

Supplementary Information

Integrated metabolomic and transcriptomic analyses revealed the distribution of saponins in *Panax notoginseng*

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Results

The resulting dataset of all components between different parts were analyzed to examine the clustering of each group using multivariate statistical analysis. Five parts of two-year *P. notoginseng* showed separation; in the five parts of three-year *P. notoginseng*, principal component 1, which is the key component for sample separation, identified the underground parts (root and fibril) and the aerial parts (stem, leaf, flower); however, the flower overlapped the stem, and the root clustered with the fibril (Fig. S1). Meanwhile, chemical components in *P. notoginseng* at different developmental stages were also compared; differences are found between two- and three-year-old *P. notoginseng* and principal component 1 identified all parts between two- and three-year-old *P. notoginseng* (Fig. S2).

Table S1 Calibration curves, linearity, precision, repeatability, stability and recovery rate of seven saponins.

Saponins	Calibration curves	R^2	Linearity (ug)	RSD% ($n=5$)			Recovery rate (%) (RSD%)
				Precision	Repeatability	Stability	
NG-R1	$Y=278.3X+8.81$	0.9997	0.102-2.04	0.1	1.55	2.08	95.84(2.09)
G-Rg1	$Y=112.83X+21.97$	0.9998	0.101-10.1	0.03	0.94	2.99	98.25(2.87)
G-Re	$Y=237.94X+20.335$	0.9998	0.098-1.96	0.06	2.03	2.22	102.37(1.41)
G-Rb1	$Y=298.38X+3.3239$	0.9999	0.096-1.92	0.2	0.19	2.94	100.43(0.56)
G-Rc	$Y=181.18X+2.2452$	0.9991	0.099-1.98	0.52	0.41	2.63	100.60(1.25)
G-Rb2	$Y=231.26X+3.6762$	0.9999	0.094-1.88	1.12	2.68	2.80	96.68(2.13)
G-Rd	$Y=290.72X+1.686$	1.0000	0.099-1.98	0.07	0.93	1.21	100.31(1.22)

NG: notoginsenoside; G: ginsenoside

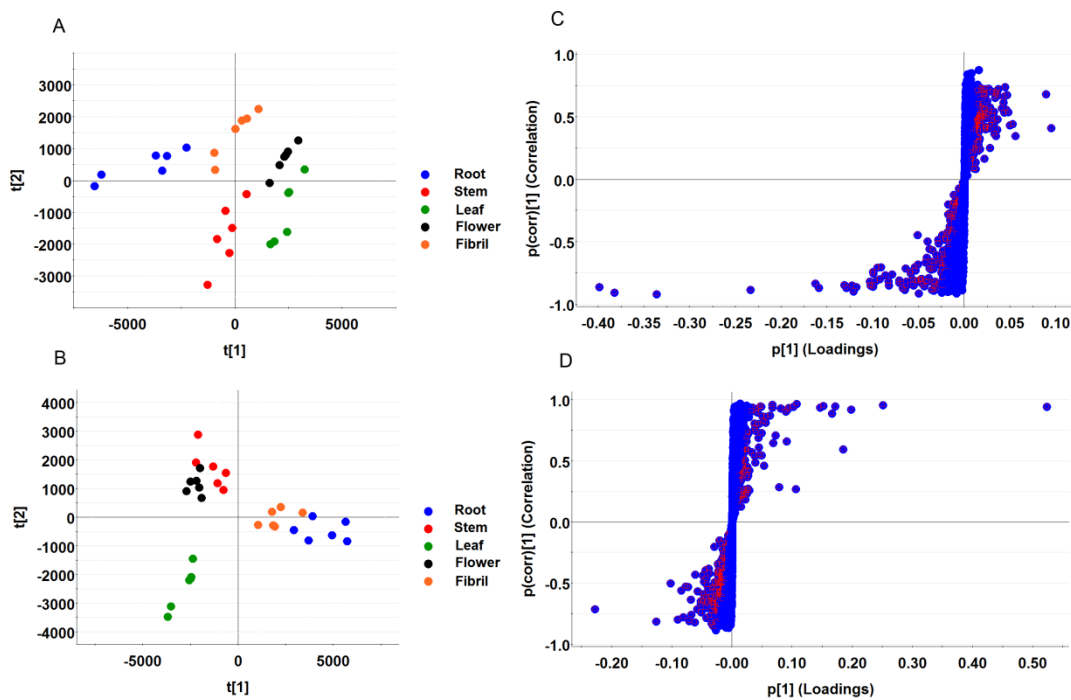


Figure S1 Metabolic analysis of all components in the five parts during the two- and three-year-old of *P. notoginseng* plants. (A, C) PCA score plots and S-plot of the five parts in two-year-old *P. notoginseng*; (B, D) PCA score plots and S-plot of the five parts in three-year-old *P. notoginseng*.

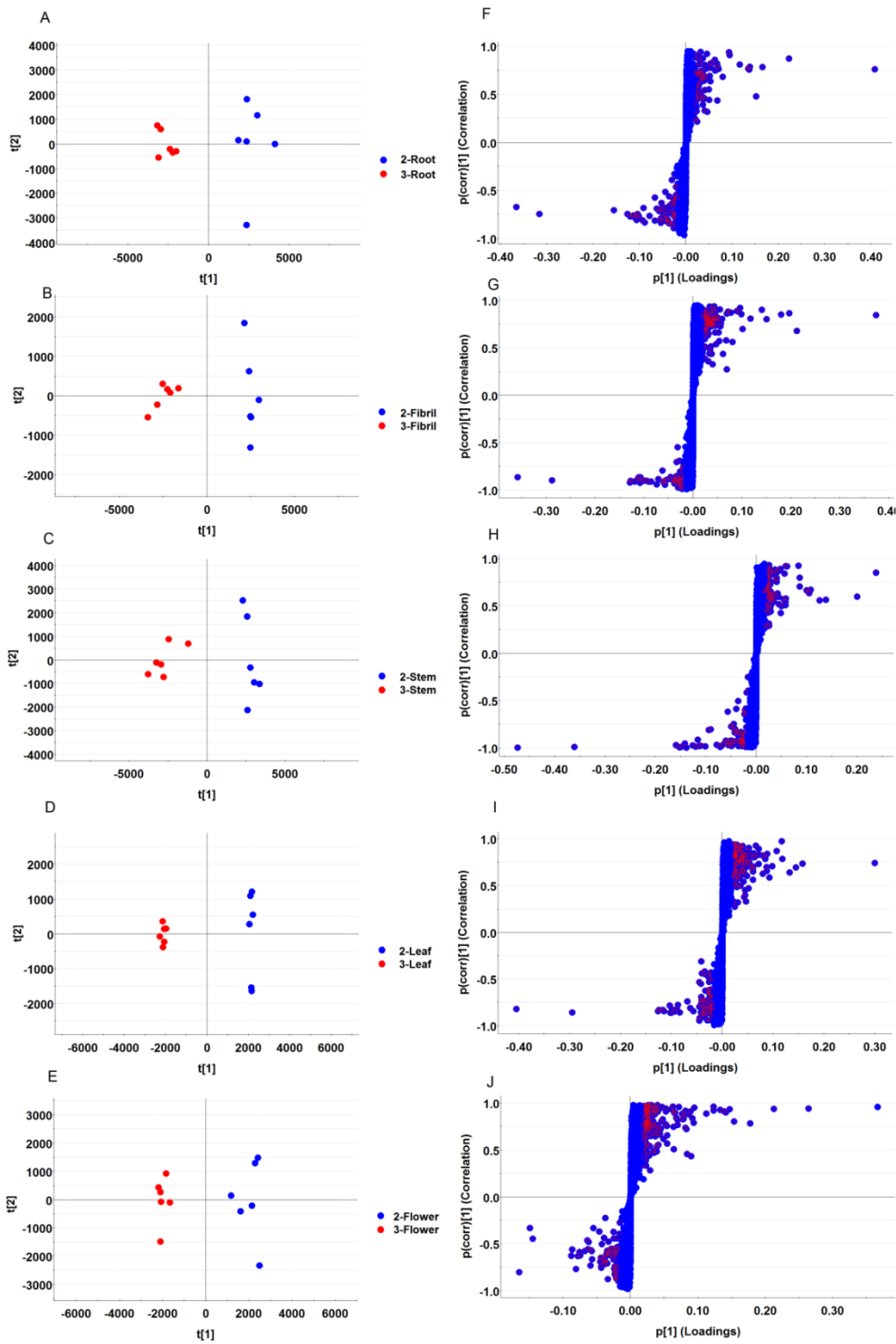


Figure S2 Metabolic analysis of all components in the same parts of two- and three-year-old of *P. notoginseng* plants. (A, B, C, D, E) PCA score plots of root, fibril, stem, leaf and flower at two developmental stages, respectively; (F, G, H, I, J) S-plot of root, fibril, stem, leaf and flower at three developmental stages, respectively.

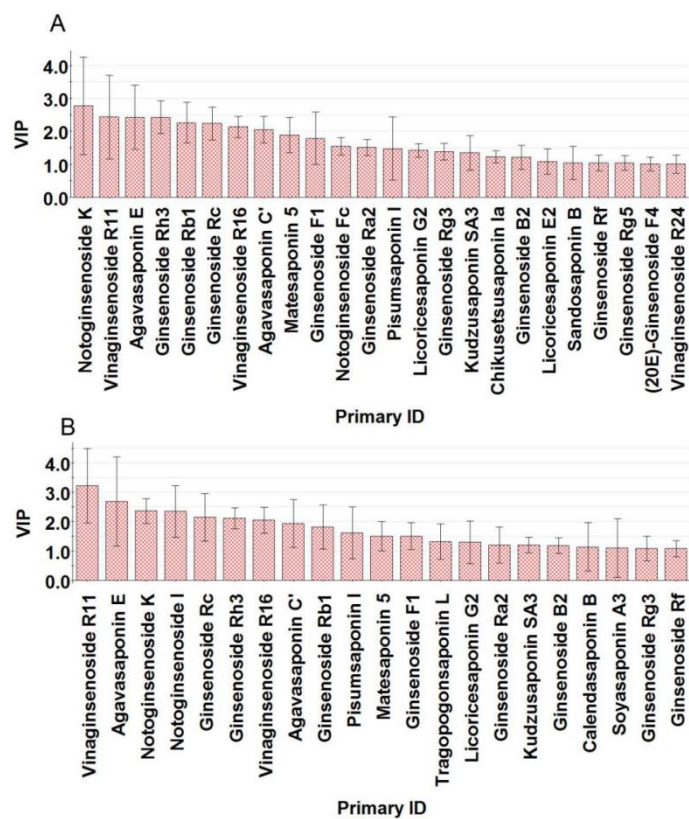


Figure S3 VIP of saponins in the five parts at the same developmental stages. (A) VIP of root, fibril, stem, leaf and flower in two-year-old *P. notoginseng*. (B) VIP of root, fibril, stem, leaf, and flower in three-year-old *P. notoginseng*.

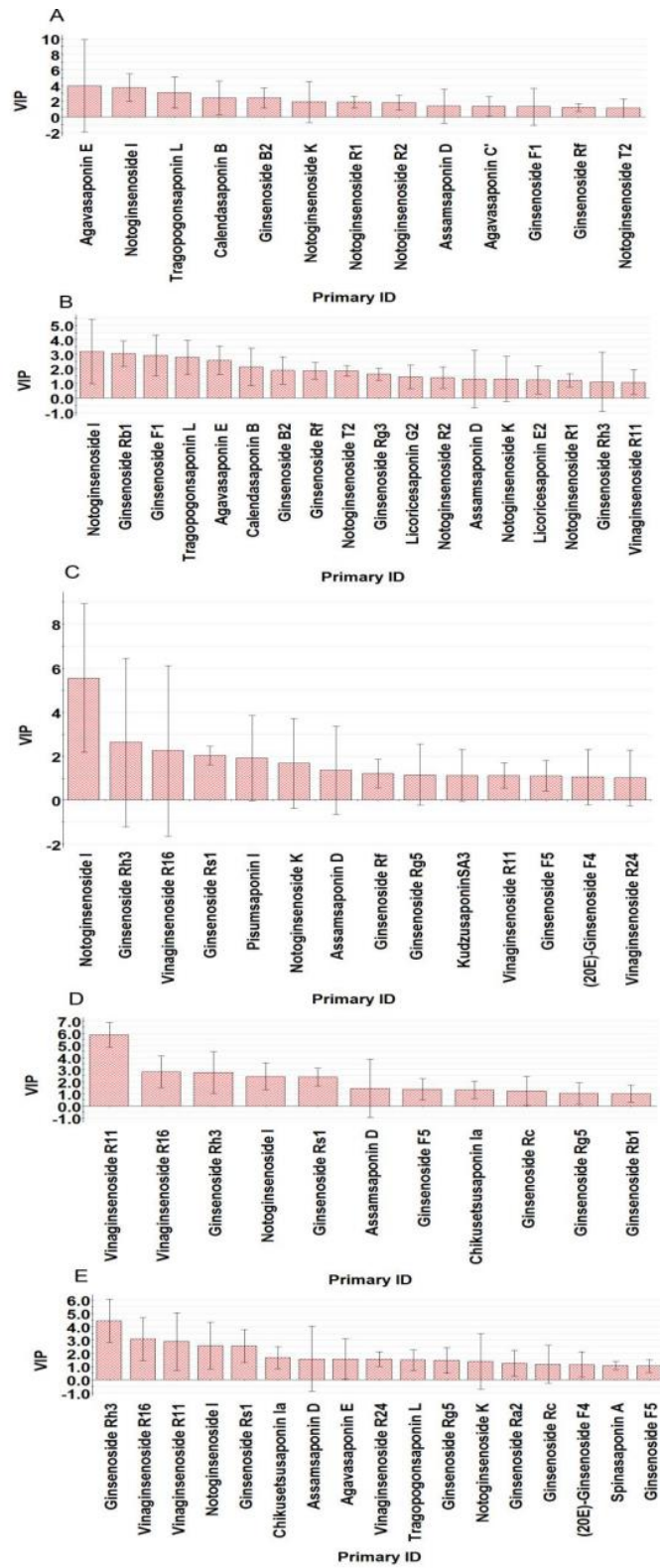


Figure S4 VIP of saponins in the same parts of two- and three-year-old *P. notoginseng*. (A–E) VIP of roots, fibrils, stems, leaves and flowers in two- and three-year-old *P. notoginseng*.

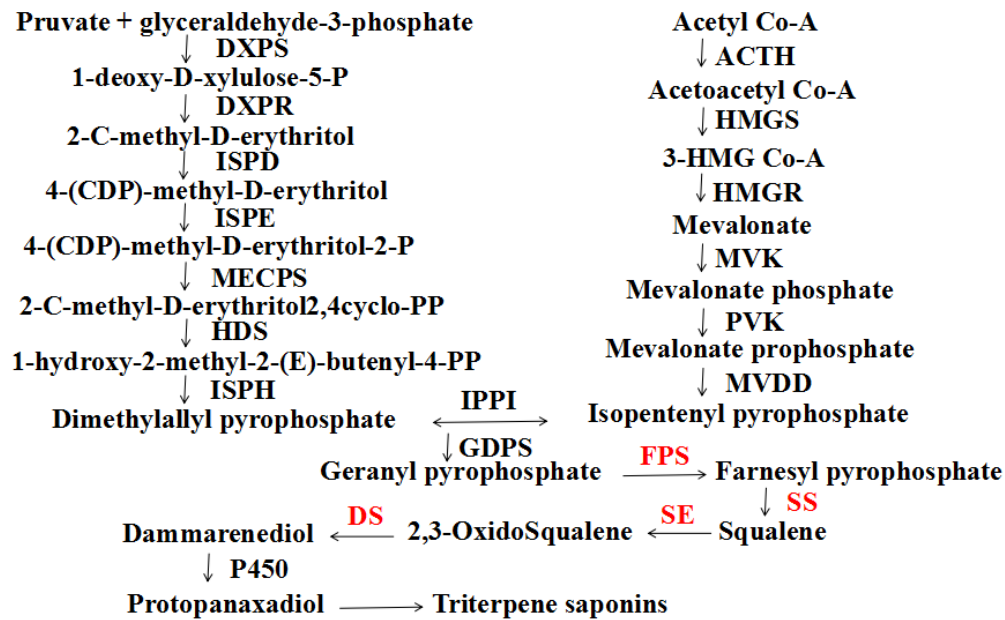


Figure S5 Biosynthetic pathways of triterpene saponins in *P. notoginseng* plants. MVA pathway: AACT acetoacetyl-CoA acyltransferase; HMGS 3-hydroxy-3-methylglutaryl-CoA synthase; HMGR 3-hydroxy-3-methylglutaryl-CoA reductase; MVK mevalonate kinase; PMK phosphomevalonate kinase; MVDD mevalonate diphosphate decarboxylase; IPPI isopentenyl pyrophosphate isomerase; GDPS geranyl diphosphatesynthase. MEP pathway: DXPS 1-deoxy-o-xylulose 5-phosphate synthase; DXPR 1-deoxy-o-xylulose 5-phosphate reductoisomerase; ISPD 2-C-methylerythritol 4-phosphatecytidyl transferase; ISPE 4-(cytidine-5'-diphospho)-2-C-methylerythritol kinase; MECPS 2-C-methylerythritol-2,4-cyclophosphate synthase; HDS 1-hydroxy-2-methyl-2-(E)-butenyl 4-diphosphate synthase; ISPH 1-hydroxy-2-methyl-2-(E)-butenyl 4-diphosphate reductase; FPS farnesyl pyrophosphate synthase; SS squalene synthase; SE squalene epoxidase; DS dammarenediol-II synthase; P450 P450-monooxygenase.