ACCSCIENCE PUBLISHING

Eurasian Journal of Medicine and Oncology

ORIGINAL RESEARCH ARTICLE

Comprehensive characterization of the material basis and network pharmacology of Dan-Shen-Yin in the treatment of gastritis

Supplementary File

1. Materials and methods

1.1. Reference compounds

The details of reference standards used in this study are presented in Table S1.

Table S1. Lot number and source of reference compounds

Standard samples	Lot number	Source
Salvianolic acid A	wkq22050609	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Salvianolic acid B	wkq22051904	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Epicatechin	wkq23073106	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Dihydrotanshinone I	wkq23052211	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Cryptotanshinone	wkq22011809	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Orientin	wkq23080310	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Danshensu	wkq22052410	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Salvianolic acid D	wkq22072012	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Ferulic acid	wkq22010705	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Isosalvianolic acid C	wkq22042702	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Lithospermic	wkq23060109	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Rosmarinic acid	wkq23020112	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Quercitrin	wkq23011612	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Neocryptotanshinone	wkq22050913	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Isoorientin	wkq23030802	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Isovitexin	wkq23030802	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Vitexin	wkq23031407	Ichuan Weikeqi Biological Technology CO., LTD (Chengdu, China)
Tanshinone IIA	P21J11F118380	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)
Catechin	J10GB151070	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)
Glucose	B21882	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)
Rhamnose	B21172	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)
Arabinose	B25845	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)

1.2. Gas chromatography–mass spectrometry (GC-MS) analysis conditions of Dan-Shen-Yin (DSY)

MS was conducted using an electron ionization source. The ion source temperature was set at 230°C, and the quadrupole temperature was maintained at 150°C. The scanning range was set to 40–450 m/z, with a solvent delay

Table S1. ***(Continued)***

Standard samples	Lot number	Source
Lyxose	B25436	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)
Glucuronic acid	B25302	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)
Galacturonic acid	S11020	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)
Xylose	S45224	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)
M-hydroxybiphenyl	S30798	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)
Borax decahydrate	S24099	Shanghai Yuanye Bio-Technology Co., Ltd (Shanghai, China)

Table S2. Heating program for gas chromatography–mass spectrometry analysis

Gradient	Velocity of flow (□/min)	Temperature (□)
Initial value	/	50
Gradient 1	4	70
Gradient 2	5	90
Gradient 3	5	135
Gradient 4	7	170
Gradient 5	1	185
Gradient 6	3	190
Gradient 7	10	220

time of 3.6 min. The detailed heating program for the chromatographic column is shown in Table S2.

2. Results

2.1. Optimization of Headspace GC-MS (HS-GC-MS) analysis conditions

To improve the accuracy of the volatile component profiling of DSY, headspace analysis conditions, including split ratio, equilibrium temperature, and equilibrium time, were assessed and optimized. The results are presented in Figure S1.

2.2. Identification of volatile compounds in *Salvia miltiorrhiza Bge.* (DS), *Amomum villosum Lour.* (SR), and *Santalum album L.* (TX)

The nonvolatile compounds in the individual herbs were identified using GC-MS, and detailed information is provided in Table S3 (DS), Table S4 (SR), and Table S5 (TX).

2.3. Identification of nonvolatile compounds in DS, SR, and TX

The nonvolatile compounds in the individual herbs were identified using liquid chromatography–mass spectrometry (LC-MS), and detailed information is provided in Table S6 (DS), Table S7 (SR), and Table S8 (TX).

2.4. Determination of total sugar, galacturonic acid, and protein content in DSY

To quantify the total sugar, uronic acid, and protein content in DSY decoction, standard curves were established using respective standard solutions. For total sugar determination, glucose standards at concentrations of 0.025 mg/mL, 0.05 mg/mL, 0.1 mg/mL, 0.2 mg/mL, 0.3 mg/mL, and 0.5 mg/mL were used (Figure S2A). Uronic acid content was determined using galacturonic acid standards at concentrations of 0.02 mg/mL, 0.04 mg/mL, 0.06 mg/mL, 0.08 mg/mL, 0.10 mg/mL, 0.14 mg/mL, and 0.18 mg/mL (Figure S2B). Finally, the standard curve for protein quantification was generated using bovine serum albumin standards at concentrations of 0.02 mg/mL, 0.04 mg/mL, 0.06 mg/mL, 0.08 mg/mL, 0.12 mg/mL, and 0.16 mg/mL (Figure S2C).

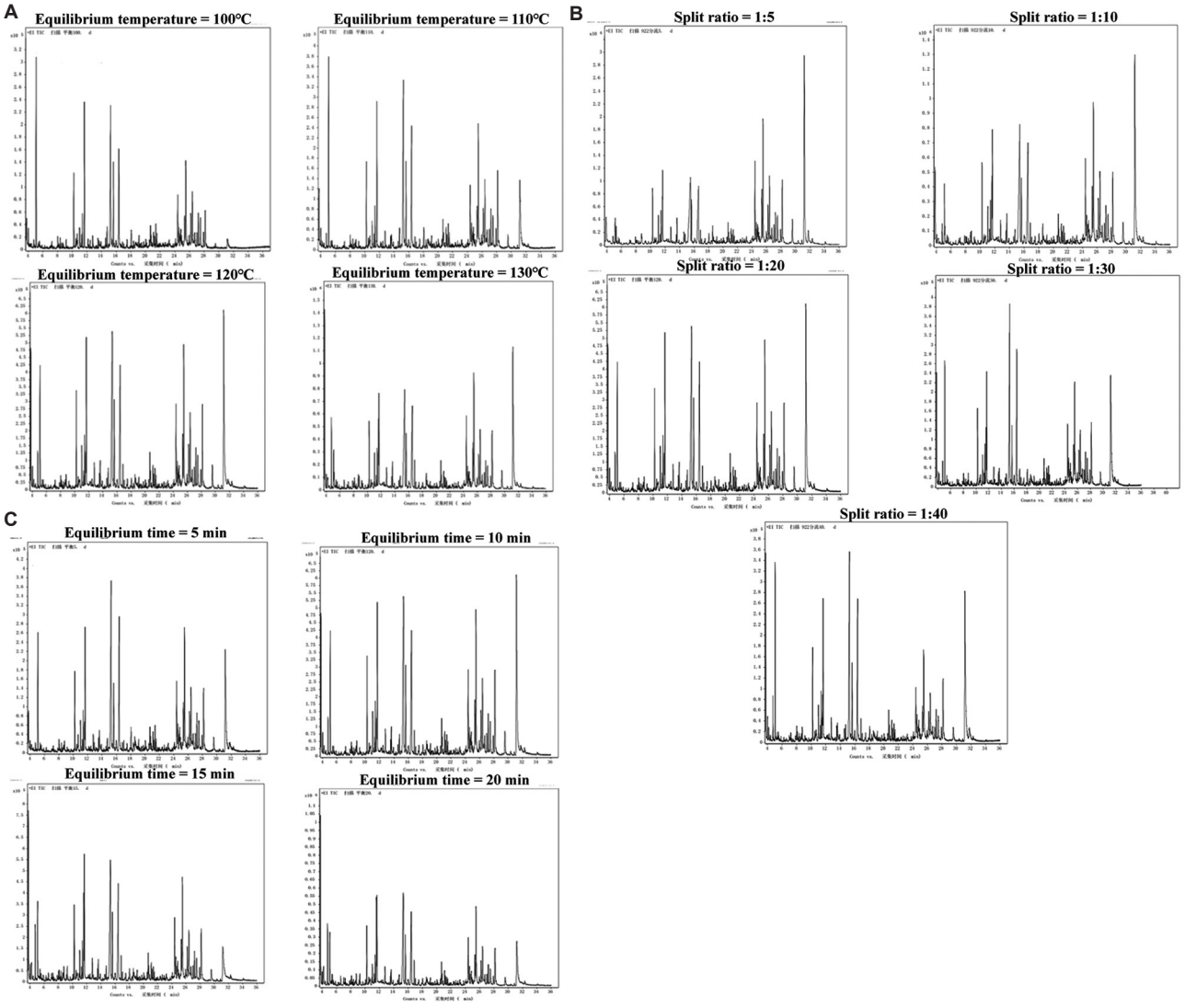

Figure S1. Optimization of HS-GC-MS sampling conditions. (A) Effect of the equilibrium temperature. (B) Effect of the split ratio. (C) Effect of the equilibrium time

Abbreviations: DSY: Dan-Shen-Yin; HS-GC-MS: Headspace gas chromatography–mass spectrometry

Table S3. Identified volatile compounds in DS based on GC-MS

No.	t_R (min)	Molecular formula	CAS number	Compound name	Match degree		Relative content (%)
					P.Match	R.Match	
1	3.806	$C_5H_4O_2$	98-01-1	Furfural	826	898	4.056
2	4.235	$C_5H_6O_2$	98-00-0	2-Furanmethanol	873	884	2.527
3	5.430	$C_4H_6O_2$	96-48-0	Butyrolactone	906	972	1.801
4	6.968	$C_6H_{12}O_2$	142-62-1	Hexanoic acid	885	899	1.227
5	7.044	$C_6H_8O_4$	10230-62-3	2,4-Dihydroxy-2,5-dimethyl-3 (2H)-furanone	824	834	1.332
6	7.835	C_5H_5NO	1003-29-8	1H-Pyrrole-2-carboxaldehyde	912	963	2.116
7	8.778	C_8H_8O	122-78-1	Benzeneacetaldehyde	917	957	3.083
8	9.140	$C_6H_8O_3$	3658-77-3	Furaneol	881	893	0.596

(Cont'd...)

Table S3. ***(Continued)***

No.	t_R (min)	Molecular formula	CAS number	Compound name	Match degree		Relative content (%)
					P.Match	R.Match	
10	10.902	$C_8H_{16}O_2$	149-57-5	Hexanoic acid, 2-ethyl-	815	869	0.806
11	11.568	$C_6H_8O_4$	28564-83-2	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	925	927	15.484
12	12.416	$C_8H_{16}O_2$	124-07-2	Octanoic acid	824	824	0.956
13	15.135	$C_9H_{18}O_2$	112-05-0	Nonanoic acid	868	904	1.988
14	18.573	$C_8H_8O_3$	621-59-0	Isovanillin	837	883	1.981
15	19.016	$C_{14}H_{26}O_2$	126-86-3	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	829	829	1.453
16	20.773	$C_{19}H_{40}$	629-92-5	Nonadecane	808	825	0.732
17	21.126	$C_{14}H_{22}O$	96-76-4	2,4-Di-tert-butylphenol	913	919	3.908
18	23.659	$C_{15}H_{26}O$	23811-08-7	Hinesol	911	937	2.430
19	23.893	$C_{15}H_{26}O$	473-15-4	Beta-Eudesmol	935	940	6.530
20	24.412	$C_{15}H_{24}O$	115-71-9	α-Santalol	871	877	3.094
21	25.821	$C_{15}H_{26}O_2$	1911-78-0	Oplopane	804	861	1.485
22	27.783	$C_{15}H_{28}O_2$	4666-84-6	Cryptomeridiol	861	861	3.218
23	29.355	$C_{19}H_{28}O_4$	/	Phthalic acid, hept-4-yl isobutyl ester	906	931	4.034
24	30.878	$C_{17}H_{24}O_3$	82304-66-3	7,9-Di-tert-butyl-1- oxaspiro (4,5) deca-6,9-diene-2,8-dione	896	909	4.523
25	32.174	$C_{16}H_{22}O_4$	84-74-2	Dibutyl phthalate	944	953	10.710

Abbreviations: DS: *Salvia miltiorrhiza Bge.*; GC-MS: Gas chromatography–mass spectrometry; P.Match: Positive match score; R.Match: Reverse match score; t_R: Retention time.

Table S4. Identified volatile compounds in SR based on GC-MS

No.	t_R (min)	Molecular formula	CAS number	Compound name	Match degree		Relative content (%)
					P.Match	R.Match	
1	3.792	$C_5H_4O_2$	98-01-1	Furfural	893	915	4.732
2	4.192	$C_5H_6O_2$	98-00-0	2-Furanmethanol	923	948	2.634
3	5.078	$C_8H_{14}O_2$	24070-70-0	3-Methylcyclopentyl acetate	878	909	0.564
4	5.197	C_4H_8OS	3268-49-3	Methional	828	836	0.525
5	5.344	$C_6H_6O_2$	1192-62-7	Ethanone, 1-(2-furanyl)-	828	904	0.284
6	5.454	$C_4H_6O_2$	96-48-0	Butyrolactone	828	947	1.028
7	5.882	$C_{10}H_{16}$	4889-83-2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	828	882	0.454
8	6.249	$C_{10}H_{16}$	79-92-5	Camphene	893	925	0.654
9	6.397	$C_6H_8O_2$	3857-25-8	2-Furanmethanol, 5-methyl-	863	863	0.574
10	6.611	$C_6H_6O_2$	620-02-0	2-Furancarboxaldehyde, 5-methyl-	879	917	0.631
11	7.059	$C_6H_8O_4$	10230-62-3	2,4-Dihydroxy-2,5-dimethyl-3 (2H)-furan-3-one	925	939	1.736
12	7.340	$C_{10}H_{16}$	18172-67-3	(1S)-(1)-beta-Pinene	809	904	0.357
13	7.844	C_5H_5NO	1003-29-8	1H-Pyrrole-2-carboxaldehyde	866	938	0.240
14	8.363	$C_{10}H_{16}$	5989-27-5	D-Limonene	913	913	0.837
15	8.644	$C_5H_6O_3$	19322-27-1	3 (2H)-Furanone, 4-hydroxy-5-methyl-	823	931	0.566
16	8.773	C_8H_8O	122-78-1	Benzeneacetaldehyde	930	957	1.901
17	9.178	$C_6H_8O_3$	68755-49-7	2.5-Dimethyl-3.4-dioxofuran	920	944	0.364
18	9.292	C_6H_7NO	1072-83-9	2-Acetyl pyrrole	936	939	3.656
19	10.073	$C_7H_8O_2$	90-05-01	Phenol, 2-methoxy-	880	891	0.963

(Cont'd...)

Table S4. ***(Continued)***

No.	t_R (min)	Molecular formula	CAS number	Compound name	Match degree		Relative content (%)
					P.Match	R.Match	
20	10.511	$C_{10}H_{16}O$	29957-43-5	HOTRIENOL	827	901	0.313
21	11.616	$C_6H_8O_4$	28564-83-2	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	936	940	12.419
22	12.368	$C_{10}H_{18}O_2$	39028-58-5	Linalool oxide C	856	885	0.436
23	12.506	$C_{10}H_{18}O_2$	14049-11-7	2H-Pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-	805	856	0.351
24	12.944	$C_{10}H_{18}O_2$	13741-21-4	2,6-Dimethyl-3,7-octadiene-2,6-diol	910	942	3.314
25	14.921	$C_{12}H_{22}O$	/	Cis, trans-4-n-Propyl-3-oxabicyclo[4.4.0]decane	806	840	1.457
26	15.264	$C_{10}H_{18}O_2$	51276-33-6	2,6-Dimethyl-1,7-octadiene-3,6-diol	860	865	1.167
27	15.568	$C_{10}H_{14}O$	/	2-Caren-10-al	864	884	1.291
28	15.630	$C_{12}H_{20}O_2$	76-49-3	Bornyl acetate	909	912	1.355
29	16.354	$C_9H_{10}O_2$	7786-61-0	2-Methoxy-4-vinylphenol	927	971	1.251
30	17.040	$C_{10}H_{18}O_2$	1946-00-5	Limonene glycol	870	899	2.301
31	17.635	$C_{16}H_{30}O_2$	/	1,12-Di (oxiran-2-yl) dodecane	803	803	0.504
32	18.045	$C_{15}H_{24}$	469-61-4	α-Cedrene	809	821	3.795
33	18.445	$C_{15}H_{26}O$	21698-41-9	(-)-Pogostol	845	862	1.370
34	18.697	$C_6H_{13}ClOSi$	/	Trans-(2-Chlorovinyl) dimethylethoxysilane	812	812	0.506
35	19.121	$C_{15}H_{24}$	512-61-8	Alpha-Santalene	876	915	0.845
36	19.197	$C_{10}H_{18}O_3$	87096-70-6	1,2-cis-1,5-trans-2,5-dihydroxy-4-methyl-1-(1-hydroxy-1-isopropyl) cyclohex-3-ene	803	825	0.361
37	19.488	$C_{15}H_{24}$	18252-46-5	Cis- alpha-Bergamotene	876	890	0.275
38	19.954	$C_{12}H_{18}O_3$	55658-18-9	5-Ketobornyl acetate	802	807	0.495
39	20.530	$C_{15}H_{24}$	23986-74-5	Germacrene D	864	918	0.252
40	20.859	$C_{15}H_{24}$	24703-35-3	(1S,2E,6E,10R)-3,7,11,11-Tetramethylbicyclo[8.1.0] undeca-2,6-diene	899	910	0.965
41	21.402	$C_{17}H_{28}O_2$	149197-48-8	Tau-Cadinol acetate	807	828	1.222
42	22.488	$C_{15}H_{24}O$	6750-60-3	Spathulrnol	874	892	0.206
43	22.616	$C_{10}H_{12}O_4$	617-05-0	Ethyl Vanillat	824	841	0.489
44	25.359	$C_{15}H_{26}O_2$	1212211-43-2	1,1,4,7-Tetramethyldecahydro-1H-cyclopropa[e] azulene-4,7-diol	880	947	2.585
45	29.364	$C_{18}H_{26}O_4$	/	Phthalic acid, hex-3-yl isobutyl ester	816	867	0.279
46	30.874	$C_{17}H_{24}O_3$	82304-66-3	7,9-Di-tert-butyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione	890	891	0.420
47	32.169	$C_{16}H_{22}O_4$	84-74-2	Dibutyl phthalate	880	921	0.323

Abbreviations: GC-MS: Gas chromatography–mass spectrometry; P.Match: Positive match score; R.Match: Reverse match score; t_R: Retention time; SR: *Amomum villosum Lour.*

Table S5. Identified volatile compounds in TX based on GC-MS

No.	t_R (min)	Molecular formula	CAS	Compound name	Match degree		Relative content (%)
					P.Match	R.Match	
1	3.787	$C_5H_4O_2$	98-01-1	Furfural	922	943	2.114
2	4.773	C_9H_{14}	529-16-8	Santene	898	918	0.802
3	5.078	$C_8H_{14}O_2$	24070-70-0	3-Methylcyclopentyl acetate	897	939	2.724
4	8.659	$C_5H_6O_3$	19322-27-1	Norfuraneol	857	939	0.688
5	11.268	$C_9H_{14}O$	6090-9-1	4-Acetyl-1-methylcyclohexene	843	915	0.350
6	11.659	$C_{10}H_{16}O$	464-49-3	(+)-2-bornanone	942	956	2.739
7	12.783	$C_9H_{10}O$	122-00-9	Ethanone, 1-(4-methylphenyl)-	878	960	0.752
8	14.750	$C_{14}H_{22}$	1014-60-4	Benzene, 1,3-bis (1,1-dimethylethyl)-	876	910	0.373
9	15.407	$C_{10}H_{14}O_2$	562-66-3	Alpha-Teresantalic acid	937	959	9.437
10	15.630	$C_{12}H_{20}O_2$	76-49-3	Bornyl acetate	926	928	1.795
11	16.511	$C_{10}H_{14}O_2$	562-66-3	Alpha-Teresantalic acid	804	832	5.244
12	17.040	$C_{12}H_{18}O$	16933-18-9	Tricycloekasantalal	880	894	0.128
13	18.554	$C_8H_8O_3$	121-33-5	Vanillin	892	908	0.734
14	19.121	$C_{15}H_{24}$	512-61-8	Alpha-Santalene	847	897	0.148
15	20.050	$C_{15}H_{24}O$	115-71-9	α-Santalol	824	838	0.147
16	20.535	$C_{15}H_{22}$	644-30-4	α-Curcumene	836	915	0.282
17	24.402	$C_{15}H_{24}O$	115-71-9	α-Santalol	927	936	2.650
18	24.574	$C_{15}H_{26}O$	/	7-Epi-trans-sesquisabinene hydrate	806	827	0.880
19	24.745	$C_{15}H_{24}O$	88034-74-6	Alpha-Bergamotenol	876	888	0.538
20	25.350	$C_{15}H_{26}O$	4602-84-0	Farnesyl alcohol	830	841	2.472
21	25.502	$C_{15}H_{22}O$	39599-18-3	Cis-nuciferol	907	915	4.975
22	31.193	$C_{15}H_{24}O$	/	Diepicedrene-1-oxide	804	811	20.300
23	31.769	$C_{15}H_{26}O_2$	201731-87-5	FUCSWNUANQRDFQ-VZUCSPMQSA-N	854	928	2.372

Abbreviations: GC-MS: Gas chromatography–mass spectrometry; P.Match: Positive match score; R.Match: Reverse match score; t_R: Retention time; TX: *Santalum album L.*

Table S6. Identified nonvolatile compounds in DS based on LC-MS

No.	t_R (min)	Mass (ppm)	Formula	Selected ion	ESI-MS²	Compound name	Error (ppm)
1	0.83	665.2148	$C_{24}H_{42}O_{21}$	$[M-H]^-$	485.1528, 383.1202, 341.1098	Tetrose	1.948
2	0.85	341.1090	$C_{12}H_{22}O_{11}$	$[M-H]^-$	179.0565	Disaccharide	3.436
3	1.12	191.0197	$C_6H_8O_7$	$[M-H]^-$	173.0093, 111.0088	Citric Acid	5.607
4	2.06	151.0402	$C_8H_8O_3$	$[M-H]^-$	123.0453	2-Anisic acid	8.272
5	2.07	197.0455	$C_9H_{10}O_5$	$[M-H]^-$	179.0352, 135.0453, 123.0453, 72.9932	Danshensu	−0.135
6	2.18	167.0351	$C_8H_8O_4$	$[M-H]^-$	123.0453	Vanillic acid	7.452
7	2.35	153.0193	$C_7H_6O_4$	$[M-H]^-$	109.0295, 91.0191	Protocatechuic acid	−0.274
8	2.63	181.0506	$C_9H_{10}O_4$	$[M-H]^-$	163.0402, 135.0453	3,4-Dihydroxyhydro cinnamic acid	7.538
9	3.06	137.0245	$C_7H_6O_3$	$[M-H]^-$	119.0139, 108.0218, 91.0190	Protocatechualdehyde	0.273
10	3.27	193.0506	$C_{10}H_{10}O_4$	$[M-H]^-$	149.0608	Ferulic acid	0.425
11	3.63	179.0349	$C_9H_8O_4$	$[M-H]^-$	135.0436, 107.0487	Caffeic acid	−0.123
12	4.54	537.1043	$C_{27}H_{22}O_{12}$	$[M-H]^-$	493.1135, 295.0611, 185.0244, 109.0295	Salvianolic acid h	2.788

(Cont'd...)

Table S6. ***(Continued)***

No.	t_R (min)	Mass (ppm)	Formula	Selected ion	ESI-MS^2	Compound name	Error (ppm)
137	4.58	313.0718	$C_{17}H_{14}O_6$	[M-H]$^-$	313.0717, 269.0821, 203.0352, 159.0453, 109.0296	Salvianolic acid f	0.059
14	4.90	493.1143	$C_{26}H_{22}O_{10}$	[M-H]$^-$	295.0612, 185.0244, 109.0295	Salvianolic acid a or its isomer	0.547
15	4.90	537.1042	$C_{27}H_{22}O_{12}$	[M-H]$^-$	493.1135, 295.0611, 109.0295	Salvianolic acid u	0.634
16	5.00	537.1041	$C_{27}H_{22}O_{12}$	[M-H]$^-$	493.1135, 295.0611, 109.0295	Salvianolic acid t	0.392
17	5.21	417.0829	$C_{20}H_{18}O_{10}$	[M-H]$^-$	197.0444, 175.0388	Salvianolic acid d	0.408
18	5.39	551.1198	$C_{28}H_{24}O_{12}$	[M-H]$^-$	353.0668, 321.0405	Monomethyl lithospermate	0.564
19	5.44	717.1459	$C_{36}H_{30}O_{16}$	[M-H]$^-$	519.0937, 339.0511, 321.0405	Salvianolic acid b or its isomer	−0.234
20	5.56	537.1041	$C_{27}H_{22}O_{12}$	[M-H]$^-$	493.1135, 295.0611, 185.0244, 109.0295	Salvianolic acid j	2.565
21	5.66	359.0772	$C_{18}H_{16}O_8$	[M-H]$^-$	197.0444, 197.0444, 161.0230	Rosmarinic acid	−0.002
22	5.79	493.1142	$C_{26}H_{22}O_{10}$	[M-H]$^-$	295.0611, 185.0243, 109.0295	Salvianolic acid a or its isomer	0.365
23	5.98	717.1460	$C_{36}H_{30}O_{16}$	[M-H]$^-$	295.0606, 519.0930, 339.0503, 321.0399	Salvianolic acid b or its isomer	−0.150
24	5.99	339.0511	$C_{18}H_{12}O_7$	[M+H]$^-$	295.0615, 185.0244, 109.0295	Salvianolic acid g	0.262
25	6.01	537.1041	$C_{27}H_{22}O_{12}$	[M-H]$^-$	493.1135, 295.0611, 185.0244, 109.0295	Lithospermic	2.434
26	6.07	493.1142	$C_{26}H_{22}O_{10}$	[M-H]$^-$	295.0612, 185.0244, 109.0295	Salvianolic acid a or its isomer	0.304
27	6.21	717.1459	$C_{36}H_{30}O_{16}$	[M-H]$^-$	519.0937, 339.0511, 321.0405	Salvianolic acid e	1.295
28	6.33	717.1462	$C_{36}H_{30}O_{16}$	[M-H]$^-$	519.0937, 339.0511, 321.0405	Salvianolic acid b	0.184
29	6.64	493.1141	$C_{26}H_{22}O_{10}$	[M-H]$^-$	295.0612, 185.0244, 109.0295	Salvianolic acid a or its isomer	0.243
30	7.16	493.1142	$C_{26}H_{22}O_{10}$	[M-H]$^-$	295.0611, 185.0243, 109.0295	Salvianolic acid a its isomer	0.487
31	7.17	731.1619	$C_{37}H_{32}O_{16}$	[M-H]$^-$	533.1094, 353.0666, 335.0563	9'''-Methyl salvianolate B	0.153
32	7.50	491.0986	$C_{26}H_{20}O_{10}$	[M-H]$^-$	293.0455, 265.0506, 197.0455	Isosalvianolic acid c	0.468
33	8.65	491.0986	$C_{26}H_{20}O_{10}$	[M-H]$^-$	293.0455, 249.0555, 135.0451	Salvianolic acid c	0.529
34	10.57	311.1277	$C_{19}H_{18}O_4$	[M+H]$^-$	267.1377, 203.0853	Tanshinaldehyde	−3.929
35	10.80	327.1238	$C_{19}H_{20}O_5$	[M-H]$^-$	283.1340, 239.1441	1S-hydroxy-anhydride of 16Rcryptotanshinone	0.040
36	10.83	311.1277	$C_{19}H_{18}O_4$	[M+H]$^-$	293.1191, 275.1058, 203.0852	Tanshinone IIB	−0.307
37	10.94	309.1119	$C_{19}H_{16}O_4$	[M+H]$^-$	265.1223, 223.0755, 203.0854	Salvianolic aldehyde	−0.438
38	11.03	313.1445	$C_{19}H_{22}O_4$	[M-H]$^-$	269.1543, 213.0914	Neocryptotanshinone	−0.008
39	11.04	297.1484	$C_{19}H_{20}O_3$	[M+H]$^-$	253.1586, 203.0853	Isocryptotanshinone	−0.674
40	11.23	279.1014	$C_{18}H_{14}O_3$	[M+H]$^-$	261.0907, 203.0852	Dihydrotanshinone I	−0.469
41	11.51	295.1327	$C_{19}H_{18}O_3$	[M+H]$^-$	267.1379, 249.1266, 203.0853	Tanshinone IIA	−4.431
42	11.79	297.1482	$C_{19}H_{20}O_3$	[M+H]$^-$	279.1378, 203.0852	Cryptotanshinone	−4.704

Abbreviations: DS: *Salvia miltiorrhiza Bge.*; ESI-MS_2: Electrospray ionization tandem mass spectrometry; LC-MS: Liquid chromatography–mass spectrometry; t_R: Retention time.

Table S7. Identified nonvolatile compounds in SR based on LC-MS

No.	t_R (min)	Mass (ppm)	Formula	Selected ion	ESI-MS^2	Compound name	Error (ppm)
1	0.74	169.0498	$C_8H_8O_4$	$[M+H]^-$	151.0385, 125.0597, 111.0440, 65.0386,	Isovanillic acid	−0.035
2	0.91	133.0142	$C_4H_6O_5$	$[M-H]^-$	115.0040, 71.0141	Malic Acid	−0.079
3	1.65	191.0197	$C_6H_8O_7$	$[M-H]^-$	111.0090, 87.0090	Limonexic acid	−0.083
4	1.92	329.0879	$C_{14}H_{18}O_9$	$[M-H]^-$	269.0667, 209.0457, 167.0351	Vanillin hexoside	0.166
5	2.18	167.0350	$C_8H_8O_4$	$[M-H]^-$	152.0115, 123.0452, 108.0217, 91.0191	Vanillic acid	0.287
6	2.35	153.0193	$C_7H_6O_4$	$[M-H]^-$	109.0296, 91.0191	Protocatechuic acid	−0.274
7	2.58	329.0879	$C_{14}H_{18}O_9$	$[M-H]^-$	269.0667, 209.0457, 167.0351	Vanillin hexoside or its isomer	0.166
8	2.59	188.0706	$C_{11}H_9NO_2$	$[M+H]^-$	146.0601, 118.0652	3-Indoleacrylic acid	0.079
9	2.69	577.1354	$C_{30}H_{26}O_{12}$	$[M-H]^-$	425.0873, 407.0764, 289.0715, 125.0242	Proanthocyanidin B or its isomer	0.278
10	2.72	579.1494	$C_{30}H_{26}O_{12}$	$[M+H]^-$	407.0770, 289.0718, 125.0244	Vitexin 2”-O-p-coumarate	−0.609
11	2.84	451.1232	$C_{21}H_{24}O_{11}$	$[M-H]^-$	289.0714	Catechin hexoside	−0.258
12	3.01	289.0718	$C_{15}H_{14}O_6$	$[M-H]^-$	245.0812, 205.0495, 123.0448, 109.0291	Catechin or its isomer	0.064
13	3.04	289.0710	$C_{15}H_{14}O_6$	$[M-H]^-$	245.0812, 205.0498, 151.0394, 123.0448, 109.0292	Epicatechin	−2.807
14	3.06	137.0245	$C_7H_6O_3$	$[M-H]^-$	119.0140, 108.0219, 91.0191	Protamine sulfates	0.676
15	3.2	137.0247	$C_7H_6O_3$	$[M-H]^-$	93.0346, 65.0398	4-hydroxybenzhydrazide	1.379
16	3.31	577.1351	$C_{30}H_{26}O_{12}$	$[M-H]^-$	425.0873, 407.0764, 289.0715, 125.0242	Procyanidin B	0.278
17	3.34	579.1494	$C_{30}H_{26}O_{12}$	$[M-H]^-$	407.0770, 289.0718, 125.0244	Vitexin 2”-O-p-coumarate	−0.384
18	3.81	289.0718	$C_{15}H_{14}O_6$	$[M+H]^-$	245.0812, 205.0495, 123.0448, 109.0291	Catechin	0.023
19	4.11	865.1987	$C_{45}H_{38}O_{18}$	$[M-H]^-$	695.1429, 577.1353, 425.0874, 287.0562	Procyanidin C	0.153
20	4.39	577.1354	$C_{30}H_{26}O_{12}$	$[M-H]^-$	425.0873, 407.0764, 289.0715, 125.0242	Proanthocyanidin B or its isomer	0.504
21	4.58	577.1354	$C_{30}H_{26}O_{12}$	$[M-H]^-$	425.0873, 407.0764, 289.0715, 125.0242	Proanthocyanidin B or its isomer	0.504
22	4.73	163.0400	$C_9H_8O_3$	$[M-H]^-$	119.0502, 93.0347	Cis-4-coumaric acid	−0.291
23	4.94	463.0884	$C_{21}H_{20}O_{12}$	$[M-H]^-$	300.0277, 271.0249, 243.0295, 151.0039	Isoquercitrin	0.326
24	5.37	447.0939	$C_{21}H_{20}O_{11}$	$[M-H]^-$	300.0278, 271.0252, 255.0303, 243.0299, 151.0040	Quercitrin	0.281
25	10.46	318.3001	$C_{18}H_{39}NO_3$	$[M+H]^-$	256.2636, 203.0854	2-Amino-1,3,4-octadecanetriol	−0.505
26	11.08	415.2114	$C_{24}H_{30}O_6$	$[M+H]^-$	203.0855, 119.0855	Bis (4-ethylbenzylidene) sorbitol	−0.518

Abbreviations: ESI-MS_2: Electrospray ionization tandem mass spectrometry; LC-MS: Liquid chromatography–mass spectrometry; SR: *Amomum villosum Lour*.; t_R: Retention time.

Table S8. Identified nonvolatile compounds in TX based on LC-MS

No.	t_R (min)	Mass (ppm)	Formula	Selected ion	ESI-MS²	Compound name	Error (ppm)
1	1.29	165.0560	$C_9H_{10}O_3$	[M-H]⁻	150.0325, 122.0376, 93.0348	Acetovanillone	1.359
2	2.42	153.0559	$C_8H_{10}O_3$	[M-H]⁻	123.0454, 109.0297	Syringol	1.299
3	3.62	151.0402	$C_8H_8O_3$	[M-H]⁻	136.0167	Vanillin	0.944
4	4.17	123.0453	$C_7H_8O_2$	[M-H]⁻	108.0218	Guaiacol	1.214
5	4.86	431.0999	$C_{21}H_{20}O_{10}$	[M-H]⁻	341.0645, 311.0563, 228.1595, 203.0871	Vitexin	3.572
6	5.07	199.1481	$C_{15}H_{18}$	[M+H]⁻	157.1010, 143.0855	Guaiazulene	−0.035
7	5.19	415.1001	$C_{21}H_{20}O_9$	[M-H]⁻	289.0714,109.0294	Chrysin-8-C-glucoside	−1.538
8	5.20	219.1743	$C_{15}H_{22}O$	[M+H]⁻	203.0855	Anaephene A	−0.100
9	5.22	415.1001	$C_{21}H_{20}O_9$	[M-H]⁻	289.0714,109.0294	Chrysin-6-C-glucoside	−2.259
10	5.34	447.0944	$C_{21}H_{20}O_{11}$	[M-H]⁻	332.0857, 228.1654, 203.0869	Orientin	2.472
11	5.38	447.0944	$C_{21}H_{20}O_{11}$	[M-H]⁻	332.0857, 228.1654, 203.0869	Isoorientin	0.773
12	5.52	345.1345	$C_{19}H_{22}O_6$	[M-H]⁻	297.0768, 256.0382	Cedrusin	1.096
13	5.62	195.0665	$C_{10}H_{12}O_4$	[M-H]⁻	180.0429, 162.0323	Acetosyringone	0.963
14	5.65	359.1500	$C_{20}H_{24}O_6$	[M-H]⁻	223.0979, 180.0793, 135.0454	Dihydrodehydroconiferyl alcohol	0.385
15	5.67	177.0559	$C_{10}H_{10}O_3$	[M-H]⁻	162.0324	Coniferaldehyde	0.240
16	6.06	431.0999	$C_{21}H_{20}O_{10}$	[M-H]⁻	341.0645, 311.0563, 228.1595, 203.0871	Isovitexin	3.572
17	8.35	201.1638	$C_{15}H_{20}$	[M+H]⁻	159.1168, 145.1012	Hexahydrodibenzsuberane	−0.036
18	8.70	219.1743	$C_{15}H_{22}O$	[M+H]⁻	203.0855	Anaephene A isomer	−0.054
19	10.80	203.1794	$C_{15}H_{22}$	[M+H]⁻	131.0703, 83.0493	Cis-calamenene	−2.820
20	11.05	255.1955	$C_{15}H_{26}O_3$	[M+H]⁻	203.0856, 131.0704, 83.0492	Isocadinanol A	0.152
21	11.50	415.2114	$C_{24}H_{30}O_6$	[M+H]⁻	203.0855, 119.0855	Bis (4-ethylbenzylidene) sorbitol	−0.227

Abbreviations: ESI-MS_2: Electrospray ionization tandem mass spectrometry; LC-MS: Liquid chromatography–mass spectrometry; TX: *Santalum album L.*; t_R: Retention time

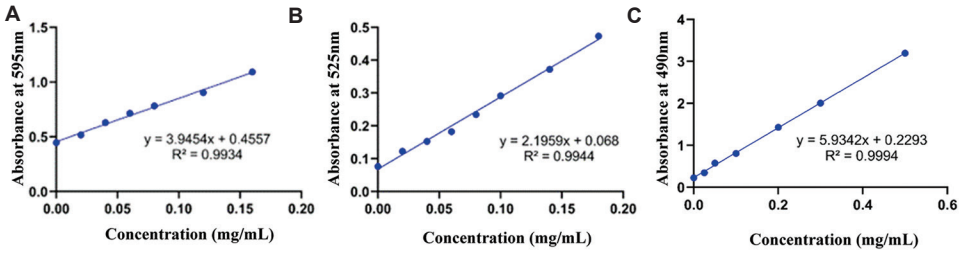

Figure S2. Standard curves for quantification. (A) Linear standard curve of glucose for total sugar analysis. (B) Linear standard curve of galacturonic acid for uronic acid determination. (C) Linear standard curve of bovine serum albumin or protein analysis