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The analysis of 15 inorganic elements across 8 components in Chuanxiong Cha Tiao San

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ABSTRACT

This resarch aims to study the characteristics of fifteen inorganic elements in eight components of Chuanxiong Cha Tiao San by the ICP-MS method. An ICP-MS method is established to determine the content of 15 inorganic elements in the 8-component medicines of Chuanxiong Cha Tiao San. A characteristic profile for these 15 inorganic elements in the medicines is created. We use SIMCA-PCA to analyze the differences among the 8 components medicines, and principal component analysis (PCA) is also employed to identify the common inorganic elements responsible for the wind-dispelling and pain-relieving effects of Chuanxiong, Qianghuo, Baizhi, Xixin, Jingjie, Fangfeng, and Bohe. The Student-Newman-Keuls is used to compare the differences in the common efficacy-related inorganic elements among these 7 herbs. We found that the characteristic profile of fifteen inorganic elements in the eight component medicine of Chuanxiong Cha Tiao San are strongly defined. From SIMCA-PCA, the 3D scatter plot shows a significant difference between Licorice and the other 7 herbs. By analysising the main component, it indicates that the common inorganic elements contributing to the wind-dispelling and exterior-releasing effects of Chuanxiong, Qianghuo, Baizhi, Xixin, Jingjie, Fangfeng, and Bohe are Mg, K, and S. Among the 7 herbs, the differences in Mg and S were not statistically significant, while the difference in K was statistically significant. From this research, we can know that the ICP-MS method is accurate, reliable and reproducible, the difference in the inorganic element profiles among the 8 components is significant, and the common efficacy-related inorganic elements is Mg, K and S.

Keywords: Chuanxiong Cha Tiao San; component medicine; inorganic elements; fingerprint; principal component analysis; inorganic elements of common efficacy

Chuanxiong Cha Tiao San was first published in "Tai Ping Hui Min He Ji Ju Fang", by Chuan Xiong. Notopterygium. Angelica dahurica. Windproof Asarum. Mint. Herba schizonepetae. Licorice consists of 8 herbs, mainly for headache caused by exogenous wind evil. Aversion to cold. Fever. Nasal congestion[1] is a classic prescription of traditional Chinese medicine for the clinical treatment of exogenous wind evil headache[2].

Inorganic elements have many functions. They have a strong ability to form complexes and are easy to interact with nitrogen contained in organisms. Oxygen. Sulfur ligands form coordination bonds, coordinate the material balance in the body, and inorganic elements have a certain synergistic effect on the exertion of drug efficacy[3–5]. Current research shows that the content of inorganic elements. Species can affect the nature, taste and efficacy of traditional Chinese medicine. In the traditional Chinese medicine compound, there may be differences in the types and contents of inorganic elements in the tastes with different properties, tastes and effects, while the tastes with similar taste effects may have similarities in the types of inorganic elements. As the basis of efficacy, the difference of inorganic element content may lead to the strength of efficacy[6–8].

According to the classification of traditional Chinese medicine, among the eight constituent drugs of Chuanxiong Tea-Tiao Powder, there are seven exterior relieving drugs (dispelling wind and relieving pain) and one tonic drug (reconciling various drugs), indicating that there may be differences in the composition of inorganic elements, while the drugs with similar effects may have common inorganic elements. Chuanxiong Tea-Tiao Powder is a mixture of different medicinal powders. Without extraction and other processes, the efficacy of the medicinal flavor is strongly related to the compound.

At present, there is no research on the inorganic elements of Chuanxiong tea. Therefore, starting from the eight components of Chuanxiong Cha Tiao San, this study established an ICP-MS method to determine the content of 15 inorganic elements, studied the characteristic Atlas of inorganic elements of the eight components of Chuanxiong Tea-Tiao Powder, and analyzed Chuanxiong. Notopterygium. Angelica dahurica. Asarum. Herba schizonepetae. Windproof Based on the differences of 15 inorganic elements between mint and licorice, Ligusticum chuanxiong was screened by principal component analysis. Notopterygium. Angelica dahurica. Asarum. Herba schizonepetae. Windproof Peppermint exerts the common effect inorganic elements of dispelling wind and relieving pain, and defines the differences between the common effect inorganic elements of different medicinal flavors, in order to provide a research basis for the clinical application of Chuanxiong Tea-Tiao Powder.

1. Instruments and reagents

Cemmars_6 microwave digestion instrument (German Berghof company); 7900 inductively coupled plasma mass spectrometry (ICP-MS, Agilent); bas_2245 electronic analytical balance (Germany sedoli company); DHG-9013a electric blast drying oven (Shanghai Yiheng Instrument Co., Ltd.); milli-Q ultra pure water machine (milliporebedfordma, USA).

Spexertificate15 standard solutions contain B. Na. Mg. Al. K. Ca. Mn. Fe. Co. Ni. Cu. Zn. As. Se. Cd. BA (batch No. 2-192AB, SPEX, USA), mass concentration 1000 μg/mL; internal standard solution: ^{73}Ge (batch number GSB04-1728-2004), ^{115}In (batch number gsb04-1731-2004), Single element standard solution (1000 μG/mL)of ^{209}Bi (batch number GSB04-1719-2004), purchased from the national reference material research center of the Chinese Academy of metrology; the concentrated nitric acid is MOS grade (Tianjin kemio Chemical Reagent Co., Ltd.).

40 samples were collected from the Lotus Chi Chinese Medicinal Materials Market in Chengdu, Sichuan Province. The samples were collected from the Chinese herbal medicine market in Puning City, Guangdong Province. See **Table 1** for the source information of the samples. The samples were identified as the dried rhizome of Ligusticum chuanxiong Hort., the dried rhizome of Notopterygium incisum Ting ex H.T.Chang, the dried rhizome of the Umbelliferae plant, Notopterygium incisum Ting ex H.T.Chang, and the dried rhizome of the Umbelliferae plant. Dried roots and rhizomes of Angelica dahurica (Fisch.ex Hoffm.) Benth.et Hook.f., Aristolochiaceae Asarum heterotropodes Fr.Schmidt var. mandshurica (Maxim.)Kitag. Dried aerial parts of Schizonepeta tenuifolia Briq., Umbelliferae Sposhnikovia divaricata (Turcz.) Schischk., Dried aerial parts of

Lamiaceae Mentha haplocalyx Briq., Legume Glycyrrhiza uralensis Dried roots and rhizomes of Fisch.

Table 1. Sample information of 8 components of Chuanxiong Cha Tiao San.

Number	Product name	Collection location	Collection time
CX-1, CX-2	Rhizome of chuanxiong	Sichuan Chengdu lotus pond traditional Chinese medicine market	2019. 04
CX-3, CX-4, CX-5	Rhizome of chuanxiong	Puning traditional Chinese medicine market, Guangdong Province	2019. 04
QH-1, QH-2	Notopterygium	Lotus Pond Traditional Chinese Medicine Market in Chengdu, Sichuan Province	2019. 04
QII-3, QH-4, QH-5	Notopterygium	Puning traditional Chinese medicine market, Guangdong Province	2019. 04
BZ-1, BZ-2	Angelica dahurica	Lotus Pond Traditional Chinese Medicine Market in Chengdu, Sichuan Province	2019. 04
BZ-3, BZ-4, BZ-5	Angelica dahurica	Puning traditional Chinese medicine market, Guangdong Province	2019. 04
XX-1, XX-2	Asarum	Lotus Pond Traditional Chinese Medicine Market in Chengdu, Sichuan Province	2019. 04
XX-3, XX-4, XX-5	Asarum	Puning traditional Chinese medicine market, Guangdong Province	2019. 04
JJ-1, JJ-2	Herba schizonepetae	Lotus Pond Traditional Chinese Medicine Market in Chengdu, Sichuan Province	2019. 04
JJ-3, JJ-4, JJ-5	Herba schizonepetae	Puning traditional Chinese medicine market, Guangdong Province	2019. 04
FF-1, FF-2	Windproof	Lotus Pond Traditional Chinese Medicine Market in Chengdu, Sichuan Province	2019. 04
FF-3, FF-4, FF-5	Windproof	Puning traditional Chinese medicine market, Guangdong Province	2019. 04
BH-1, BII-2	Mint	Lotus Pond Traditional Chinese Medicine Market in Chengdu, Sichuan Province	2019. 04
BII-3, BH-4, BH-5	Mint	Puning traditional Chinese medicine market, Guangdong Province	2019. 04
GC-1, GC-2	Licorice	Lotus Pond Traditional Chinese Medicine Market in Chengdu, Sichuan Province	2019. 04
GC-3, GC-4, GC-5	Licorice	Puning traditional Chinese medicine market, Guangdong Province	2019. 04

2. Method

2.1. Sample pretreatment

0.2 g (80 mesh) of the sample powder is accurately weighed, placed in a polytetrafluoroethylene digestion tank, placed in a fume hood, added 8mL of concentrated nitric acid, and placed overnight. On the second day, it was put into the microwave digestion instrument and treated according to the set digestion procedure: first, it was heated from room temperature to 130 ℃ in 10 min and maintained for 5 min digestion, then it was heated from 130 ℃ to 165 ℃ in 10 min and maintained for 10 min digestion, and then it was heated from 165 ℃ to 180 ℃ in 15 min and maintained for 30 min digestion. After digestion, cool to room temperature, take out the digestion tank, volatilize the acid in the fume hood, and add deionized water to fix the volume to 50 mL. Simultaneously conduct blank test with 8 mL concentrated nitric acid without adding samples.

2.2. Optimization of determination conditions

The instrument automatically tunes and sets working parameters to improve sensitivity. Background. Stability and other indicators to optimize the working parameters of the instrument. Measurement conditions: plasma RF power: 1550 W, plasma gas: 15 l/min, auxiliary gas flow: 1 l/min, atomization gas flow: 1 l/min, compensation/dilution gas: 1 l/min, atomization chamber temperature: 2 °C, peristaltic pump speed: 0.3 rps. Integration time: 1 s, delay time: 1 s, repetition times: 3 times. Measurement method: standard curve method, reading method: peak intensity. ^{73}Ge, ^{115}In, ^{209}Bi is the internal standard, which can effectively overcome the drift of the instrument signal and correct the matrix effect by monitoring the change of the signal.

2.3. Preparation of standard curve

Take B. Na. Mg. Al. K. Ca. V. Cr. Mn. Fe. Co. Ni. Cu. Zn. As. Se. Sr. Cd. Mixed standard mother liquor of Ba, use 10% HNO_3 as blank solution, and dilute the mother liquor to 5, 10, 20, 50, 100 μg/mL.

Prepare the standard solution according to the level of the elements to be tested in the sample, successively determine the series mass concentration standard solution of 15 inorganic elements, and add ^{73}Ge, ^{115}In, ^{209}Bi internal standard solution and prepare standard blank solution at the same time. Take the mass concentration of the standard as the abscissa (x), and the ratio of the analytical peak signal value of the element to be tested to the reference peak response value of the internal standard element as the ordinate (y), draw the standard curve, and obtain the regression equation of each element standard. Correlation coefficient and linear range. The Results shows that the linearity of each element with the ratio in the concentration range of 0–100 μg/L was good, see **Table 2** for details.

Table 2. Linear regression equations of 15 inorganic elements. Correlation coefficient. Detection limit and linear range.

Element	Regression equation	R	Detection limit (μg/mL)	Linear range (μg/mL)
B	$Y = 0.1138X + 0.0711$	0.9992	0.0609	0–100
Mg	$Y = 1.3332X + 0.1325$	0.9996	0.0123	0–100
A$_1$	$Y = 0.0607X + 0.0010$	0.9992	0.0066	0–100
S	$Y = 1.8718 \times 10^{-4}X + 0.0023$	0.9991	0.4192	0–100
K	$Y = 0.1542X + 0.0087$	0.9999	0.0111	0–100
Ca	$Y = 0.0046X + 2.2888 \times 10^{-4}$	0.9999	0.0241	0–100
Mn	$Y = 2.0325X + 0.0154$	0.9998	0.0009	0–100
Fe	$Y = 4.5207X + 0.0802$	1.0000	0.0142	0–100
Co	$Y = 14.5814X + 00172$	0.9996	0.0004	0–100
Cu	$Y = 10.7285X + 0.0369$	0.9990	0.0006	0–100
Zn	$Y = 0.8232X + 0.0520$	0.9998	0.0043	0–100
As	$Y = 0.6339X + 0.0012$	0.9999	0.0004	0–100
Se	$Y = 0.0206X + 5.6313 \times 10^{-5}$	0.9997	0.0025	0–100
Cd	$Y = 0.1848X + 2.94618 \times 10^{-4}$	0.9994	0.0004	0–100
Ba	$Y = 0.1401X + 4.80818 \times 10^{-4}$	1.0000	0.0007	0–100

2.4. Methodological review

2.4.1. Precision test

Take the mixed standard solution and inject it for 6 consecutive times to determine the content of elements. The RSD value of the content of 15 inorganic elements is 0.45%–2.30%, indicating that the precision of the instrument is good.

2.4.2. Stability test

Take the same portion containing Ligusticum chuanxiong. Notopterygium. Angelica Asarum.Herba schizonepetae.windproof Mint. Put the liquorice sample solution to be tested at 0, 4, 8, 12, 16, 20. After 24 h, the contents of 15 elements were determined, and the RSD values were respectively 0.65%–2.15%, 0.62%–2.31%, 0.59%–2.01%, 0.76%–2.12%, 0.76%–1.78%, 0.68%–2.09%, 0.76%–1.83%, 0.78%–2.87%, indicating that the solution to be tested is stable within 24 h. The results are shown in **Table 3**.

Table 3. Methodological investigation of 8 components of Chuanxiong Cha Tiao San (%).

Element	RSD	Rhizome of chuanxiong					Notopterygium			
		RSD		Sample recovery			RSD		Sample recovery	
	Precision	Stability	Repeatability	Mean value	RSD		Stability	Repeatability	Mean value	RSD
B	0.65	0.88	0.45	97.10	2.64		0.68	1.82	101.42	3.12
Na	0.98	0.92	0.71	96.21	1.98		1.22	1.01	100.98	2.93
Mg	1.20	0.56	1.33	100.29	1.73		1.34	0.89	98.48	1.89
Al	0.75	1.22	1.04	101.24	3.01		1.29	0.92	99.29	2.67
S	1.33	1.12	0.93	103.47	2.54		0.98	1.92	96.53	2.53
K	0.45	0.73	1.03	100.57	1.35		0.62	1.75	95.26	1.94
Ca	0.98	0.65	0.97	98.34	3.15		0.99	1.39	97.33	2.33
Mn	1.26	1.68	1.07	98.76	2.98		1.97	2.33	97.45	1.45
Fe	0.94	1.54	1.21	97.99	2.76		2.11	2.10	101.29	2.39
Cu	0.57	2.15	1.89	95.98	3.99		1.76	2.80	103.58	3.19
Zn	1.02	0.59	0.71	96.33	3.76		1.87	1.92	104.32	3.29
As	1.62	1.48	1.97	98.49	3.64		2.31	1.49	101.34	2.98
Se	2.10	1.88	1.65	102.04	2.10		1.93	1.94	95.89	1.49
Cd	2.30	1.92	1.29	103.41	2.03		1.87	2.11	102.35	2.01
Ba	1.08	2.10	1.77	101.26	1.65		2.19	1.87	100.92	1.78

Element	RSD	Angelica dahurica					Asarum			
		RSD		Sample recovery			RSD		Sample recovery	
	Precision	Stability	Repeatability	Mean value	RSD		Stability	Repeatability	Mean value	RSD
B	0.65	1.01	2.11	99.19	2.97		1.27	2.09	96.28	3.56
Na	0.98	0.92	1.46	97.32	3.01		1.02	2.11	95.88	2.47
Mg	1.20	0.87	2.08	102.08	1.63		1.08	1.96	101.34	1.98
Al	0.75	1.34	1.07	100.32	1.96		0.76	1.75	100.02	2.01
S	1.33	1.09	1.96	100.98	2.19		0.88	2.30	103.45	1.86
K	0.45	0.81	1.47	98.23	1.99		1.97	2.01	98.28	1.77
Ca	0.98	0.92	1.88	102.89	2.71		1.29	1.86	102.38	2.81
Mn	1.26	1.32	2.05	96.33	1.68		1.49	1.98	104.39	1.38
Fe	0.94	1.45	2.31	98.25	2.38		1.30	2.79	97.34	2.05
Cu	0.57	1.28	1.87	101.29	3.09		0.77	2.69	96.33	1.90
Zn	1.02	0.59	1.59	103.19	3.18		0.89	2.37	99.54	2.33
As	1.62	1.98	2.87	98.34	2.70		1.28	0.98	103.20	3.68
Se	2.10	2.01	2.98	95.64	1.69		2.01	1.28	102.10	2.96
Cd	2.30	1.39	2.30	101.22	3.28		2.12	1.77	98.32	1.78

Ba	1.08	1.78	1.57	103.68	2.69	1.59	1.49	95.69	2.05

Element	Herba schizonepetae				Windproof			
	RSD		Sample recovery		RSD		Sample recovery	
	Stability	Repeatability	Mean value	RSD	Stability	Repeatability	Mean value	RSD
B	1.33	2.11	102.34	2.89	1.09	1.89	102.09	2.89
Na	0.97	2.07	101.22	2.01	0.87	2.49	97.33	1.78
Mg	1.37	1.65	98.34	1.95	0.84	3.19	98.29	1.49
Al	0.78	1.38	97.49	1.33	0.69	2.05	95.33	3.01
S	1.32	1.98	99.87	2.08	1.43	2.09	99.39	2.79
K	1.66	2.06	95.34	1.58	1.28	1.59	103.24	2.66
Ca	1.39	1.49	101.23	2.37	0.68	1.49	100.98	3.05
Mn	1.51	1.27	104.07	1.83	1.12	1.88	104.39	1.97
Fe	1.02	1.84	97.65	1.76	1.29	2.09	101.28	1.43
Cu	1.78	2.05	99.86	1.49	1.98	2.33	97.39	2.49
Zn	1.67	1.48	101.29	2.09	0.89	2.49	98.49	3.98
As	1.29	1.39	103.49	1.39	1.58	1.29	101.29	2.69
Se	0.76	1.68	97.93	1.74	1.93	1.59	95.89	1.78
Cd	0.98	1.86	98.78	1.09	2.09	1.28	95.33	2.59
Ba	1.24	0.99	102.39	2.33	1.77	1.58	102.39	3.07

Element	Mint				Licorice				
	RSD		Sample recovery		RSD		Sample recovery		
	Stability	Repeatability	Mean value	RSD	Stability	Repeatability	Mean value	RSD	
	0.97	2.03	103.22	2.18	0.78	2.87	95.69	3.06	0.97
	1.32	2.33	101.28	3.09	1.44	3.45	97.39	2.87	1.32
	1.83	1.58	97.34	4.01	1.82	3.01	103.42	3.96	1.83
	0.76	1.67	96.59	3.28	2.33	1.59	101.29	3.19	0.76
	1.26	2.32	98.49	2.19	1.89	1.49	97.77	1.89	1.26
	1.19	1.78	101.39	1.87	1.23	1.98	98.39	3.78	1.19
	0.89	1.68	102.59	1.39	1.49	1.25	96.49	2.58	0.89
	1.52	2.33	95.38	2.43	2.87	1.09	102.39	2.45	1.52
	1.23	3.19	97.68	1.28	0.99	3.23	99.34	1.39	1.23
	1.76	1.49	102.69	2.65	1.49	1.68	103.24	3.45	1.76
	0.79	2.71	97.66	2.55	1.02	2.07	95.39	2.67	0.79
	1.45	2.45	98.34	2.31	2.56	2.19	97.19	3.48	1.45
	1.29	1.68	99.30	1.69	1.44	2.67	101.29	2.87	1.29
	0.79	2.18	96.28	2.48	1.98	1.89	98.39	1.98	0.79
	1.82	1.39	104.29	2.19	0.98	1.77	97.65	2.48	1.82

2.4.3. Repeatability test

Weigh Ligusticum chuanxiong accurately. Notopterygium. Angelica dahurica. Asarum. Herba schizonepetae. Windproof Mint. Six samples of licorice were made into the test solution, and the contents of 15 elements were determined. The RSD values were respectively 0.45%–1.97%, 0.89%–2.80%, 1.07%–2.98%, 0.98%–2.79%, 0.99%–2.11%, 1.28%–3.19%, 1.39%–2.71%, 0.78%–2.87%, indicating that the repeatability

of the method is good. The results are shown in **Table 3**.

2.4.4. Sampling recovery test

Precisely weigh 0.2 g of the samples of Chuanxiong, Qianghuo, Angelica, Asarum, Nepeta, Fangfeng, Mint and Licorice with the determined contents respectively, a total of 6 samples, add a certain amount of standard solution of each element accurately, and then determine the content, calculate 15. The recoveries of the elements were 95.98%–103.47%, 95.89%–104.32%, 95.64%–103.68%, 95.69%–104.39%, 95.34%–104.07%, 95.33%–104.39%, 95.38%–104.29%, 95.39%, respectively. ~103.42%, RSD values were 1.35%–3.99%, 1.45%–3.29%, 1.63%–3.28%, 1.38%–3.56%, 1.33%–2.89%, 1.43%–3.98%, 1.28%–4.01%, 1.39%–3.78%, indicating that the recovery rate of the method meets the requirements. The results are shown in **Table 3**.

2.5. Determination of samples

Prepare Ligusticum chuanxiong according to the method under "2.1". Notopterygium. Angelica dahurica. Asarum. Herba schizonepetae. Windproof Mint. The content of 15 inorganic elements in the test solution of licorice sample was determined under the set experimental conditions. The contents of 15 inorganic elements in 40 samples are shown in **Table 4**.

Table 4. Contents of 15 inorganic elements in 8 components of Chuanxiong Cha Tiao San (mg/kg).

No.	B	Na	Mg	Al	S	K	Ca	Mn	Fe	Cu	Zn	As	Se	Cd	Ba
CX-1	66.05	1323.12	6516.11	639.52	2788.30	8389.08	374.67	59.04	413.35	11.44	43.94	0.24	0.20	0.56	27.36
CX-2	75.76	2782.06	6365.89	156.94	2498.14	9140.33	278.99	28.73	60.44	9.61	43.97	0.21	0.04	0.78	13.35
CX-3	144.89	2485.51	11,782.73	191.71	10,719.65	7745.64	271.54	32.74	92.01	9.43	28.87	0.24	0.06	0.42	10.78
CX-4	63.49	3177.47	6812.28	139.63	2496.43	8855.76	257.92	49.16	32.93	9.44	25.50	0.17	0.08	0.49	11.53
CX-5	47.54	2882.67	5940.69	146.71	2356.39	7846.41	252.88	44.05	51.01	9.84	40.40	0.15	0.07	0.59	11.32
QH-1	73.06	580.23	7370.92	1176.66	1525.86	7405.57	386.43	52.92	1079.64	6.65	19.99	0.59	0.36	0.14	14.55
QH-2	80.99	180.64	9671.62	283.06	1833.17	7270.34	356.53	30.48	244.73	8.11	21.31	0.15	0.09	0.25	11.91
QH-3	63.43	2444.52	74,641.76	727.50	34,850.52	7422.65	301.08	76.85	724.40	6.45	18.64	0.50	0.42	0.16	37.51
QH-4	84.93	872.92	7709.50	639.43	4091.30	8003.25	393.44	39.46	756.71	8.12	16.47	0.73	0.17	0.14	16.02
QH-5	90.89	323.76	8186.34	355.71	1681.45	7461.56	353.88	34.94	434.82	7.46	17.84	0.29	0.10	0.14	13.21
BZ-1	45.77	472.91	4438.63	489.66	5668.89	6928.94	196.64	28.84	253.43	6.65	38.80	0.21	0.16	0.05	7.33
BZ-2	46.40	886.15	4064.33	259.46	1109.06	7370.14	139.23	12.94	222.73	6.95	12.36	0.12	0.07	0.03	6.01
BZ-3	30.20	915.89	3825.45	371.76	6351.09	5743.90	165.12	24.17	224.71	6.83	11.44	0.25	0.23	0.02	5.68
BZ-4	40.96	522.99	4006.06	237.09	1116.22	7852.84	166.58	15.91	89.45	7.88	12.95	0.15	0.05	0.02	5.68
BZ-5	51.77	693.43	4217.63	151.59	1166.23	7567.42	153.79	12.56	67.81	7.49	10.19	0.12	0.02	0.02	4.68
XX-1	57.05	127.49	6515.72	1016.09	5775.77	9287.17	249.65	180.23	931.82	21.21	75.36	0.36	0.79	1.94	25.79
XX-2	56.41	157.32	5927.85	824.20	3027.29	7375.21	252.01	197.99	588.97	8.60	45.42	0.24	0.38	1.24	29.60
XX-3	50.70	98.22	5933.34	1480.65	4956.57	6944.05	230.99	299.07	1282.34	5.98	37.80	0.41	0.24	1.18	41.02
XX-4	67.93	69.41	5574.49	887.85	2635.21	7015.42	258.09	236.80	1112.14	6.97	39.45	0.61	0.24	0.98	38.18
XX-5	56.15	96.77	4619.16	751.90	2326.45	6404.08	240.86	146.58	585.27	4.52	34.46	0.25	0.18	0.52	31.57
JJ-1	90.69	169.10	14,267.62	588.21	2754.45	16,274.06	923.99	24.29	215.47	12.27	28.55	0.43	0.23	0.06	71.67
JJ-2	95.74	328.96	12,723.69	354.05	2037.21	18,806.02	972.43	15.17	493.14	10.88	24.69	0.39	0.21	0.10	89.67
JJ-3	75.71	45.27	10038.02	262.99	2230.68	13,496.11	796.52	16.23	247.27	12.93	26.00	0.18	0.12	0.03	48.24
JJ-4	59.89	108.03	9561.46	38.11	976.01	12,349.14	538.00	5.94	67.84	7.03	6.12	0.09	0.02	0.05	75.60
JJ-5	74.63	370.60	12,970.24	259.28	1329.06	13,878.10	862.43	14.95	358.00	7.56	9.76	0.19	0.14	0.09	93.78

FF-1	109.50	1498.59	5576.70	297.86	1755.54	13,904.00	296.51	13.51	182.20	11.73	27.36	0.16	0.11	0.26	30.42
FF-2	109.29	1412.59	7314.36	767.64	1529.95	6997.65	603.28	25.70	570.45	8.23	29.92	0.33	0.31	0.01	50.55
FF-3	75.96	1266.87	1266.87	510.07	1773.35	9560.27	267.01	19.61	161.33	11.74	21.38	0.29	0.18	0.07	21.78
FF-4	103.24	3265.33	8341.94	1030.27	1842.84	9079.74	490.48	32.83	787.99	11.47	38.26	0.49	0.37	0.06	34.18
FF-5	101.97	2197.93	7769.00	704.02	1931.39	9759.29	466.01	26.32	499.52	11.44	40.12	0.33	0.33	0.12	53.63
BH-1	79.87	136.99	11,683.37	322.84	3478.29	13,870.85	1336.77	53.99	426.19	10.05	26.43	0.21	0.16	0.02	23.84
BH-2	80.58	176.72	12,920.66	359.59	2999.12	13,192.29	1345.68	146.06	354.41	10.33	27.51	0.19	0.12	0.06	25.54
BH-3	60.92	308.71	12,813.75	3120.64	2835.06	16,043.41	971.02	190.20	2201.34	9.23	34.64	0.91	0.91	0.13	43.52
BH-4	106.83	102.07	12,415.73	369.82	3166.31	14,044.77	1632.02	38.29	382.82	9.70	22.78	0.21	0.11	0.08	28.05
BH-5	97.51	600.25	13,675.55	283.70	2259.60	17,057.70	1314.80	139.19	345.08	10.08	17.62	0.23	0.08	0.11	40.14
GC-1	58.32	550.11	6022.75	48.12	2744.96	5486.57	335.12	7.63	60.53	4.84	10.72	0.07	-	-	1.23
GC-2	76.09	1460.50	7239.21	185.49	1133.08	6342.10	649.09	10.95	215.26	6.41	12.83	0.10	0.08	0.01	1.87
GC-3	76.28	614.75	6734.88	69.09	2866.85	6439.96	335.58	9.05	113.44	6.36	12.87	0.11	0.10	-	1.39
GC-4	89.36	1258.48	8075.82	54.23	1124.87	6385.29	429.43	10.74	76.81	7.16	11.62	0.09	-	-	1.20
GC-5	90.69	1135.79	8417.03	98.77	1033.42	6937.32	733.24	9.91	121.69	6.90	7.00	0.12	0.01	0.01	2.17

Note: "-" is not detected.

3. Results and analysis

3.1. Establishment of characteristic maps of 15 inorganic elements in 8 constituent medicines

Calculate the average value of each inorganic element of each flavor and the average value of each inorganic element in 40 samples respectively, then calculate the ratio of the average value of each inorganic element of each flavor to the average value of each inorganic element in 40 samples, and draw the broken line diagram of 15 inorganic elements of each flavor as the characteristic map. It can be seen that there are great differences in the characteristic maps of inorganic elements between different drug flavors. See **Figure 1** for the results.
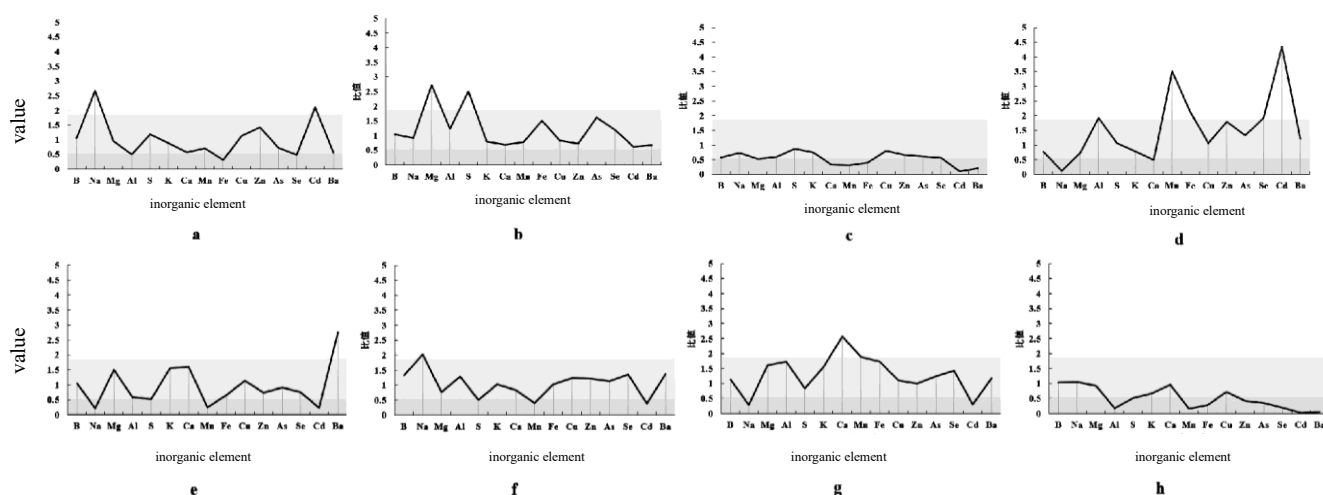

Figure 1. Characteristic Atlas of inorganic elements of different medicinal flavors, **(a)** Ligusticum chuanxiong; **(b)** Notopterygium; **(c)** Angelica dahurica; **(d)** Asarum; **(e)** Schizonepeta; **(f)** Fangfeng; **(g)** Mint; **(h)** Licorice.

3.2. SIMCA-PCA analysis of eight components of Chuanxiong tea Tiao powder

The results of 40 samples were substituted into SIMCA14.1 software for pca-x analysis. Select the first two principal components, R^2X is 0.412, Q^2 is 0.15, and the Score Scatter 3D Plot is obtained. The results are shown in **Figure 2**. It can be seen from the figure that there are obvious differences between the five licorice samples and the other seven drugs, indicating that there are great differences in 15 inorganic elements between licorice and the other seven drugs, which may be due to the great differences in the efficacy of licorice and the other seven drugs. There is a cross phenomenon in the remaining seven drugs, which may be related to the similar effect of these seven drugs—dispelling wind and relieving pain.
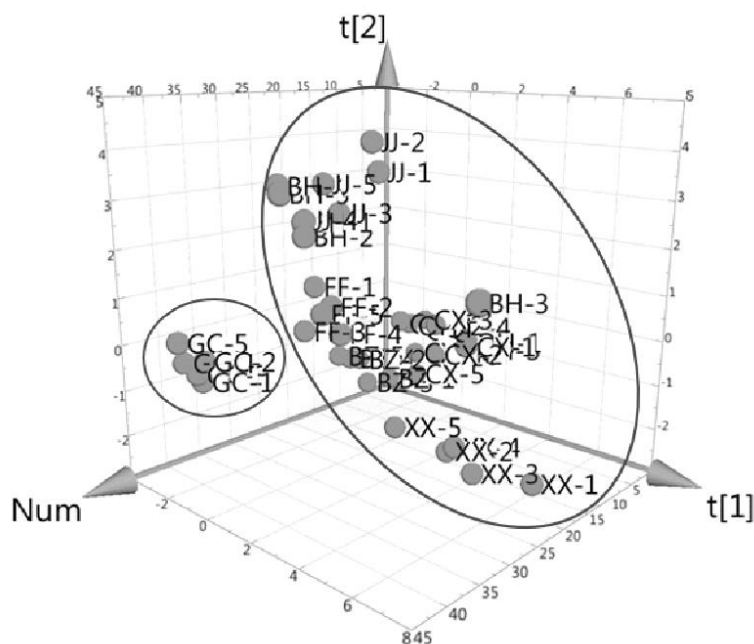

Figure 2. PCA Score Scatter 3D Plot for 40 samples.

3.3. Analysis of inorganic elements with the common effect of dispelling wind and relieving pain in Chuanxiong Cha Tiao San

Among the 8 ingredients of Chuanxiong Cha Tiao San, except licorice, the other 7 ingredients have the effect of dispelling wind and relieving exterior symptoms. It can be seen from the results under "3.2" that these seven drugs have common parts in 15 inorganic elements. To this end, Chuanxiong. Notopterygium. Angelica dahurica. Asarum. Herba schizonepetae. Windproof The content of 15 inorganic elements in peppermint was analyzed by principal component analysis to find out the common inorganic elements with the function of dispelling wind and relieving pain. Six principal components are selected to extract, and the cumulative percentage of initial eigenvalues is 89.384% (greater than 85%) and the component matrix of six principal components is obtained. Set the correlation coefficient as A, the total value of the initial eigenvalues of each component is x, and the corresponding coefficient of each component element is y, that is, $A = (\sum_1^n x\,y)/n$. Calculate the correlation coefficient between each inorganic element of each drug and the comprehensive score of principal component analysis. At the same time, calculate the average value (b) of the content of each inorganic element of 35 samples, and calculate the comprehensive score of the average value (C), $C = \sum_1^n A B$. Calculate the contribution rate (D) of each inorganic element, $D = (B \times A)/C \times 100\%$. The results are shown in **Tables 5–7**.

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Table 5. Total variance explained by principal component analysis.

Ingredients	Initial eigenvalue			Extract sum of squares load		
	Total	% of variance	Cumulative%	Total	% of variance	Cumulative%
1	4.931	32.865	32.865	4.93	32.865	32.870
2	2.754	18.363	51.228	2.754	18.363	51.225
3	2.146	14.31	65.538	2.147	14.31	65.533
4	1.783	11.866	77.404	1.78	11.866	77.419
5	1.125	7.498	84.903	1.125	7.498	84.921
6	0.671	4.482	89.384	0.672	4.482	89.392

Table 6. Composition matrix.

Element	Ingredients					
	1	2	3	4	5	6
B	0.036	0.557	0.025	0.434	−0.4	0.502
Na	−0.182	−0.218	0.319	0.646	−0.462	−0.014
Mg	0.201	0.158	0.878	0.206	0.314	0.011
Al	0.883	−0.068	0.077	−0.283	−0.282	−0.064
S	0.218	−0.148	0.848	0.285	0.308	0.020
K	0.284	0.874	−0.138	0.059	0.134	−0.126
Ca	0.128	0.844	−0.047	−0.114	0.117	0.217
Mn	0.753	−0.267	−0.137	−0.184	0.303	0.391
Fe	0.904	−0.046	0.111	−0.325	−0.192	0.062
Cu	0.405	0.256	−0.402	0.657	0.044	−0.261
Zn	0.674	−0.264	−0.361	0.492	0.067	0.019
As	0.801	0.047	0.263	−0.174	−0.365	−0.020
Se	0.906	−0.062	0.078	0.035	−0.119	−0.259
Cd	0.554	−0.495	−0.358	0.334	0.343	0.176
Ba	0.399	0.638	−0.002	0.013	0.220	−0.169

The contribution rate of 15 inorganic elements ranks in the top 3 are Mg, K, S, the contribution rate is 42.04%, 38.66%, 13.26% respectively, followed by Aal, Fe, Ca, Mn, B, Ba, Zn, Cu, As, Se, Cd, Na, Mg, K. The cumulative contribution rate of S is 94.32%, which is the main component of 15 inorganic elements, indicating that Ligusticum chuanxiong. Notopterygium. Angelica dahurica. Asarum. Herba schizonepetae. Windproof The main common inorganic element of mint is Mg, K, S. The results are shown in **Table 7**.

The location of exogenous wind chill is the lung. In the basic theory of traditional Chinese medicine, the lung governs the skin, emphasizing the correlation between the lung and the skin. Relevant literature reports that the content of Mg in the hair of rats with wind cold and deficiency invading the lung is lower than that of normal rats, indicating that Mg is closely related to the etiology and pathogenesis of exogenous wind pathogens[9]. The content of Mg in the serum of migraine patients is low. Taking $mgso_4$ can effectively alleviate migraine, indicating that Mg can treat nervous system diseases. At the same time, $mgso_4$ can act on the lungs and treat bronchial asthma, indicating that mg has a strong correlation with the efficacy of eliminating wind and relieving pain[10,11]. S is not an essential element in the body and often exists in combination with other ions. $MgSO_4$ can effectively alleviate migraine and treat bronchial asthma, indicating that s may play a therapeutic effect in the form of sulfate, that is, Mg and s have a synergistic effect. K contributes to the normal

operation of nerve conduction function, can coordinate the physiological state of the body, and is also conducive to oxygen supply to the brain, indicating that K may have a synergistic effect in alleviating migraine[12], Mg, K, S is closely related to the effect of dispelling wind and relieving pain.

Table 7. Correlation coefficients of 15 inorganic elements in 7 components of Chuanxiong Cha Tiao San. Average content. Contribution rate.

Ranking	Element	Correlation coefficient	Average value (mg/kg)	Contribution rate (%)
1	Mg	0.673	6681.89	42.05
2	K	0.614	6142.56	38.66
3	S	0.559	2106.85	13.26
4	Al	0.578	333.45	2.10
5	Fe	0.636	300.55	1.89
6	Ca	0.488	252.42	1.59
7	Mn	0.493	33.33	0.21
8	B	0.404	30.22	0.19
9	Ba	0.646	20.19	0.13
10	Zn	0.464	12.95	0.08
11	Cu	0.48	4.45	0.03
12	As	0.652	0.2	0.00
13	Se	0.703	0.15	0.00
14	Cd	0.283	0.09	0.00
15	Na	−0.032	−30.25	−0.19

3.4. Difference analysis of Mg, K and S in 7 expelling wind and analgesic flavors

In SPSS19.0 statistical software, students-Newman-Keuls in one-way ANOVA were selected to compare mg in 7 components of Chuanxiong Cha Tiao San. The difference of K. In the subset of student-Newman-Keuls with alpha = 0.05, the difference between the same subset is not statistically significant, and the difference between different subsets is statistically significant. K: Ligusticum chuanxiong Hort. Asarum. There is no significant difference in the cross phenomenon of notopterygium; herba schizonepetae. Mint. There was no significant difference between Angelica dahurica. Herba schizonepetae. Mint and windbreak.Asarum. The difference between Angelica dahurica was statistically significant, and the specific order of content was jingmustard > Mint > Fangfeng > Ligusticum chuanxiong > notopterygium > Asarum > Angelica dahurica. Mg: there was no statistically significant difference between the seven drugs, and the specific content order was notopterygium > Mint > Schizonepeta tenuifolia > Ligusticum chuanxiong > Fangfeng > Asarum > Angelica dahurica; S: The specific content order is notopterygium > Ligusticum chuanxiong > Asarum > Angelica dahurica > Schizonepeta > Mint > Fangfeng. The results are shown in **Table 8**.

Table 8. Student-Newman-keulsa analysis results.

Group	N	K			Mg	S
		Subset of alpha = 0.05				
		1	2	3	1	1
BZ	5	7092.648	4110.42	3082.2980		
XX	5	7405.186	7405.186		5714.112	3744.2580
QII	5	7512.674	7512.674		21,516.028	8796.4600

CX	5	8395.444	8395.444		7483.54	4171.7820
FF	5		9860.19		6053.774	1766.6140
BI	5			14841804	12701812	1780.6360
JJ	5			14,960.686	11,912.206	1865.4820
Significance		0216	0068	0902	0196	0473

Note: the group mean value in the same subset will be displayed. A. The harmonic mean sample size = 5.000 will be used.

4. Discussion

Among the 40 samples, although the CD content of 5 samples of Ligusticum chuanxiong is between 0.42–0.78 mg/kg, and the Cu content of 1 sample of Asarum is 21.21 mg/kg, which is not in line with the regulations (CD ≤ 0.3 mg/kg, Cu ≤ 20 mg/kg)[13]. However, due to the different dosage proportions of different medicinal flavors in Chuanxiong Cha Tiao San (Chuanxiong 16.33%, asarum 4.08%)[1], the calculated CD content of Chuanxiong is 0.08−0.13 mg/kg, and the Cu content of Asarum is 0.87 mg/kg, which meets the limit requirements. Traditional Chinese medicine serves the clinic of traditional Chinese medicine, and prescription preparation is the final application form of traditional Chinese medicine in clinic. The quality control of traditional Chinese medicine needs to be treated systematically, and it can't just stay on the quality evaluation of single drugs.

The maps of 15 inorganic elements in the 8 components of Chuanxiong Cha Tiao San are different and have strong characteristics. There are significant differences in 15 inorganic elements between licorice and the other seven drugs, indicating that it may be related to the difference in drug efficacy. Rhizome of chuanxiong. Herba schizonepetae. Mint. Notopterygium. Angelica dahurica. The inorganic element of Asarum is Mg, K, S. And there are differences between different drug flavors, which is likely to be the reason why the effects of different drug flavors in Chuanxiong Cha Tiao San are both similar and different. The role of inorganic elements in the efficacy of traditional Chinese medicine can not be ignored, and the material basis of Chuanxiong Cha Tiao San needs to be further clarified in combination with clinical efficacy research.

Conflict of interest

The authors declare no conflict of interest.

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