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Phenotypic and genotypic signature of saponin chemical composition in Chinese wild soybean (*Glycine soja*): revealing genetic diversity, geographical variation and dispersal history of the species

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Supplementary Table 1. Retention times (RT) under UV chromatograms and molecular ion masses ($[M+H]^+$) of saponin components in Chinese wild soybeans

No.	RT (min)	$[M+H]^+$	Identification				
			Saponin	Group	Aglycone	C-3 sugar	C-22 sugar
1	24.9	1107.6	A0- α g	A	SS-A	Glc-Gal-GlcUA-	Ara-
2	25.6	1077.5	A0- α a	A	SS-A	Glc-Ara-GlcUA-	Ara-
3	31.8	1033.5	KA- α g	β	SS-KA	Glc-Gal-GlcUA-	H-
4	33.1	975.5	A- α g	A	SS-A	Glc-Gal-GlcUA-	H-
5	33.3	973.5	H- α g	α	SS-H	Glc-Gal-GlcUA-	O=
6	33.3	1453.6	HAb- α g	β	SS-HA	Glc-Gal-GlcUA-	acetylGlc-Ara-
7	34.1	987.5	I- α g	α	SS-I	Glc-Gal-GlcUA-	O=
8	35.2	1059.5	J- α g	α	SS-J	Glc-Gal-GlcUA-	O=
9	35.4	1365.6	Aa	A	SS-A	Glc-Gal-GlcUA-	acetylXyl-Ara-
10	36.2	1349.6	Au	A	SS-A	Rha-Gal-GlcUA-	acetylXyl-Ara-
11	36.2	1335.6	Ax	A	SS-A	Glc-Ara-GlcUA-	acetylXyl-Ara-
12	36.2	1029.5	J- α a	α	SS-J	Glc-Ara-GlcUA-	O=
13	36.8	1437.7	Ab	A	SS-A	Glc-Gal-GlcUA-	acetylGlc-Ara-
14	37.4	1421.7	Ac	A	SS-A	Rha-Gal-GlcUA-	acetylGlc-Ara-
15	37.6	1203.6	Ae	A	SS-A	Gal-GlcUA-	acetylXyl-Ara-
16	37.6	1407.6	Ad	A	SS-A	Glc-Ara-GlcUA-	acetylGlc-Ara-
17	39.0	1275.6	Af	A	SS-A	Gal-GlcUA-	acetylGlc-Ara-
18	39.1	959.5	Ba	B	SS-B	Glc-Gal-GlcUA-	H-
19	39.3	1015.5	K- α g	α	SS-K	Glc-Gal-GlcUA-	O=
20	40.1	943.5	Bb	B	SS-B	Rha-Gal-GlcUA-	H-
21	40.8	797.5	Bb'	B	SS-B	Gal-GlcUA-	H-
22	41.7	913.5	Bc	B	SS-B	Glc-Ara-GlcUA-	H-
23	42.0	957.5	Bd	E	SS-E	Glc-Gal-GlcUA-	O=
24	42.9	1085.6	α g	DDMP	SS-B+DDMP	Glc-Gal-GlcUA-	(DDMP-)
25	44.0	1069.6	β g	DDMP	SS-B+DDMP	Rha-Gal-GlcUA-	(DDMP-)
26	45.2	1039.5	β a	DDMP	SS-B+DDMP	Rha-Ara-GlcUA-	(DDMP-)
27	46.1	923.5	γ g	DDMP	SS-B+DDMP	Gal-GlcUA-	(DDMP-)