Supplementary Materials

Multidimensional Quality Evaluation of Drying Methods on the Bioactive Components and Antioxidant Activity of *Astragalus membranaceus* var. *mongholicus* Slices

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Materials and methods

S1. Measurement of antioxidant capacity

S1.1. DPPH Assay

The DPPH assay was performed using a commercially available kit according to the manufacturer's instructions. Briefly, 0.1 g (DW) of sample powder was homogenized with 1 mL of pre-cooled extraction buffer (provided with the kit) on ice, then centrifuged at 10,000×g for 10 min at 4°C; the supernatant was collected as the sample extract. In a reaction mixture, 50 μL of sample extract (or extraction buffer for the blank) was mixed with 950 μL of DPPH reagent (freshly provided in the kit). The mixture was incubated at room temperature in the dark for 20 min. Absorbance was measured at 515 nm against a blank (the blank was used to zero the spectrophotometer). All measurements were performed in biological triplicate. DPPH radical scavenging rate (%) = $(A_1 - A_2) / A_1 \times 100$ %, where A_1 and A_2 are the absorbances of the blank and sample, respectively.

S1.2. ABTS Assay

The ABTS assay was performed using a commercially available kit in accordance with the manufacturer's instructions. Sample extraction was carried out according to the method described in S1.1. The ABTS working solution was prepared as follows: dissolve 1 vial of reagent 2 in 25 mL of reagent 1, mix thoroughly, and let stand for 20 minutes; then use the supernatant. Next, mix 50 μL of the sample extract (or the extraction buffer from the blank control) with 950 μL of the ABTS working solution. After mixing thoroughly, measure the absorbance at a wavelength of 734 nm within 10 minutes. All measurements were performed in biological triplicate. ABTS radical scavenging rate (%) = $(A_1 - A_2) / A_1 \times 100$ %, where A_1 and A_2 are the absorbances of the control and sample, respectively.

S1.3. FRAP Assay

The total antioxidant capacity of plant or herbal extracts and various antioxidant solutions can be determined using the ferric reducing antioxidant power (FRAP) assay. Under acidic conditions, the ability of a substance to reduce Fe^{3+}-tripyridyltriazine (Fe^{3+}-TPTZ) to form the blue-colored Fe^{2+}-TPTZ reflects its total antioxidant capacity. The absorbance changes were detected at 593 nm, and a standard curve was established based on the concentration of Fe^{2+} (0.075, 0.05, 0.025, 0.0125, 0.00625, 0.003125, 0.00156, 0.00078 μmol/mL) and the standard absorbance values (y). Then, the standard curve was used to calculate the sample concentration by substituting the measured y-values into the equation. All measurements were performed in biological triplicate. Net absorbance ΔA = A(sample) – A(blank). A standard curve was plotted using the Trolox standards provided in the kit, yielding the following equation: $y = 8.7339x + 0.0095$, $R^2 = 0.9703$, where y is ΔA and x is the concentration of Trolox (μM/mL). The formula for total antioxidant capacity (μmol Trolox/g dry weight) is: $0.4027 \times (\Delta A - 0.0134) / W$, where W is the dry weight of the sample (g).

S1.4. Total Flavonoids Assay

Total flavonoid content was determined using a commercial kit (Solarbio BC1335) according to the manufacturer's instructions. Dried sample powder (0.1 g, dry weight) was mixed with 1 mL of extraction buffer (60% ethanol) and ultrasonicated at 300 W and 60 °C for 30 min, then centrifuged at 12,000 rpm for 10 min at 25 °C; the supernatant was collected as the sample extract. For each sample, a control tube (60 μL sample extract + 15 μL reagent 1 + 120 μL reagent 3 + 90 μL 60% ethanol) and a test tube (60 μL sample extract + 15 μL reagent 1 + 15 μL reagent 2 + 120 μL reagent 3) were prepared. A standard curve was constructed using rutin standards (0.039–2.5 mg/mL) with a blank (60 μL distilled water instead of standard) and standard tubes (60 μL standard solution + 15 μL reagent 1 + 15 μL reagent 2 + 120 μL reagent 3). After each addition, the mixtures were vortexed

and incubated at room temperature for 5 min (twice: after adding reagent 1 and after adding reagent 2), then incubated at 37 °C for 45 min and centrifuged at 10,000×g for 10 min at room temperature. The supernatant (200 μL) was transferred to a microplate, and the absorbance was measured at 470 nm (A-test, A-control, A-standard, A-blank). The net absorbance ΔA-test = A-test – A-control, and ΔA-standard = A-standard – A-blank. The concentration (x, mg/mL) of total flavonoids in the extract was calculated from the rutin standard curve. The content in the dry sample was expressed as mg rutin equivalents per gram dry weight (mg RE/g DW) using the following formula: total flavonoids (mg/g) = x / W, where W is the sample dry weight (g). All measurements were performed in biological triplicate.

S1.5. Total Sugar Assay

Total sugar content was measured using a commercial kit (Solarbio BC2715) according to the manufacturer's protocol. Dried sample powder (0.1 g, dry weight) was mixed with 1 mL of reagent 1 and 1.5 mL of distilled water, homogenized, and heated in a boiling water bath for 30 min (sealed with Parafilm). After cooling, 1 mL of reagent 2 was added, and the mixture was vortexed and diluted with distilled water to a final volume of 10 mL, then centrifuged at 8,000×g for 10 min at 25 °C; the supernatant was used as the sample extract. A standard curve was prepared using glucose standards (0.1–1.6 mg/mL). For each assay, a blank (30 μL distilled water + 30 μL reagent 3 + 180 μL distilled water), a test tube (30 μL sample extract + 30 μL reagent 3 + 180 μL distilled water), and a standard tube (30 μL glucose standard + 30 μL reagent 3 + 180 μL distilled water) were prepared. After vortexing, the tubes were heated in a boiling water bath for 10 min, cooled to room temperature, and 200 μL of each mixture was transferred to a microplate. The absorbance was measured at 540 nm (A-test, A-blank, A-standard). The net absorbance ΔA-test = A-test – A-blank, and ΔA-standard = A-standard – A-blank. The glucose concentration (x, mg/mL) in the extract was

calculated from the standard curve. The total sugar content in the dry sample was calculated as: total sugars (mg/g dry weight) = (10 × x) / W, where 10 is the total extraction volume (mL) and W is the sample dry weight (g). All measurements were performed in biological triplicate.

S1.6. Total Phenols Assay

Total phenolic content was determined using a commercial kit (Solarbio BC1340) according to the manufacturer's instructions. Dried sample powder (0.1 g, dry weight) was mixed with 2.5 mL of extraction buffer (60% ethanol) and ultrasonicated at 300 W and 60 °C for 30 min (sealed with Parafilm), then centrifuged at 12,000 rpm for 10 min at 25 °C; the supernatant was collected as the sample extract. A standard curve was prepared using gallic acid standards (0.0025–0.15625 mg/mL). For each sample, a control tube (50 μL sample extract + 250 μL reagent 1 + 250 μL reagent 2 + 700 μL distilled water) and a test tube (50 μL sample extract + 250 μL reagent 1 + 250 μL reagent 2 + 450 μL distilled water) were prepared. Similarly, a blank (50 μL distilled water + 250 μL reagent 1 + 250 μL reagent 2 + 450 μL distilled water) and standard tubes (50 μL gallic acid standard + 250 μL reagent 1 + 250 μL reagent 2 + 450 μL distilled water) were prepared. After adding reagent 1, the mixtures were vortexed and allowed to stand at room temperature for exactly 2 min; then reagent 2 was added, followed by distilled water. After vortexing, the mixtures were allowed to stand at room temperature for exactly 10 min. The absorbance was measured at 760 nm (A-test, A-control, A-standard, A-blank). The net absorbance ΔA-test = A-test − A-control, and ΔA-standard = A-standard − A-blank. The gallic acid concentration (x, mg/mL) in the extract was calculated from the standard curve. The total phenolic content in the dry sample was expressed as mg gallic acid equivalents per gram dry weight (mg GAE/g DW) using the following formula: total phenols (mg/g) = (2.5 × x) / W, where 2.5 is the extraction volume (mL) and W is the sample dry weight (g). All measurements were performed in biological triplicate.

S2. Detection of active substances

S2.1. Sample pre-treatment

The *Astragalus membranaceus* var. *mongholicus* slices were ground into powder, and 1 g of the sample was accurately weighed and placed in a 50 mL centrifuge tube. Then, 10 mL of methanol was added. The prepared sample was ultrasonically extracted (power: 100 W, temperature maintained at 25 ℃) for 120 min (ice was added during the sonication process to maintain the temperature). After centrifugation at 5000 rpm for 10 min, 1 mL of the supernatant was passed through a 0.22 μm filter membrane and then analyzed by UPLC-MS/MS.

S2.2. UPLC-MS/MS analysis

The analytes were separated using an HPLC system (Xevo TQ-S micro-Triple Quadrupole, Waters, Milford, MA, USA). A CORTECS® UPLC®C18 column (2.1×100 mm, 1.6 μm) was used for active substances. The column temperature was set at 35 °C, and a 3 μL aliquot of sample was injected into the column. The mobile phase flow rate is 0.3 mL/min, with mobile phase A being 0.1% formic acid in water and mobile phase B being methanol. The elution gradient is as follows: 0-10 min, 95% A; 10-13 min, 10% A; 13-14 min, 40% A; 14-20 min, 95% A. The total chromatographic run time was 20 min.

Electrosprayed positive ions (ESI+, capillary: 3.5 kV) were used to detect the active substances in multiple reaction monitoring (MRM) mode. The ion source temperature was 150 °C, the desolvation temperature was 500 °C, and the flow rates of the cone gas and the desolvation gas were 150 l/h and 1000 l/h, respectively. Data were analyzed qualitatively by comparing retention times and ion-pair data and quantitatively using the parent and product ions with the highest response values.

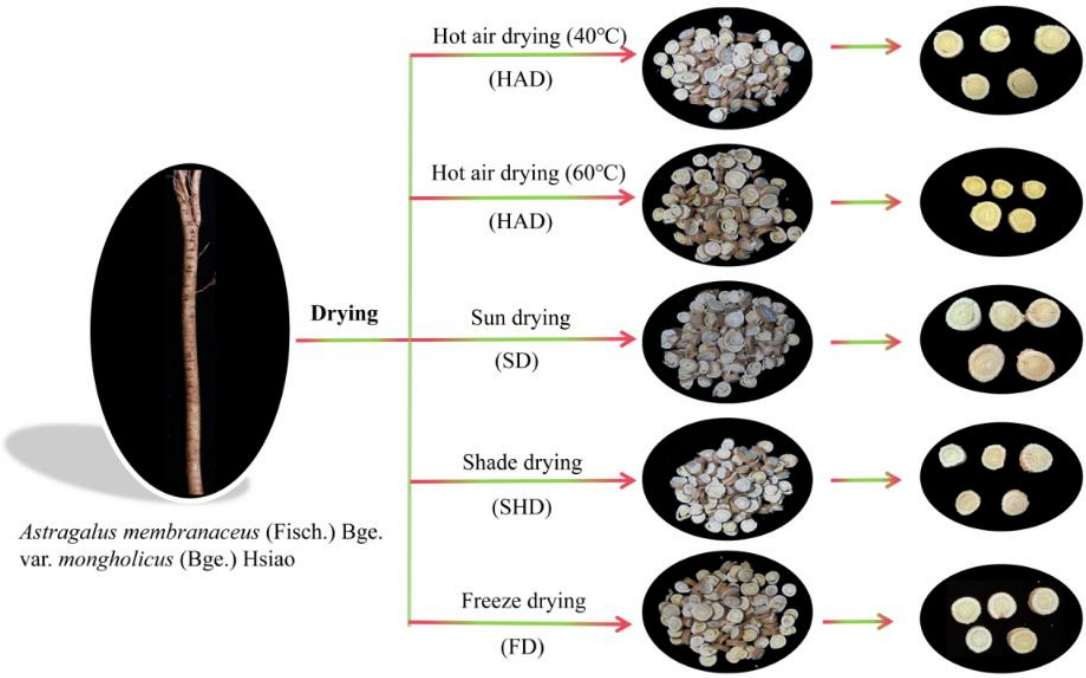


Figure S1. The appearance of *Astragalus membranaceus* var. *mongholicus* slices under different drying treatments. FS: fresh sample; SD: sun-dried; FD: freeze-dried; SHD: shade-dried; HAD40: 40°C hot-air-dried; HAD60: 60°C hot-air-dried.

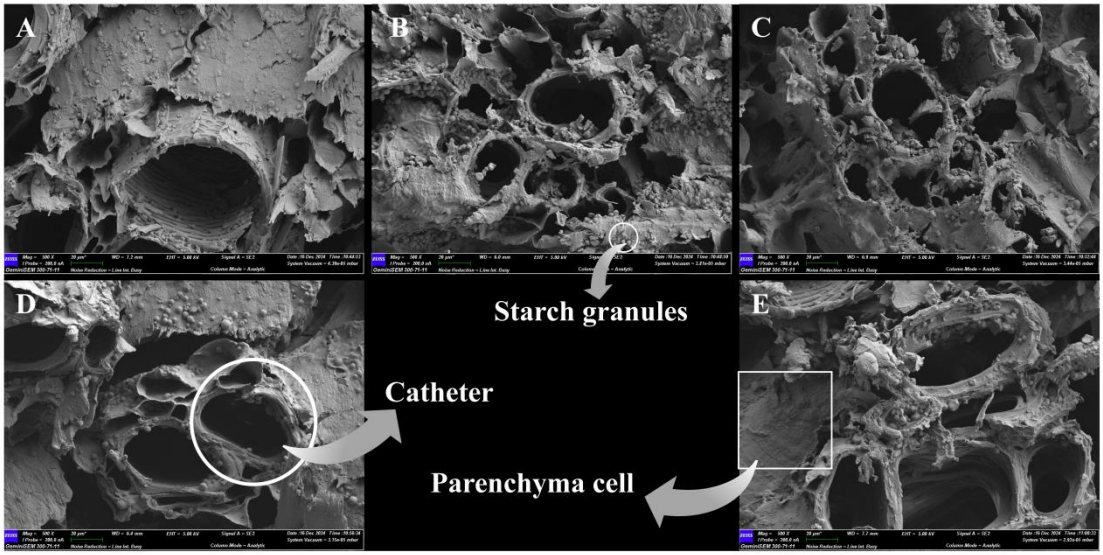


Figure S2. Microstructure of *Astragalus membranaceus* var. *mongholicus* slices under different drying conditions (Magnification 500x). A. SD; B. SHD; C. FD; D. HAD 40; E. HAD 60.

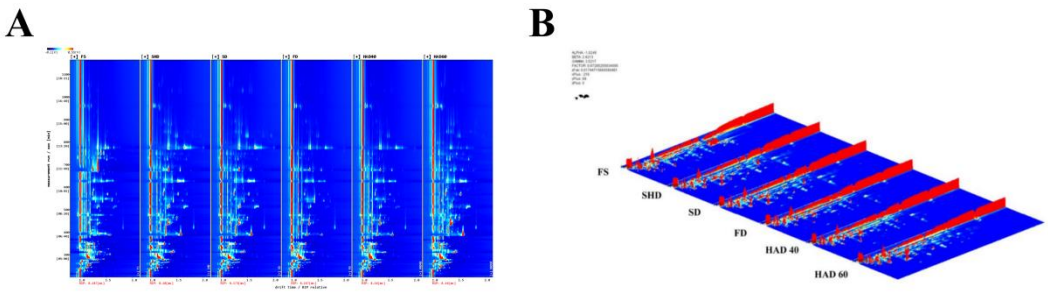


Figure S3. Three-dimensional GC-IMS spectral visualization. (A) GC-IMS topographic map. (B) Three-dimensional spectra of different treatment drying methods.

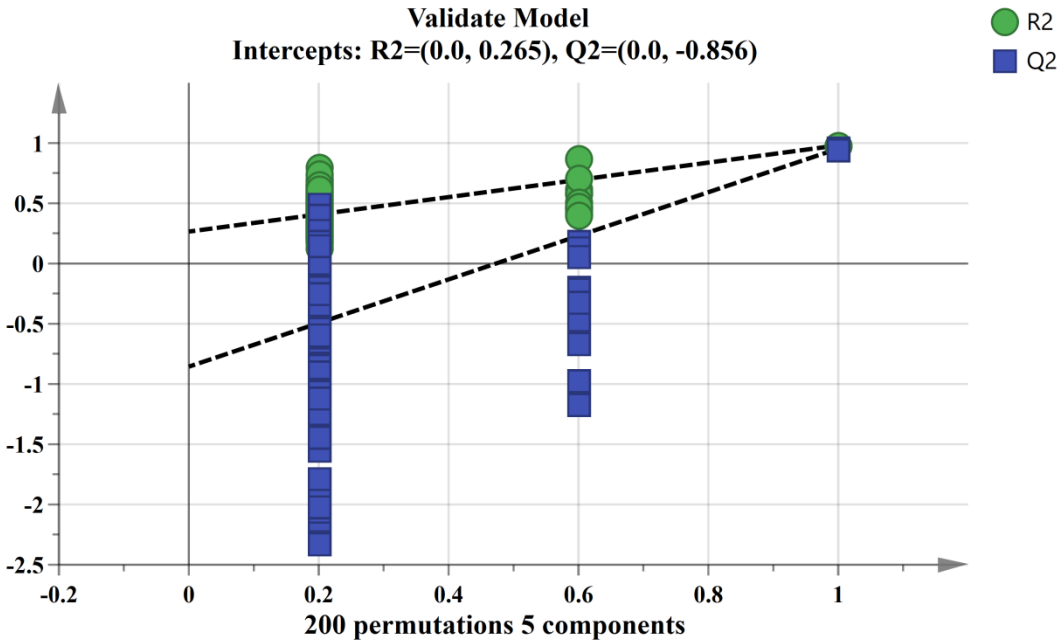


Figure S4. Plot of cross-validation of 200-substitution test.

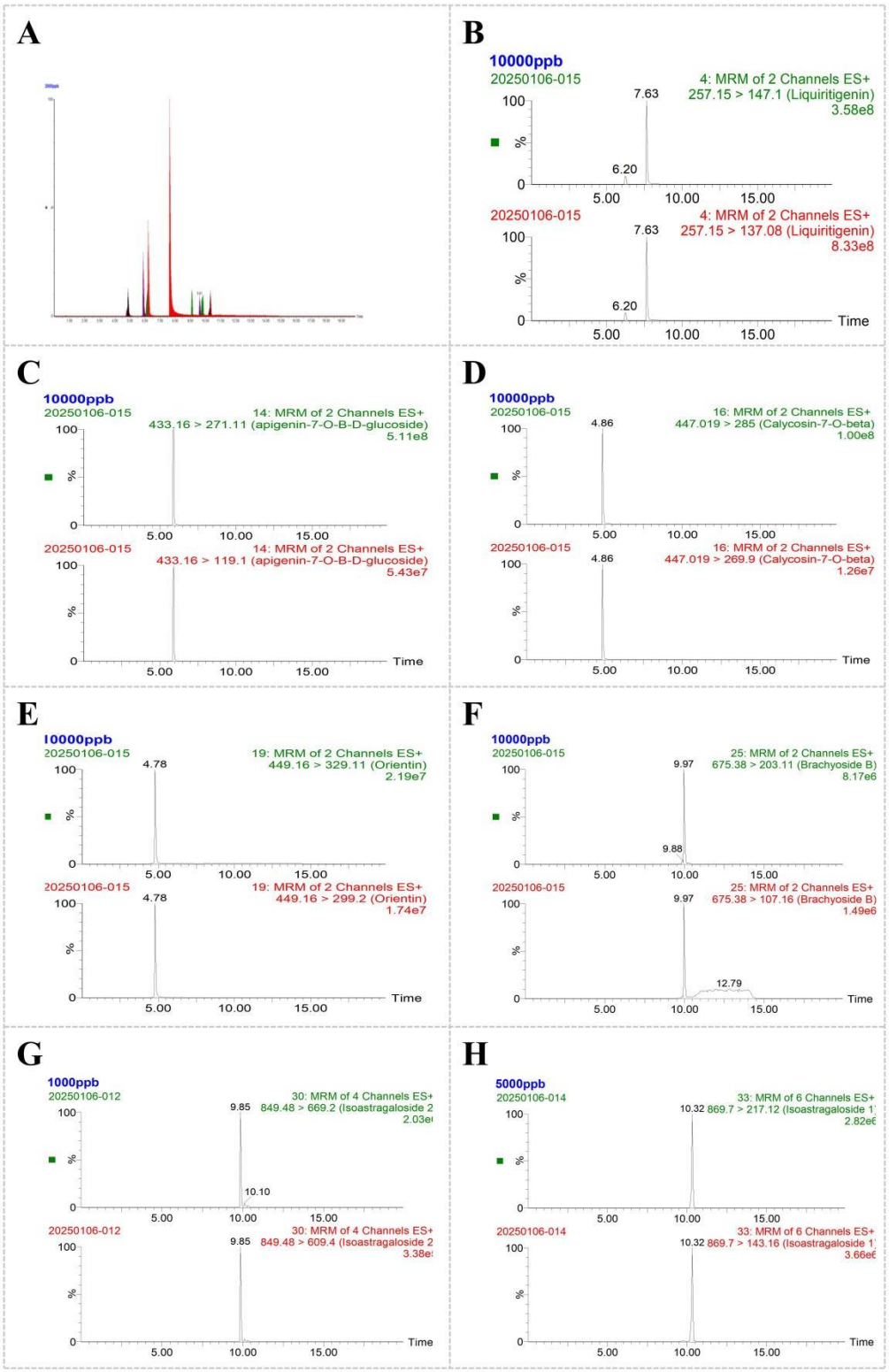


Figure S5. UPLC-MS/MS ion chromatogram of 13 active substance mixed control solutions in positive mode. (A) Thirteen active substances. (B) Liquiritigenin. (C) Apigenin-7-O-β-D-glucopyranoside. (D) Calycosin-7-O-β-D-glucoside. (E) Orientin. (F) Brachyoside B. (G) Isoastragaloside II. (H) Isoastragaloside I.

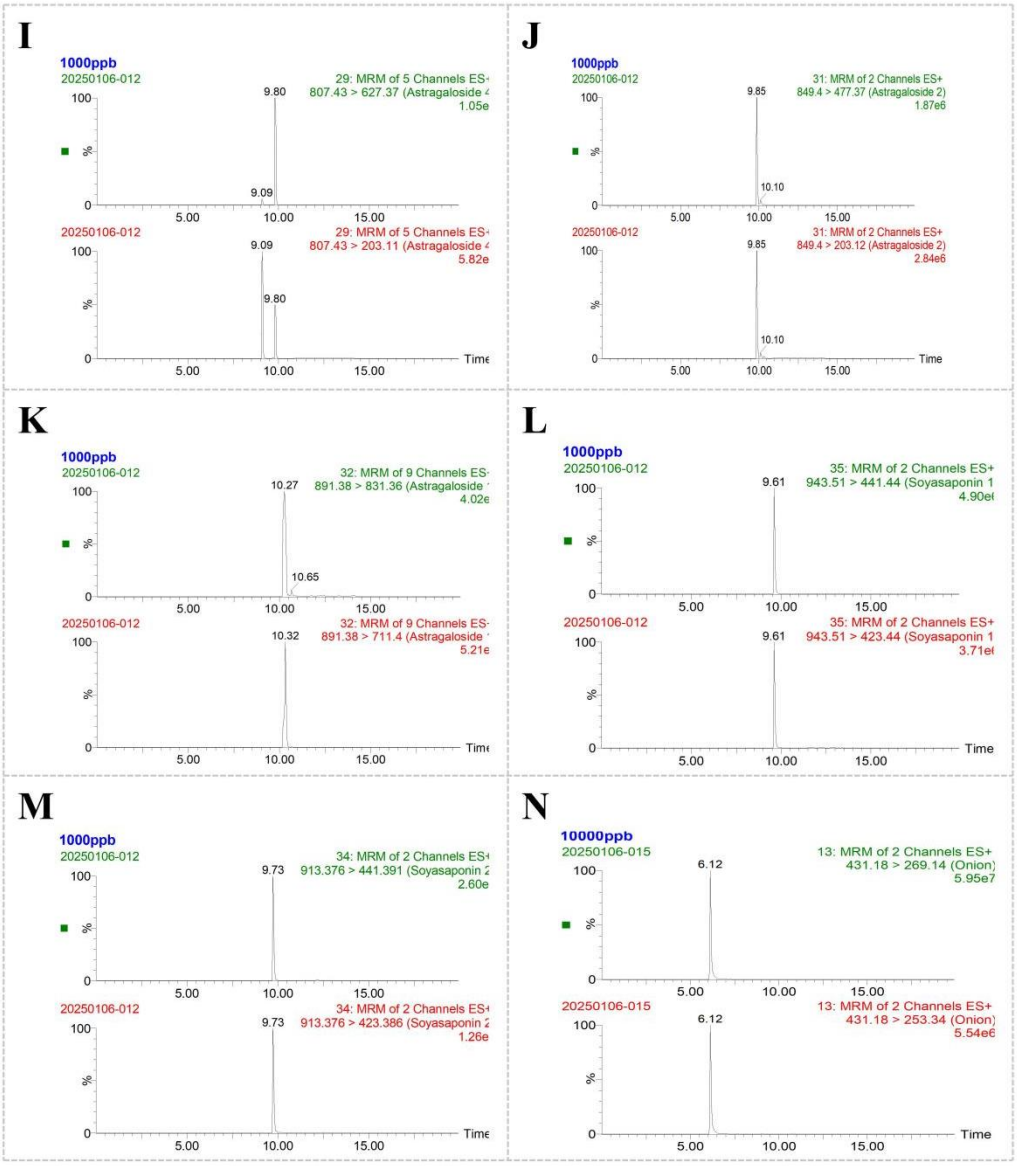


Figure S5 (continued). UPLC-MS/MS ion chromatogram of 13 active substance mixed control solutions in positive mode. (I) Astragaloside IV. (J) Astragaloside II. (K) Astragaloside I. (L) Soyasaponin I. (M) Soyasaponin II. (N) Ononin.

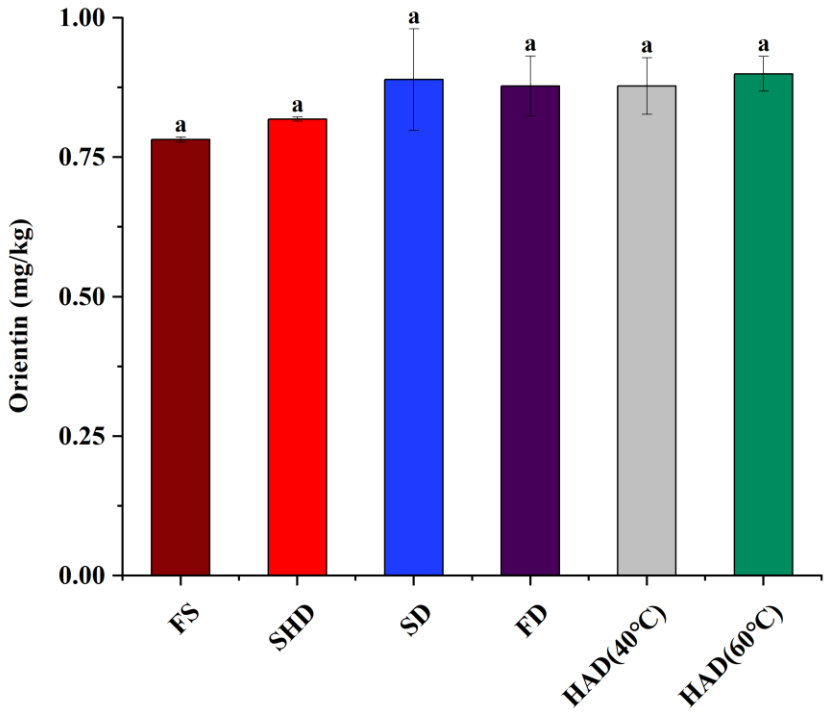


Figure S6. The orientin content of different dried samples. Different lowercase letters (a - f, etc.) indicate significant differences between groups at the $P < 0.05$ level.

Table S1 Calibration parameters, regression equations, and sensitivity for 13 active constituents by UPLC-MS/MS.

Active constituents	Linear range (ng/mL)	R^2	Regression equation	S/N	LOD (ng/mL)	LOQ (ng/mL)
Liquiritigenin	50–10000	0.9907	y = 5827.28x + 622420	98.68	1.52	5.07
Apigenin-7-O-β-D-glucopyranoside	50–10000	0.9954	y = 2436.57x + 40699	26.50	5.66	18.87
Calycosin-7-O-β-D-glucoside	50–10000	0.9922	y = 949.30x + 64324	71.34	2.10	7.01
Orientin	50–10000	0.9912	y = 179.54x + 15920	81.65	1.84	6.12
Brachyoside B	50–10000	0.9915	y = 63.41x + 15865	73.22	2.05	6.83
Isoastragaloside II	50–10000	0.9929	y = 13.41x + 575	60.18	2.49	8.31
Isoastragaloside I	50–10000	0.9969	y = 31.32x + 961	49.84	3.01	10.03
Astragaloside IV	50–10000	0.9999	y = 286.98x + 17473	23.59	6.36	21.20
Astragaloside II	50–10000	0.9947	y = 13.55x + 401	86.02	1.74	5.81
Astragaloside I	50–10000	0.9974	y = 790.48x + 25553	31.23	4.80	16.01
Soyasaponin I	50–10000	0.9928	y = 350.22x + 20876	102.92	1.46	4.86
Soyasaponin II	50–10000	0.9991	y = 86.81x + 16244	108.53	1.38	4.61
Ononin	50–10000	0.9937	y = 1308.45x + 255739	156.27	0.96	3.20

Note: Signal-to-noise ratio (S/N) was measured at the lowest calibration level (50 ng/mL); limit of detection (LOD) and limit of quantification (LOQ) were calculated by extrapolation based on S/N = 3 and S/N = 10, respectively; In the regression equation, y represents the peak area, and x represents the analyte concentration (ng/mL); Calibration curves were constructed using eleven concentration levels (50, 100, 200, 300, 400, 500, 800, 1000, 2000, 5000, 10000 ng/mL) with three injections per level.

Table S2 Mass spectral information and retention times for 13 *Astragalus membranaceus* var. *mongholicus* active substances.

Bioactive compounds	Retention time (min)	Quantification ion pair			Qualitative ion pair			Cone energy (V)	Scan mode
		Parent ion (m/z)	Daughter ion (m/z)	Collision energy (V)	Parent ion (m/z)	Daughter ion (m/z)	Collision energy (V)		
Liquiritigenin	7.63	257.15	137.08	22	257.15	147.10	18	34	ESI+
Apigenin-7-O-β-D-glucopyranoside	5.91	433.16	119.10	50	433.16	271.11	16	24	ESI+
Calycosin-7-O-β-D-glucoside	4.86	447.02	285	20	447.02	269.20	22	12	ESI+
Orientin	4.78	449.16	299.2	30	449.16	329.11	26	22	ESI+
Brachyoside B	9.97	675.38	107.16	60	675.38	203.11	48	100	ESI+
Isoastragaloside II	9.89	849.48	609.40	60	849.48	669.20	60	10	ESI+
Isoastragaloside I	10.32	869.70	143.16	12	869.70	217.12	18	18	ESI+
Astragaloside IV	9.17	807.43	203.11	54	807.43	627.37	50	100	ESI+
Astragaloside II	10.10	849.40	203.12	56	849.40	477.37	52	100	ESI+
Astragaloside I	10.32	891.38	711.40	48	891.38	831.36	50	100	ESI+
Soyasaponin II	9.81	913.38	423.38	32	913.38	441.39	22	24	ESI+
Soyasaponin I	9.61	943.51	423.44	28	943.51	441.44	24	42	ESI+
Ononin	6.12	431.18	269.14	12	431.18	253.34	46	36	ESI+

Table S3 Component composition of the 7 functional modules.

Row	Column	Correlation
ΔE	Calycosin-7-O-β-D-glucoside	0.9428571
ΔE	Apigenin-7-O-β-D-glucoside	0.8285714
ΔE	Total flavonoids	0.9428571
ΔE	Total phenols	0.9428571
ΔE	2-Methylfuran	0.8285714
ΔE	Acetaldehyde (M)	0.8857143
ΔE	1-Penten-3-ol	-0.8857143
ΔE	3-Hydroxy-2-butanone (M)	-0.9428571
ΔE	3-Hydroxy-2-butanone (D)	-0.8285714
1.8-Cineol (D)	2-Pentylfuran	-0.9428571
1.8-Cineol (D)	1-Hexanal (D)	-1
1.8-Cineol (D)	N-Pentanal	-0.9428571
1.8-Cineol (D)	Propanal	-0.8857143
1.8-Cineol (D)	(E)-2-Hexenal	-0.9428571
1.8-Cineol (D)	2-Heptenal (M)	-0.8285714
1.8-Cineol (D)	2-Heptenal (D)	-0.8857143
1.8-Cineol (D)	(E)-2-Pentenal	-0.8857143
1.8-Cineol (D)	Tetrahydrofuran (M)	-0.8857143
1.8-Cineol (D)	Tetrahydrofuran (D)	-0.8857143
1.8-Cineol (D)	Heptanal (D)	-0.9428571
1.8-Cineol (D)	(Z)-2-Penten-1-ol	0.8285714
1.8-Cineol (M)	Acetic acid ethyl ester	-0.8857143
1.8-Cineol (M)	Allyl sulfide	-0.8857143
1-Hexanal (D)	n-Pentanal	0.9428571
1-Hexanal (D)	Propanal	0.8857143
1-Hexanal (D)	(E)-2-Hexenal	0.9428571
1-Hexanal (D)	2-Heptenal (M)	0.8285714
1-Hexanal (D)	2-Heptenal (D)	0.8857143
1-Hexanal (D)	(E)-2-Pentenal	0.8857143
1-Hexanal (D)	Tetrahydrofuran (M)	0.8857143
1-Hexanal (D)	Tetrahydrofuran (D)	0.8857143
1-Hexanal (D)	Heptanal (D)	0.9428571
1-Hexanal (D)	(Z)-2-Penten-1-ol	-0.8285714
1-Hexanal (M)	2-Butanone	0.9428571
1-Hexanal (M)	1-Pentanol (T)	0.8857143
1-Hexanal (M)	Butanal (D)	0.8857143
1-Hexanal (M)	2-Methyl-2-pentenal	0.8285714
1-Hexanal (M)	1-Propanol	0.8285714
1-Hexanal (M)	Heptanal (M)	0.8857143
1-Hexanal (M)	1-Nonanal	0.9428571

Table S3 (continued) Component composition of the 7 functional modules.

Row	Column	Correlation
1-Hexanal (M)	2-Ethyl hexanol	0.8857143
1-Hexanol (D)	1-Nonanal	0.8285714
1-Hexanol (M)	1-Hexanol (D)	0.9428571
1-Nonanal	2-Ethyl hexanol	0.9428571
1-Octanal	3-Hydroxy-2-butanone (M)	-0.8285714
1-Octen-3-ol	n-Pentanal	0.8857143
1-Octen-3-ol	1-Pentanol (T)	0.8857143
1-Octen-3-ol	Butanal (M)	0.8285714
1-Octen-3-ol	Butanal (D)	0.8857143
1-Octen-3-ol	Heptanal (M)	0.8857143
1-Octen-3-ol	Heptanal (D)	0.8285714
1-Octen-3-ol	2-Ethyl hexanol	0.8857143
1-Octen-3-ol	(Z)-2-Penten-1-ol	-0.9428571
1-Pentanol (D)	1-Pentanol (T)	0.8285714
1-Pentanol (D)	Butanal (D)	0.8285714
1-Pentanol (D)	2-Heptanone	1
1-Pentanol (D)	(E)-2-Hexenal	0.8285714
1-Pentanol (D)	Heptanal (M)	0.8285714
1-Pentanol (D)	Heptanal (D)	0.8857143
1-Pentanol (D)	2-Ethyl hexanol	0.8285714
1-Pentanol (M)	2-Butanol (D)	0.8285714
1-Pentanol (T)	Butanal (M)	0.8285714
1-Pentanol (T)	Butanal (D)	1
1-Pentanol (T)	2-Heptanone	0.8285714
1-Pentanol (T)	2-Methyl-2-pentenal	0.8285714
1-Pentanol (T)	Heptanal (M)	1
1-Pentanol (T)	Heptanal (D)	0.8857143
1-Pentanol (T)	1-Nonanal	0.9428571
1-Pentanol (T)	2-Ethyl hexanol	1
1-Penten-3-ol	2-Pentanone	0.9428571
1-Propanol	1-Hexanol (M)	0.8285714
1-Propanol	1-Hexanol (D)	0.9428571
2-Butanol (D)	2-Methylfuran	-0.8285714
2-Butanol (D)	2-Heptenal (M)	0.8285714
2-Butanol (D)	1-Penten-3-ol	0.8285714
2-Butanol (M)	2-Butanol (D)	0.8857143
2-Butanol (M)	2-Methylfuran	-0.8285714
2-Butanol (M)	2-Heptenal (M)	0.8285714
2-Butanol (M)	2-Heptenal (D)	0.8285714

Table S3 (continued) Component composition of the 7 functional modules.

Row	Column	Correlation
2-Butanol (M)	(E)-2-Pentenal	0.8285714
2-Butanone	1-Pentanol (T)	0.9428571
2-Butanone	Butanal (D)	0.9428571
2-Butanone	1-Hexanol (D)	0.8285714
2-Butanone	Heptanal (M)	0.9428571
2-Butanone	1-Nonanal	1
2-Butanone	2-Ethyl hexanol	0.9428571
2-Heptanone	(E)-2-Hexenal	0.8285714
2-Heptanone	Heptanal (M)	0.8285714
2-Heptanone	Heptanal (D)	0.8857143
2-Heptanone	2-Ethyl hexanol	0.8285714
2-Heptenal (D)	(E)-2-Pentenal	1
2-Heptenal (D)	Tetrahydrofuran (M)	0.8285714
2-Heptenal (D)	Tetrahydrofuran (D)	0.8285714
2-Heptenal (M)	2-Heptenal (D)	0.8285714
2-Heptenal (M)	(E)-2-Pentenal	0.8285714
(E)-2-Hexenal	2-Heptenal (M)	0.9428571
(E)-2-Hexenal	2-Heptenal (D)	0.9428571
(E)-2-Hexenal	(E)-2-Pentenal	0.9428571
(E)-2-Hexenal	Heptanal (D)	0.8857143
2-Methyl-2-pentenal	Tetrahydrofuran (M)	0.9428571
2-Methyl-2-pentenal	Tetrahydrofuran (D)	0.9428571
2-Methyl-2-pentenal	Heptanal (M)	0.8285714
2-Methyl-2-pentenal	2-Ethyl hexanol	0.8285714
2-Methylfuran	1-Penten-3-ol	-0.8285714
(E)-2-Pentenal	Tetrahydrofuran (M)	0.8285714
(E)-2-Pentenal	Tetrahydrofuran (D)	0.8285714
2-Pentyl furan	1-Hexanal (D)	0.9428571
2-Pentyl furan	n-Pentanal	0.8285714
2-Pentyl furan	Propanal	0.9428571
2-Pentyl furan	1-Pentanol (D)	0.8285714
2-Pentyl furan	2-Heptanone	0.8285714
2-Pentyl furan	(E)-2-Hexenal	1
2-Pentyl furan	2-Heptenal (M)	0.9428571
2-Pentyl furan	2-Heptenal (D)	0.9428571
2-Pentyl furan	(E)-2-Pentenal	0.9428571
2-Pentyl furan	Heptanal (D)	0.8857143
2-Propanol	Dimethyl sulfide (M)	1
2-Propanone	Butanal (M)	0.8285714
2-Propanone	1-Propanol	0.8857143

Table S3 (continued) Component composition of the 7 functional modules.

Row	Column	Correlation
2-Propanone	1-Hexanol (M)	0.8285714
2-Propanone	1-Hexanol (D)	0.9428571
3-Hydroxy-2-butanone (M)	3-Hydroxy-2-butanone (D)	0.9428571
a	Brachyoside B	-0.8285714
a	Total sugar	-0.8285714
a	1-Pentanol (M)	1
a	2-Butanol (D)	0.8285714
ABTS	1.8-Cineol (M)	-0.8857143
ABTS	Allyl sulfide	0.8857143
Acetaldehyde (M)	1-Penten-3-ol	-0.8285714
Acetaldehyde (M)	3-Hydroxy-2-butanone (M)	-0.9428571
Acetaldehyde (M)	3-Hydroxy-2-butanone (D)	-0.8857143
Acetic acid (D)	3-Hydroxy-2-butanone (M)	-0.8857143
Acetic acid (D)	3-Hydroxy-2-butanone (D)	-0.9428571
Acetic acid (M)	Acetic acid (D)	0.8285714
Acetic acid (M)	2-Propanone	-0.8857143
Acetic acid (M)	1-Propanol	-0.8285714
Allyl sulfide	3-Hydroxy-2-butanone (D)	-0.8285714
Apigenin-7-O-β-D-glucoside	Total phenols	0.9428571
Apigenin-7-O-β-D-glucoside	2-Butanol (M)	-0.8285714
Apigenin-7-O-β-D-glucoside	2-Butanol (D)	-0.8285714
Apigenin-7-O-β-D-glucoside	2-Methylfuran	1
Apigenin-7-O-β-D-glucoside	1-Penten-3-ol	-0.8285714
Astragaloside I	Acetaldehyde (D)	0.8857143
Astragaloside IV	ABTS	0.8285714
b	Soyasaponin II	1
b	Liquiritigenin	0.9428571
b	ABTS	0.8857143
b	1.8-Cineol (M)	-1
b	Acetic acid ethyl ester	0.8857143
b	Allyl sulfide	0.8857143
Benzaldehyde	2-Butanol (D)	0.9428571
Benzaldehyde	1-Penten-3-ol	0.9428571
Benzaldehyde	2-Pentanone	0.8857143
Brachyoside B	Benzaldehyde	-0.9428571
Brachyoside B	1-Pentanol (M)	-0.8285714
Brachyoside B	2-Butanol (D)	-0.8857143
Brachyoside B	1-Penten-3-ol	-0.8285714
Butanal (D)	2-Heptanone	0.8285714
Butanal (D)	2-Methyl-2-pentenal	0.8285714

Table S3 (continued) Component composition of the 7 functional modules.

Row	Column	Correlation
Butanal (D)	Heptanal (M)	1
Butanal (D)	Heptanal (D)	0.8857143
Butanal (D)	1-Nonanal	0.9428571
Butanal (D)	2-Ethyl hexanol	1
Butanal(M)	Butanal (D)	0.8285714
Butanal(M)	Heptanal (M)	0.8285714
Butanal(M)	2-Ethyl hexanol	0.8285714
Calycosin-7-O-β-D-glucoside	Orientin	0.8116794
Calycosin-7-O-β-D-glucoside	Total flavonoids	0.8857143
Calycosin-7-O-β-D-glucoside	Total phenols	0.8285714
Calycosin-7-O-β-D-glucoside	Ethanol	-0.8285714
Calycosin-7-O-β-D-glucoside	Acetic acid (D)	0.8857143
Calycosin-7-O-β-D-glucoside	1-Octanal	0.8285714
Calycosin-7-O-β-D-glucoside	Acetaldehyde (M)	0.9428571
Calycosin-7-O-β-D-glucoside	3-Hydroxy-2-butanone (M)	-1
Calycosin-7-O-β-D-glucoside	3-Hydroxy-2-butanone (D)	-0.9428571
Dimethyl sulfide (D)	1-Hexanol (M)	0.8285714
DPPH	Acetic acid (D)	-0.9428571
DPPH	Allyl sulfide	-0.8285714
DPPH	3-Hydroxy-2-butanone (D)	0.8857143
Ethanol	1-Octanal	-1
Ethanol	3-Hydroxy-2-butanone (M)	0.8285714
Ethanol	(Z)-2-Penten-1-ol	0.8285714
FRAP	Acetaldehyde (M)	0.8285714
Heptanal (D)	2-Ethyl hexanol	0.8857143
Heptanal (M)	Heptanal (D)	0.8857143
Heptanal (M)	1-Nonanal	0.9428571
Heptanal (M)	2-Ethyl hexanol	1
Isoastragaloside I	Astragaloside IV	0.8285714
Isoastragaloside II	Isoastragaloside I	0.8285714
Isoastragaloside II	ABTS	0.8285714
Isoastragaloside II	1-Hexanal (M)	0.8285714
Isoastragaloside II	2-Methyl-2-pentenal	0.8285714
L	a	-0.8285714
L	Astragaloside II	-0.8857143
L	Aceticacid (M)	-0.8285714
L	1-Pentanol (M)	-0.8285714
Liquiritigenin	ABTS	0.9428571
Liquiritigenin	1.8-Cineol (M)	-0.9428571

Table S3 (continued) Component composition of the 7 functional modules.

Row	Column	Correlation
Liquiritigenin	Allyl sulfide	0.9428571
Liquiritigenin	Tetrahydrofuran (M)	0.8285714
Liquiritigenin	Tetrahydrofuran (D)	0.8285714
Methyl acetate	2-Propanone	-0.9428571
Methyl acetate	1-Hexanol (D)	-0.8285714
n-Pentanal	1-Pentanol (T)	0.8285714
n-Pentanal	Butanal (D)	0.8285714
n-Pentanal	2-Methyl-2-pentenal	0.8285714
n-Pentanal	Allyl sulfide	0.8285714
n-Pentanal	(E)-2-Hexenal	0.8285714
n-Pentanal	Tetrahydrofuran (M)	0.9428571
n-Pentanal	Tetrahydrofuran (D)	0.9428571
n-Pentanal	Heptanal (M)	0.8285714
n-Pentanal	Heptanal (D)	0.8857143
n-Pentanal	2-Ethyl hexanol	0.8285714
n-Pentanal	(Z)-2-Penten-1-ol	-0.9428571
Ononin	Apigenin-7-O-β-D-glucoside	0.9428571
Ononin	Total phenols	0.8285714
Ononin	2-Methylfuran	0.9428571
Orientin	DPPH	-0.840668
Orientin	Ethanol	-0.9856108
Orientin	n-Pentanal	0.8116794
Orientin	Allyl sulfide	0.8116794
Orientin	1-Octanal	0.9856108
Orientin	3-Hydroxy-2-butanone (M)	-0.8116794
Orientin	3-Hydroxy-2-butanone (D)	-0.8116794
Orientin	(Z)-2-Penten-1-ol	-0.8116794
Propanal	2-Butanol (M)	0.8285714
Propanal	(E)-2-Hexenal	0.9428571
Propanal	2-Heptenal (M)	0.8285714
Propanal	2-Heptenal (D)	1
Propanal	(E)-2-Pentenal	1
Propanal	Tetrahydrofuran (M)	0.8285714
Propanal	Tetrahydrofuran (D)	0.8285714
Ra	Rp	0.9428571
Ra	Rq	0.9428571
Ra	Isoastragaloside I	0.9428571
Ra	Astragaloside IV	0.9428571
Rp	Rq	1
Rp	Isoastragaloside I	0.8285714

Table S3 (continued) Component composition of the 7 functional modules.

Row	Column	Correlation
Rp	Astragaloside IV	1
Rp	ABTS	0.8285714
Rq	Isoastragaloside I	0.8285714
Rq	Astragaloside IV	1
Rq	ABTS	0.8285714
Soyasaponin I	Acetaldehyde (D)	0.8285714
Soyasaponin I	2-Butanone	0.8285714
Soyasaponin I	1-Hexanol (D)	0.8285714
Soyasaponin I	1-Nonanal	0.8285714
Soyasaponin II	Liquiritigenin	0.9428571
Soyasaponin II	ABTS	0.8857143
Soyasaponin II	1.8-Cineol (M)	-1
Soyasaponin II	Acetic acid ethyl ester	0.8857143
Soyasaponin II	Allyl sulfide	0.8857143
Tetrahydrofuran (M)	Tetrahydrofuran (D)	1
Total flavonoids	Total phenols	0.8857143
Total flavonoids	2-Propanol	0.8285714
Total flavonoids	Dimethyl sulfide (M)	0.8285714
Total flavonoids	Benzaldehyde	-0.8285714
Total flavonoids	Acetaldehyde (M)	0.9428571
Total flavonoids	1-Penten-3-ol	-0.9428571
Total flavonoids	3-Hydroxy-2-butanone (M)	-0.8857143
Total flavonoids	2-Pentanone	-0.8285714
Total phenols	Benzaldehyde	-0.8285714
Total phenols	2-Methylfuran	0.9428571
Total phenols	1-Penten-3-ol	-0.9428571
Total phenols	3-Hydroxy-2-butanone (M)	-0.8285714
Total phenols	2-Pentanone	-0.8857143
Total sugar	Methyl acetate	-0.9428571
Total sugar	2-Propanone	0.8857143
Total sugar	1-Pentanol (M)	-0.8285714
Total sugar	Butanal (M)	0.8857143

Table S4 Structural composition of the 7 functional modules.

Community	1	2	3	4	5	6	7
Color	2	1	1	0	0	0	0
Microstructure	0	3	0	0	0	0	0
Active compound	2	5	2	2	2	0	0
Antioxidant	1	1	2	1	1	0	0
Volatile	5	3	6	7	9	14	12
Hub node	a	ABTS	Calycosin-7-O-β-D-glucoside	Total phenols	2-Propanone	1-Pentanol (T)	N-Pentanal
Bridge node	2-Methyl1propan-1-ol	Allyl sulfide	3-Hydroxy-2-butanone (D)	2-Butanol (D)	Acetic acid (M)	Heptanal (D)	N-Pentanal

Table S5 Component composition of the 7 functional modules.

Community	Node	Type
1	L	Color
1	a	Color
1	Astragaloside II	Active compound
1	Brachyoside B	Active compound
1	FRAP	Antioxidant
1	2-Propanol	Volatile
1	Dimethyl sulfide (M)	Volatile
1	1-Pentanol (M)	Volatile
1	2-Methyl1propan-1-ol	Volatile
1	3-Methy-l-butanol	Volatile
2	b	Color
2	Ra	Microstructure
2	Rp	Microstructure
2	Rq	Microstructure
2	Soyasaponin II	Active compound
2	Liquiritigenin	Active compound
2	Isoastragaloside II	Active compound
2	Isoastragaloside I	Active compound
2	Astragaloside IV	Active compound
2	ABTS	Antioxidant
2	1.8-Cineol (M)	Volatile
2	Acetic acid ethyl ester	Volatile
2	Allyl sulfide	Volatile
3	ΔE	Color
3	Calycosin-7-O-β-D-glucoside	Active compound
3	Orientin	Active compound
3	Total flavonoids	Antioxidant
3	DPPH	Antioxidant
3	Ethanol	Volatile
3	Acetic acid (D)	Volatile
3	1-Octanal	Volatile
3	Acetaldehyde (M)	Volatile
3	3-Hydroxy-2-butanone (M)	Volatile
3	3-Hydroxy-2-butanone (D)	Volatile
4	Ononin	Active compound
4	Apigenin-7-O-β-D-glucoside	Active compound
4	Total phenols	Antioxidant
4	Benzaldehyde	Volatile
4	2-Butanol (M)	Volatile
4	2-Butanol (D)	Volatile
4	2-Methylfuran	Volatile
4	1-Penten-3-ol	Volatile

Table S5 (continued) Component composition of the 7 functional modules.

Community	Node	Type
4	2-Pentanone	Volatile
4	Ethyl propanoate	Volatile
5	Astragaloside I	Active compound
5	Soyasaponin I	Active compound
5	Total sugar	Antioxidant
5	Acetaldehyde (D)	Volatile
5	Methyl acetate	Volatile
5	Acetic acid (M)	Volatile
5	2-Propanone	Volatile
5	Dimethyl sulfide (D)	Volatile
5	1-Propanol	Volatile
5	1-Hexanol (M)	Volatile
5	1-Hexanol (D)	Volatile
5	2-Methylbutanoic acid methyl ester	Volatile
6	1-Octen-3-ol	Volatile
6	1-Hexanal (M)	Volatile
6	2-Butanone	Volatile
6	1-Pentanol (D)	Volatile
6	1-Pentanol (T)	Volatile
6	Butanal (M)	Volatile
6	Butanal (D)	Volatile
6	2-Heptanone	Volatile
6	2-Methyl-(E)-2-Pentenal	Volatile
6	Heptanal (M)	Volatile
6	Heptanal (D)	Volatile
6	1-Nonanal	Volatile
6	2-Ethyl hexanol	Volatile
6	Ethyl 2-methylpropionate	Volatile
7	1.8-Cineol (D)	Volatile
7	2-Pentylfuran	Volatile
7	1-Hexanal (D)	Volatile
7	N-Pentanal	Volatile
7	Propanal	Volatile
7	(E)-2-Hexenal	Volatile
7	2-Heptenal (M)	Volatile
7	2-Heptenal (D)	Volatile
7	(E)-2-Pentenal	Volatile
7	Tetrahydrofuran (M)	Volatile
7	Tetrahydrofuran (D)	Volatile
7	2-Penten-1-ol	Volatile

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