Supplementary data

Soybean phytochemicals responsible for the bacterial neuraminidase inhibition and their characterization by UPLC-ESI-TOF/MS

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Table S1

Peak assignments and mass spectra of metabolite in soybean extract from positive mode using UPLC–ESI-TOF/MS.

No.	Retention times (min)	Compounds	Elemental composition	Calculated mass [M] (*m/z*)	Calculated mass $[M+H]^+$ (*m/z*)	Observed mass $[M+H]^+$ (*m/z*)	Fragmentation ions	References
1	1.95	tryptophan fragment	$C_{11}H_{12}N_2O$	187.0871	188.0950	188.0698	146.0592	Kim et al., 2013
2	2.22	phenylalanine	$C_9H_{11}NO_2$	165.0790	166.0863	166.0856	120.0799	Gu et al., 2017
3	2.84	daidzin	$C_{21}H_{20}O_9$	416.1107	417.1189	417.1171	255.0641	Duenas et al., 2012; Shen et al.,2012
4	2.96	glycitin	$C_{22}H_{22}O_{10}$	446.1213	447.1272	447.1280	285.0747	Duenas et al., 2012; Shen et al.,2012
5	3.92	genistin	$C_{21}H_{20}O_{10}$	432.1056	433.1126	433.1122	271.0590	Duenas et al., 2012; Shen et al.,2012
6	4.10	malonyldaidzin	$C_{24}H_{22}O_{12}$	502.1111	503.1191	503.1174	255.0641	Duenas et al., 2012; Shen et al.,2012
7	4.17	malonylglycitin	$C_{25}H_{24}O_{13}$	532.1217	533.1297	533.1283	285.0748	Duenas et al., 2012; Shen et al.,2012
8	5.02	acetyldaidzin	$C_{22}H_{22}O_9$	458.1213	459.1286	459.1283	255.0645	Duenas et al., 2012; Shen et al.,2012
9	5.33	malonylgenistin	$C_{24}H_{22}O_{13}$	518.1060	519.1139	519.1123	271.0590	Duenas et al., 2012; Shen et al.,2012
10	6.11	daidzein	$C_{15}H_{10}O_4$	254.0579	255.0652	255.0641		Duenas et al., 2012; Shen et al.,2012
11	10.12	soyasaponin Ab	$C_{24}H_{22}O_{13}$	1436.6460	1437.6503	1437.6503	975.5152	Decroos et al., 2005; Ha et al., 2014
12	10.26	soyasaponin Ac	$C_{67}H_{104}O_{32}$	1420.6511	1421.6506	1421.6551	959.5202	Decroos et al. 2005
13	10.71	soyasaponin Af	$C_{25}H_{24}O_{12}$	1274.5932	1275.5915	1275.5959	813.4637	Decroos et al. 2005, Guajardo-Flores et al., 2012
14	11.11	soyasaponin J-αa	$C_{51}H_{78}O_{23}$	1028.4828	1029.5255	1029.5238	423.3614	Krishnamurthy et al., 2014
15	11.47	soyasaponin Ba	$C_{48}H_{78}O_{19}$	958.5137	959.5189	959.5190	441.3725	Decroos et al. 2005, Guajardo-Flores et al., 2012
16	11.72	soyasaponin Bb	$C_{48}H_{78}O_{18}$	942.5188	943.5243	943.5244	441.3720	Decroos et al. 2005, Guajardo-Flores et al., 2012
17	12.09	soyasaponin Bb´	$C_{42}H_{67}O_{14}$	796.4609	797.4665	797.4689	441.3729, 423.3624	Decroos et al. 2005, Guajardo-Flores et al., 2012
18	12.09	soyasaponin Bc	$C_{47}H_{76}O_{17}$	912.5083	913.5133	913.5159	441.3730, 423.3623	Decroos et al. 2005
19	12.09	soyasaponin J-αg	$C_{51}H_{78}O_{23}$	1058.4934	1059.5704	1059.5709	423.3622	Krishnamurthy et al., 2014
20	12.64	soyasaponin Bd	$C_{48}H_{76}O_{19}$	956.4981	957.5037	957.5032	439.3567	Decroos et al. 2005, Guajardo-Flores et al., 2012
21	12.76	soyasaponin αg	$C_{54}H_{84}O_{22}$	1084.5454	1085.5491	1085.5492	567.4040, 423.3614	Decroos et al. 2005, Guajardo-Flores et al., 2012
22	12.91	soyasaponin Be	$C_{48}H_{76}O_{18}$	940.5032	941.5095	941.5091	439.3563	Decroos et al. 2005
23	13.04	soyasaponin βg	$C_{54}H_{84}O_{21}$	1068.5505	1069.5554	1069.5556	567.4042, 423.3615	Decroos et al. 2005, Guajardo-Flores et al., 2012
24	13.33	soyasaponin βa	$C_{47}H_{76}O_{17}$	1038.5399	1039.5430	1039.5449	567.4040, 423.3615	Guajardo-Flores et al., 2012
25	13.66	soyasaponin γg	$C_{48}H_{74}O_{17}$	922.4926	923.4999	923.4984	567.4041, 423.3616	Decroos et al. 2005, Guajardo-Flores et al., 2012
26	13.83	soyasaponin γa	$C_{47}H_{72}O_{16}$	892.4877	893.4851	893.4877	567.4072, 423.3623	Guajardo-Flores et al., 2012

Table S2

Fluorescence quenching effects of compounds **1**a and **2a** on BNA.

Compounds	K_{SV} **(× 10^5 L·mol^{-1})**	K_A **(× 10^5 L·mol^{-1})**	***n***
1a	0.08	0.19	0.92
2a	0.17	0.22	0.98

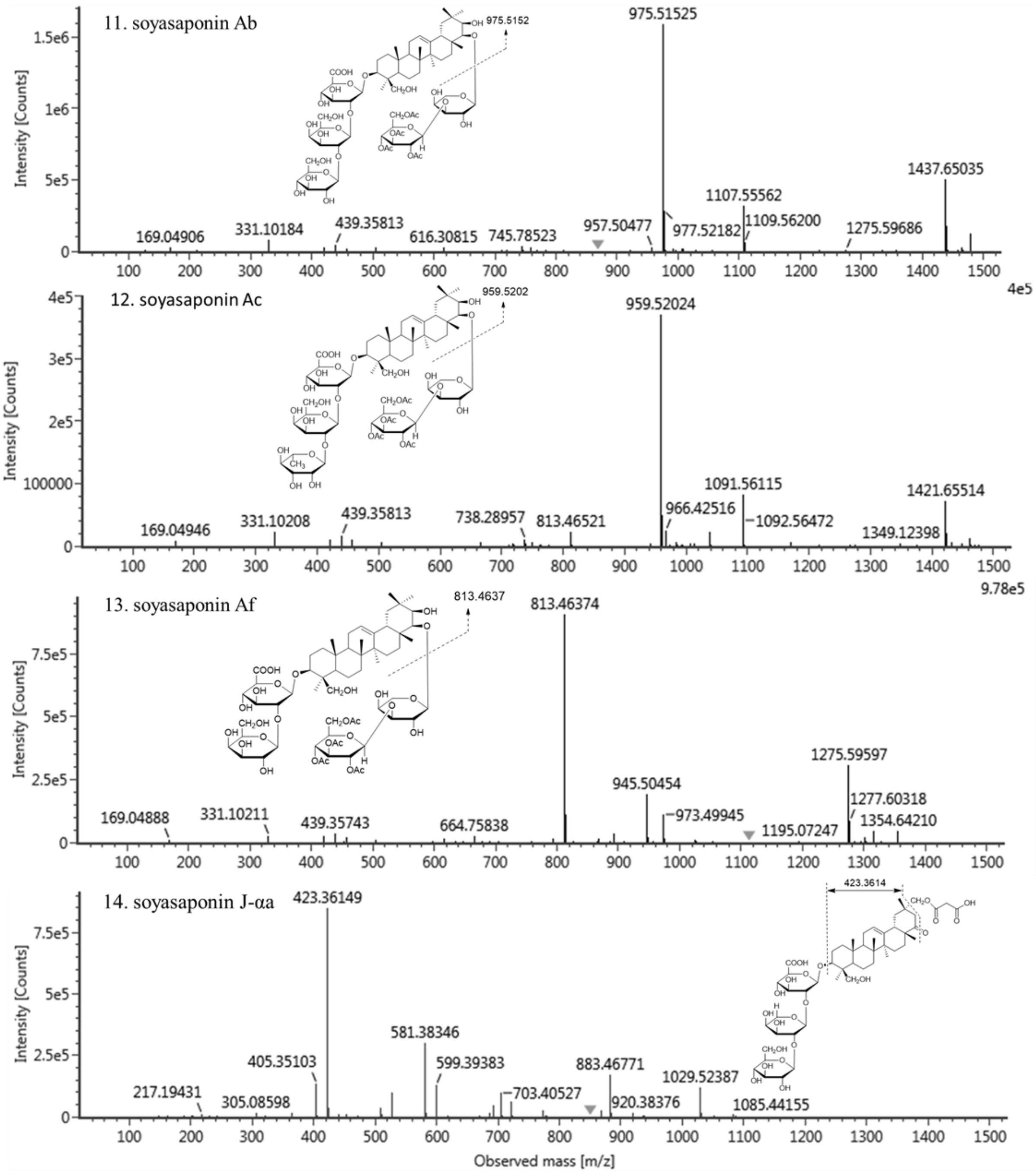

Fig. S1. Mass fragmentation patterns of the identified soyasaponins by mass spectra Mass.

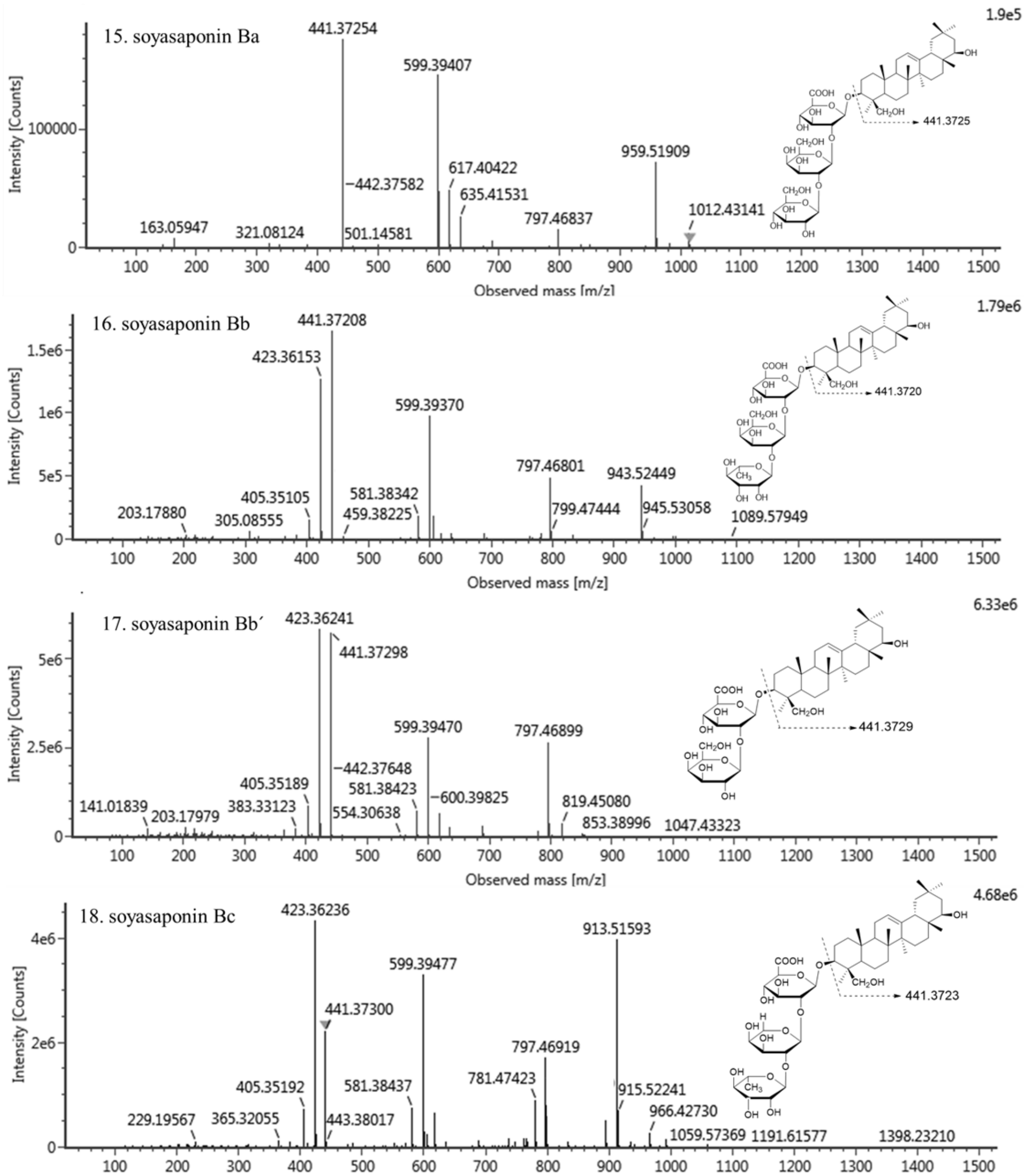

Fig. S2. Mass fragmentation patterns of the identified soyasaponins by mass spectra Mass.

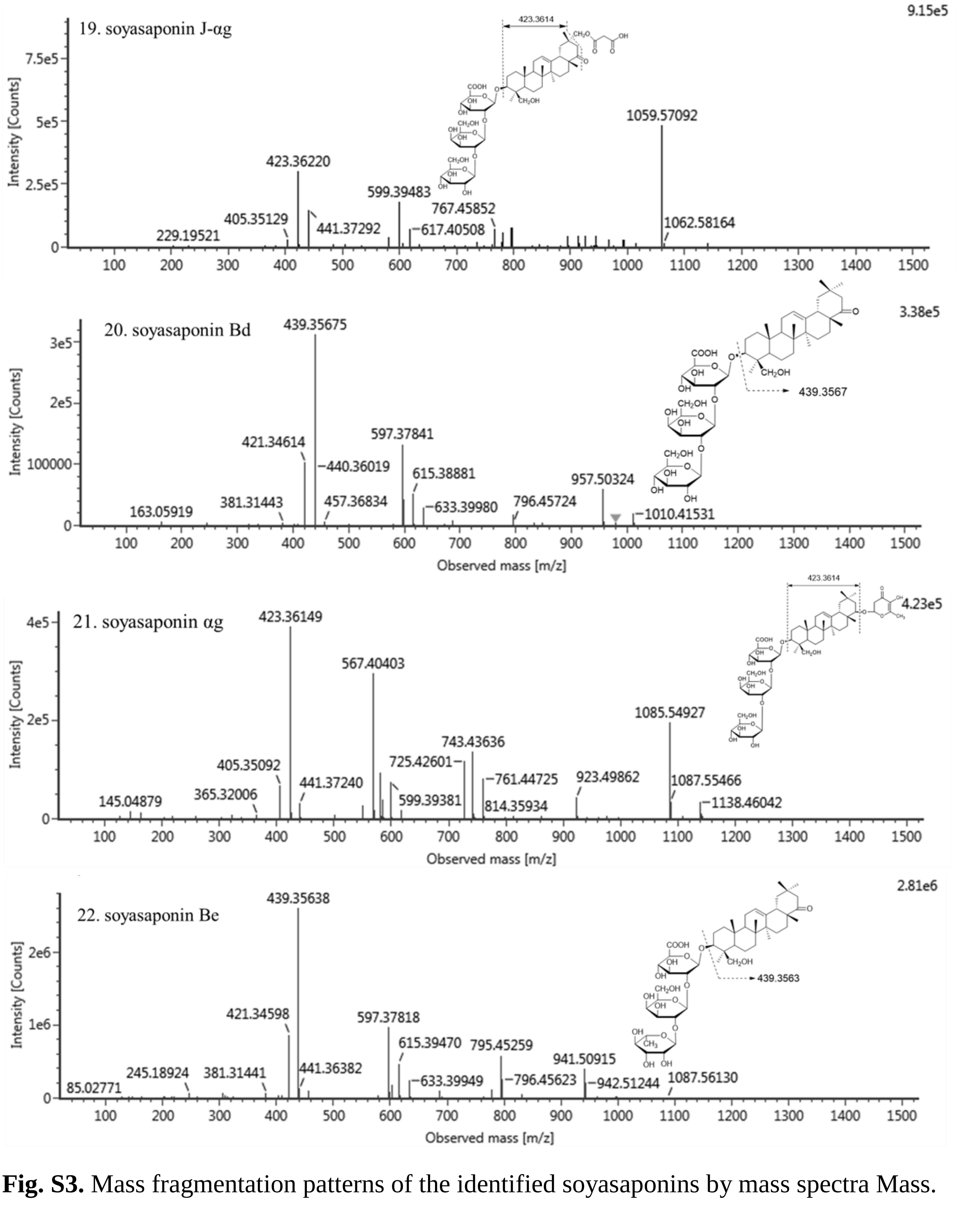

Fig. S3. Mass fragmentation patterns of the identified soyasaponins by mass spectra Mass.

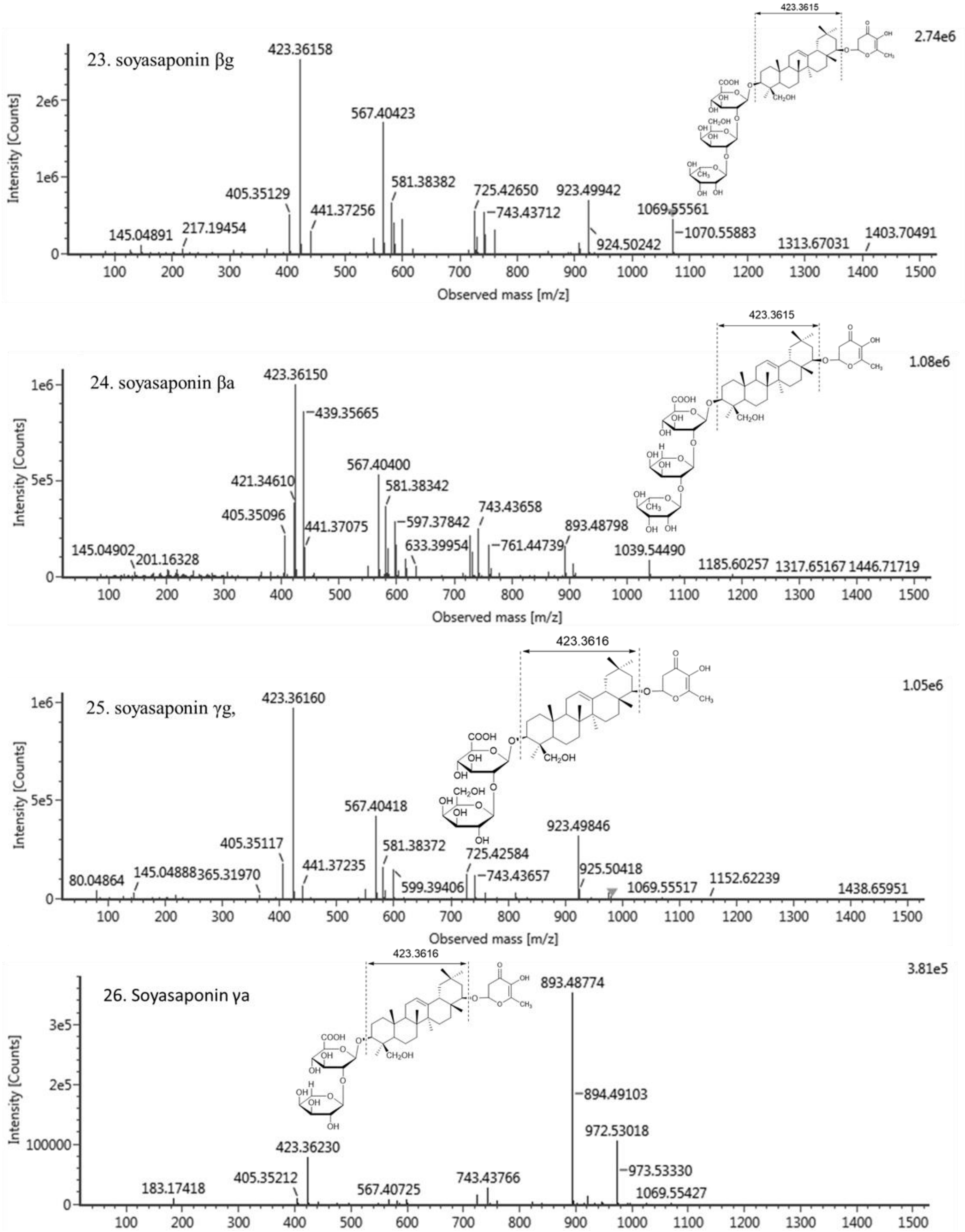

Fig. S4. Mass fragmentation patterns of the identified soyasaponins by mass spectra Mass.

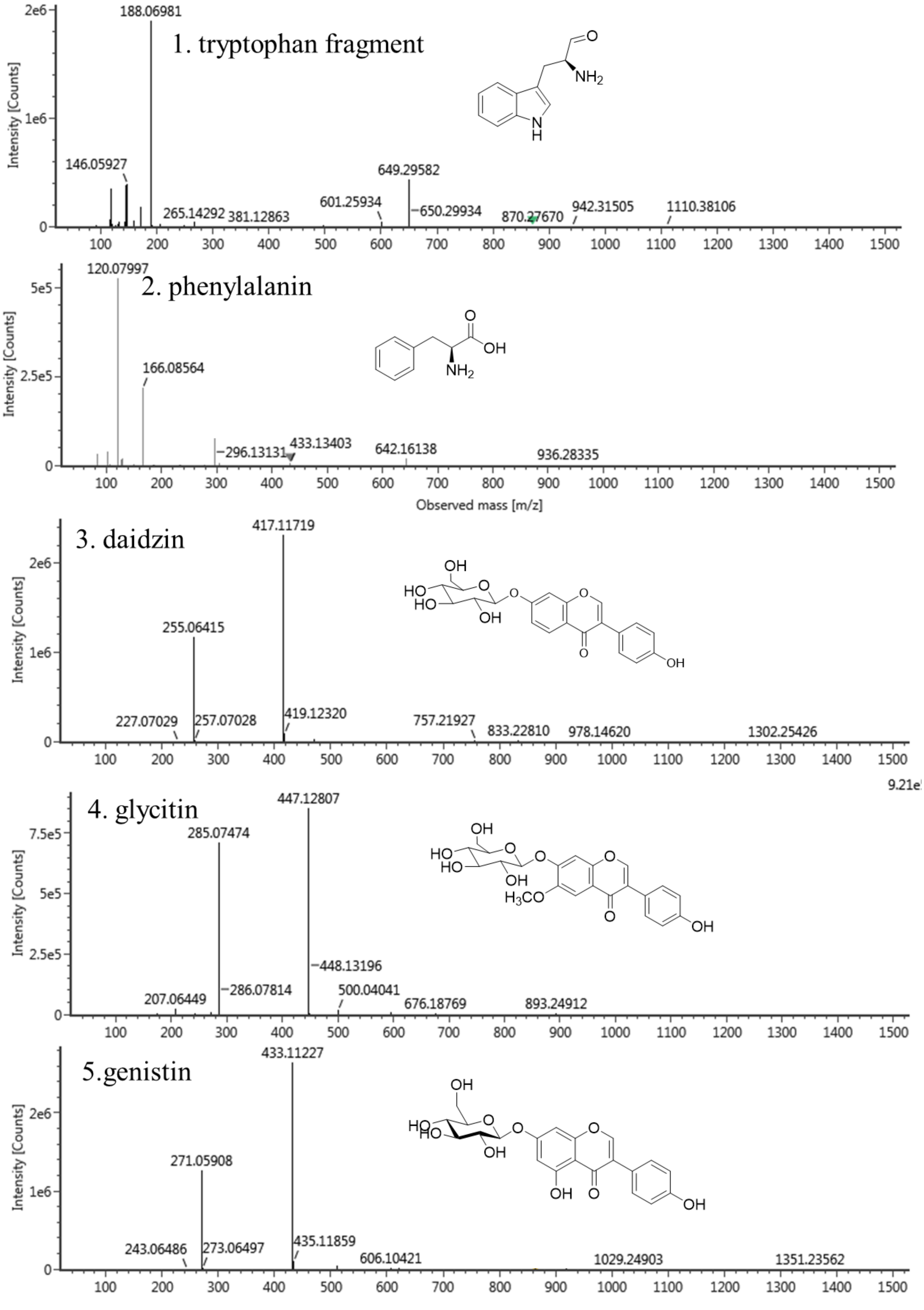

Fig. S5. Molecular ions and elementary compositions of the identified phytochemicals by mass spectra Mass fragmentation patterns of flavonoids and amino acids.

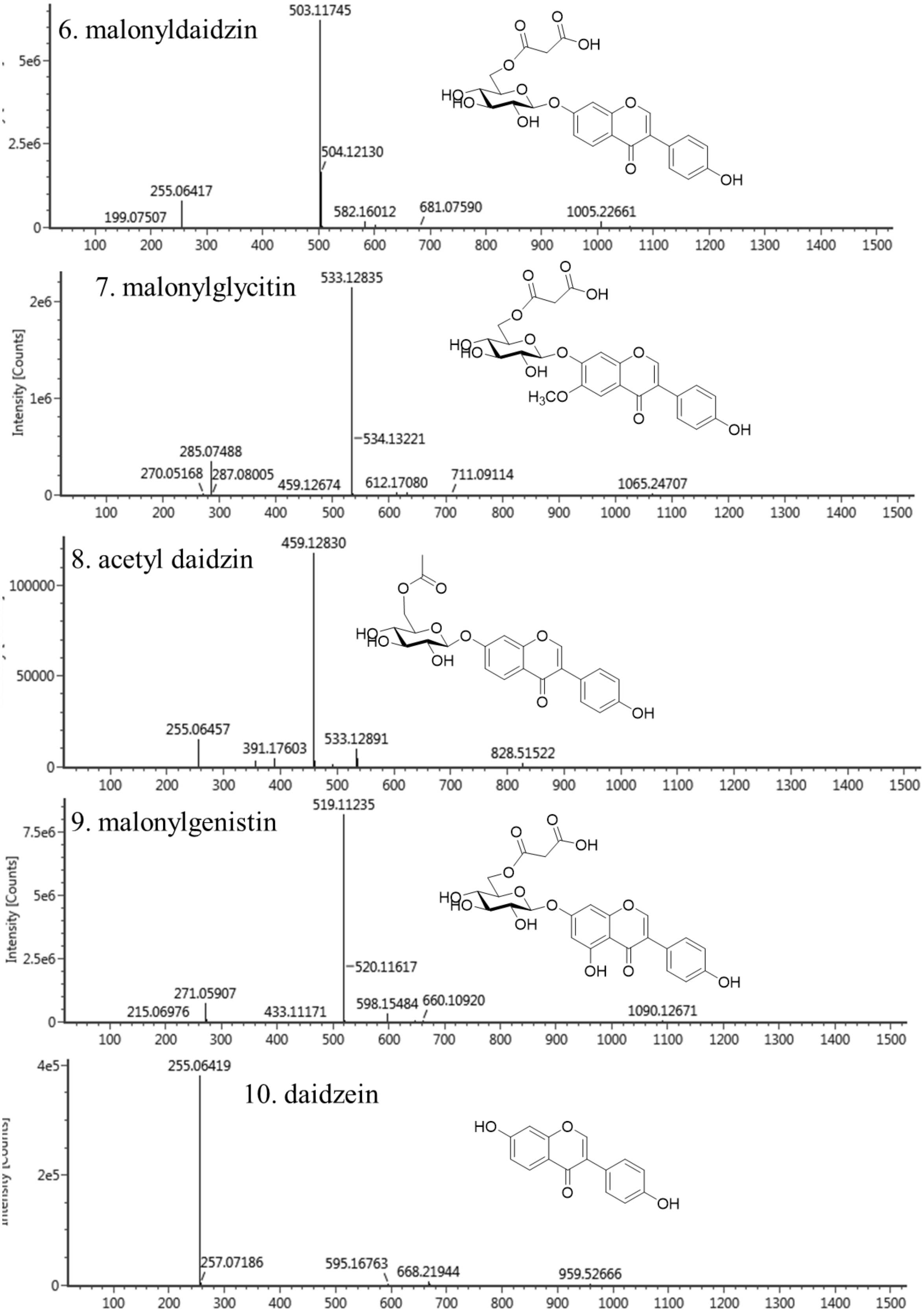

Fig. S6. Molecular ions and elementary compositions of the identified phytochemicals by mass spectra Mass fragmentation patterns of flavonoids.

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