.5438, 783.4898, 621.4371, 459.3848	PPD-mal-2xyl-3glc
97	24.54	1123.6080 <sup>b</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	1.30	357.12	+HCOO	1077.5865, 945.5421, 783.4893, 621.4356, 459.3807	notoginsenoside L or isomer
98	24.60	1255.6310 <sup>b</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	–1.45	284.63	+HCOO	1209.6256, 1077.5844, 945.5424, 783.4896, 621.4362, 459.3839	notoginsenoside-FZ or isomer
104	26.10	1163.5840 <sup>b</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	–1.11	279.06	–H	1077.5843, 945.5430, 783.4901, 621.4371, 459.3841	malonylfloralginsenoside Rc2 or isomer
108	27.10	1163.5840 <sup>b</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	–1.50	267.37	–H	1077.5833, 945.5418, 783.4889, 621.4364, 459.3841	malonylfloralginsenoside Rc1 or isomer
113	27.80	1163.5850 <sup>b</sup>	C <sub>56</sub> H <sub>92</sub> O <sub>25</sub>	–0.16	278.78	–H	1077.5831, 945.5420, 783.4892, 621.4264, 459.3834	malonylfloralginsenoside Rc4 or isomer
127	30.27	1031.5440 <sup>a</sup>	C <sub>51</sub> H <sub>84</sub> O <sub>21</sub>	1.00	340.41	–H	945.5435, 783.4904, 621.4387, 459.3845	malonylginsenoside Rd
140	32.36	1033.5570 <sup>b</sup>	C <sub>50</sub> H <sub>84</sub> O <sub>19</sub>	1.01	213.18	+HCOO	987.5544, 945.5428, 783.4905, 621.4370, 459.3838	quinquenoside III or isomer
179	34.58	961.5373 <sup>a</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	–2.92	322.31	+HCOO	915.5296, 783.4889, 621.4361, 459.3817	notoginsenoside Fe
185	35.36	961.5381 <sup>a</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	0.32	322.73	+HCOO	915.5321, 621.4382, 459.3866	ginsenoside Rd2
186	35.64	1001.5330 <sup>b</sup>	C <sub>50</sub> H <sub>82</sub> O <sub>20</sub>	0.63	319.34	–H	915.5328, 783.4955, 621.4380, 459.3850	PPD-mal-xyl-2glc
189	35.45	1093.5800 <sup>b</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>23</sub>	0.12	338.01	+HCOO	1047.5758, 915.5321, 783.4890, 621.4381, 459.3849	notoginsenoside P or isomer
196	36.25	1001.5330 <sup>b</sup>	C <sub>50</sub> H <sub>82</sub> O <sub>20</sub>	–0.07	331.19	–H	915.5347, 783.4903, 621.4380, 459.3852	PPD-mal-xyl-2glc
202	36.76	829.4961 <sup>a</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	0.73	306.82	+HCOO	783.4929, 621.4385, 459.3844, 375.2900	ginsenoside F2
217	39.39	799.4856 <sup>b</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>14</sub>	0.88	304.95	+HCOO	753.4789, 621.4361, 459.3843	gypenoside XIII or isomer

Note: The number is the same as that in the identification list Tab.1 of the flower buds of *Panax notoginseng*; a: Identification assisted with reference compounds comparison; b: Tentative characterization by analyzing the high-accuracy MS<sup>2</sup> data.

Table S4. Information for 11 metabolites identified from rat plasma.

No.	Observed RT (min)	Observed <i>m/z</i>	Formula	Mass error (ppm)	CCA (Å <sup>2</sup> )	Adducts	ESI-MS <sup>2</sup>	Metabolic pathways	Identification
M1	5.25	977.5306 <sup>b</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>20</sub>	1.07	324.23	−H	931.5275, 827.5607, 799.4864, 637.4317, 475.3791	ginsenoside Re+2O	PPT+2O+2glc+rh
M2	15.97	1107.5940 <sup>a</sup>	C <sub>54</sub> H <sub>92</sub> O <sub>23</sub>	2.88	350.46	−H	945.5427, 783.4901, 621.4381, 459.3851	notoginsenoside Fa-xyl/notoginsenoside R4-xyl	ginsenoside Rb1
M3	18.45	1209.6230 <sup>b</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	−3.10	369.83	−H	1077.5825, 945.5409, 783.4882, 621.4354, 459.3841	notoginsenoside Fh1-xyl	ginsenoside Ra1/notoginsenoside-FZ isomer
M4	19.35	1077.5820 <sup>b</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	−1.90	342.67	−H	945.5422, 783.4883, 621.4358, 459.3844	notoginsenoside Fc-xyl/notoginsenoside Fa-glc	vinaginsenoside R7
M5	23.41	783.4890 <sup>b</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	3.90	308.67	−H	783.4902, 708.3636, 642.3125	ginsenoside Re-glc	ginsenoside Rg2
M6	26.10	793.4401 <sup>b</sup>	C <sub>44</sub> H <sub>66</sub> O <sub>14</sub>	4.82	287.58	−H	−	ginsenoside Ro-glc	zingibroside R1
M7	28.38	991.5469 <sup>b</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	−0.80	327.01	+HCOO	945.5423, 783.4890, 621.4370, 459.3858	ginsenoside Rb2-ara	ginsenoside Rd
M8	28.50	991.5469 <sup>b</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	−2.00	325.96	+HCOO	945.5423, 783.4890, 621.4370, 459.3858	ginsenoside Rb1-glc	gypenoside XVII
M9	34.58	915.5311 <sup>b</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	1.41	319.12	−H	837.4027, 716.3645, 621.4389, 459.3852	notoginsenoside R4-2glc	PPD+mal+2glc+Xyl
M10	37.55	869.4884 <sup>b</sup>	C <sub>45</sub> H <sub>74</sub> O <sub>16</sub>	3.47	308.83	−H	845.6852	malonylginsenoside Rd-glc	PPD+mal+2glc
M11	37.88	885.5227 <sup>b</sup>	C <sub>46</sub> H <sub>78</sub> O <sub>16</sub>	3.02	321.52	−H	830.3231, 753.4815	notoginsenoside P-glc	PPD+glc+2xyl

a: Identification assisted with reference compounds comparison; b: Tentative characterization by analyzing the high-accuracy MS<sup>2</sup> data.

**Table S5.** CCS prediction of isomers in rat plasma based on ALLCCS and CCSbase.

No.	Observed RT (min)	Observed m/z	Formula	Adducts	Observed CCA (Å <sup>2</sup> )	Predicted CCA (Å <sup>2</sup> )			Identification
						ALLCCS [M-H] <sup>-</sup>	ALLCCS [H+HCOOH] <sup>-</sup>	CCSbase [M-H] <sup>-</sup>	
31	10.81	1285.6450 <sup>a</sup>	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	+HCOO	372.56	–	–	331.9	notoginsenosides R4
38	12.84	1285.6410 <sup>a</sup>	C <sub>59</sub> H <sub>100</sub> O <sub>27</sub>	+HCOO	372.92	–	–	331.9	notoginsenoside Fa
48	15.40	1255.6320 <sup>a</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	+HCOO	365.25	–	–	325.4	notoginsenoside FP2
61	18.4	1255.6320 <sup>a</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	+HCOO	368.97	–	–	327.0	notoginsenoside Fc
66	19.8	1255.6320 <sup>a</sup>	C <sub>58</sub> H <sub>98</sub> O <sub>26</sub>	+HCOO	363.00	–	–	327.0	ginsenoside Ra1
84	22.28	1123.5890 <sup>a</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	+HCOO	359.67	273.9	287.9	301.4	ginsenoside Rb2
90	23.43	1123.5890 <sup>a</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	+HCOO	347.37	273.9	287.9	301.4	ginsenoside Rb3
97	24.54	1123.6080 <sup>b</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	+HCOO	357.12	273.9	287.9	301.4	notoginsenoside L
M4	19.35	1077.5820 <sup>b</sup>	C <sub>53</sub> H <sub>90</sub> O <sub>22</sub>	–H	342.67	271.7	285.7	301.4	vinaginsenoside R7
179	34.58	961.5373 <sup>a</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	+HCOO	322.31	252.0	266.1	271.0	notoginsenoside Fe
185	35.36	961.5381 <sup>a</sup>	C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>	+HCOO	322.73	252.1	266.2	271.9	ginsenoside Rd2
M7	28.38	991.5469 <sup>b</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	+HCOO	327.01	255.4	269.6	274.4	ginsenoside Rd
M8	28.50	991.5469 <sup>b</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	+HCOO	325.96	257.6	269.6	274.4	gypenoside XVII
6	5.65	991.5484 <sup>a</sup>	C <sub>48</sub> H <sub>82</sub> O <sub>18</sub>	+HCOO	327.00	256.4	270.5	274.5	ginsenoside Re
202	36.76	829.4961 <sup>a</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	+HCOO	306.82	237.5	250.3	252.6	ginsenoside F2
M5	23.41	783.4890 <sup>b</sup>	C <sub>42</sub> H <sub>72</sub> O <sub>13</sub>	–H	308.67	239.0	251.8	251.6	ginsenoside Rg2

Note: The number is the same as that in the identification list Tab.1 and Tab.3.; a: Identification assisted with reference compounds comparison; b: Tentative characterization by analyzing the high-accuracy MS<sup>2</sup> data.