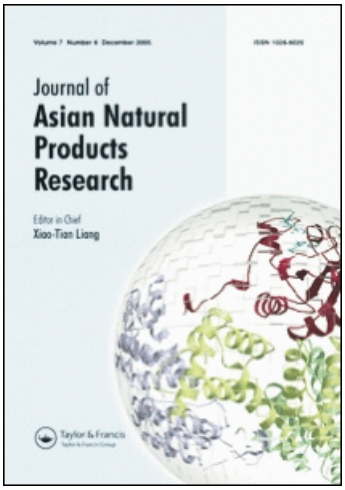

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Note: Chemical Pattern Recognition of Three Chinese Herbal Medicines from the Genus *Stephania* Lour

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Note

CHEMICAL PATTERN RECOGNITION OF THREE CHINESE HERBAL MEDICINES FROM THE GENUS *STEPHANIA* LOUR.

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Chemical pattern recognition was applied to three Chinese herbal medicines from the genus *Stephania* Lour., viz. *S. kwangsiensis* Lo, *S. viridiflavens* Lo and M. Yang and *S. mashanica* Lo and B.N. Chang. Based on the chemical features obtained from HPLC, SIMCA program was carried out and the results showed that the classification accuracy was 100%. In addition, the obtained features showed three major classes by NLM. The results of both methods were consistent with those of plant taxonomical identification. It suggested that chemical pattern recognition could be a helpful method to classify and identify Chinese herbal medicines.

Keywords: *Stephania*; Chemical pattern recognition

INTRODUCTION

Chinese herbal medicines are usually classified and identified morphologically and histologically. But sometimes it is difficult to ascertain the conclusion because those characteristics of herbal medicines can be varied with a lot of factors such as habitat, climate and collection time and because some

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species are so alike that it is hard to identify them. However, the chemical features of herbal medicines are stable. So few researchers applied chemical features to the classification and chemical pattern recognition has got some approaches in this field. But the method has not been used for the classification of herbal medicines from the genus *Stephania* Lour., many species of which were found in the passed 20 years and maybe the classification of some of these new species has not been studied adequately. In *Stephania*, many species have been used medicinally, mostly as antipyretic analgesics, antibacterials and antiinflammatory. From the plants of the genus *Stephania* Lour. in China, more than 150 alkaloids of six main types were separated, of which many exhibit bio-activites. Because of the high medicinal value of the plants from *Stephania*, richness of alkaloids and many new species, this genus has attracted many researchers in various fields. The authors collected about 70 samples of 25 species from the genus *Stephania* Lour., among which there were three species possessed enough numbers of samples to be studied by pattern recognition. These three species all belong to the same genus *Stephania* Lour., subgenus *Tuberiphania* Lo and M. Yang, sect. *Tuberiphania* Lo and M. Yang. So they are closely related species in plant taxonomy. The authors used chemical pattern recognition to classify them in order to provide a new evidence for the identification.

RESULTS AND DISCUSSION

Data

The data for this study were taken from high performance liquid chromatogram (HPLC). The chromatograms were divided into 13 time sections and the total heights of peaks in each section were used as the features (Table I).

SIMCA (Statistical Isolinear Multiple Component Analysis) [1,2]

SIMCA is a kind of supervised learning method, which classifies the samples by two steps: first, using a set of samples of known classification to develop some classification rules and second, using the classification rules to predict the classes of the samples in the unknown set. SIMCA method uses a principal-component model to describe the classes. After the method trains the known set, the class models are established. Then unknown samples can be classified by fitting them into various class models. If a sample falls

TABLE I Features of plant samples

Plant samples		*Features*												
		1	2	3	4	5	6	7	8	9	10	11	12	13
S. kwangsiensis	(1)*	40.0	1.70	3.80	4.40	0.15	0.22	0.00	19.4	1.21	0.00	0.00	20.9	0.10
	(2)	29.5	4.70	2.16	1.10	0.15	1.42	0.90	2.80	2.10	0.10	0.00	2.65	0.00
	(3)	28.0	0.69	0.98	1.50	0.10	1.20	0.00	22.5	0.20	0.00	0.00	18.2	0.67
	(4)	22.9	1.30	0.70	2.70	0.10	0.00	0.00	14.4	0.30	0.00	0.00	12.8	1.50
	(5)	27.5	0.50	0.36	4.00	0.00	0.20	0.20	20.0	0.20	0.00	0.00	18.3	0.00
S. viridiflavens	(1)	25.5	0.60	1.10	0.00	0.00	9.00	0.00	28.4	0.00	0.20	0.00	0.18	0.30
	(2)	69.0	1.60	0.75	0.40	0.10	11.7	0.00	49.5	0.00	0.10	0.00	0.20	0.20
	(3)	19.5	0.50	0.25	0.00	0.00	2.40	0.00	13.2	0.00	0.25	0.00	0.20	0.20
	(4)	14.2	1.30	1.00	0.00	0.20	7.40	0.00	36.3	0.00	0.30	0.00	0.20	0.10
	(5)	95.0	2.60	1.20	0.67	0.30	14.7	0.00	64.5	0.00	0.00	0.00	0.00	0.00
	(6)	17.7	1.70	0.20	0.30	0.10	4.25	0.00	33.3	0.00	0.20	0.00	0.20	0.10
	(7)	36.5	3.30	0.87	0.50	0.30	8.50	0.00	37.8	0.00	0.38	0.00	0.20	0.20
	(8)	16.1	3.12	0.78	1.35	0.00	1.72	0.00	32.3	0.10	0.00	0.00	18.3	0.20
S. mashanica	(1)	51.5	2.13	9.25	0.00	0.30	0.52	0.30	1.26	0.30	19.5	0.00	11.3	0.55
	(2)	85.5	3.30	16.0	0.00	3.10	0.33	1.30	10.5	0.70	17.5	0.00	26.9	0.20
	(3)	67.5	3.50	9.00	0.00	3.90	0.00	0.70	1.65	1.10	33.5	0.00	19.3	0.42
	(4)	36.5	2.20	13.5	0.00	0.20	0.20	0.70	2.20	0.50	20.5	0.10	17.6	0.54
	(5)	20.5	1.30	12.9	0.00	0.60	0.20	0.20	0.35	0.25	11.3	0.00	21.8	0.48
	(6)	54.2	4.20	7.30	0.00	0.60	2.50	0.60	1.38	1.30	24.5	0.00	14.0	0.47
	(7)	54.0	3.70	8.65	0.00	0.55	0.20	0.00	4.83	0.90	10.7	0.00	21.3	0.64

* Different number indicated the different source (see Table III).

TABLE II SIMCA testing results of three Chinese herbal medicines from the genus *Stephania* Lour.

Plant samples	*Real class*	*Predict class*	*The nearest class*	*The second nearest class*
S. kwangsiensis (5)	1	1	1	2
S. viridiflavens (5)	2	2	2	3
S. viridiflavens (6)	2	2	2	1
S. viridiflavens (7)	2	2	2	1
S. viridiflavens (8)	2	*	1	2
S. mashanica (5)	3	3	3	1
S. mashanica (6)	3	3	3	1
S. mashanica (7)	3	3	3	1

* Indicated a new class.

within a given range of classes, the sample belongs to that class. If a sample cannot fit any established model, this suggests that it is a new class.

Four samples of each species were used as the training set, and the others as the test set. The results of testing (Table II) showed that seven samples were identified as expected and the stem and leaf of *S. viridiflavens* was predicted to be a new kind. It indicated that the chemical components of the

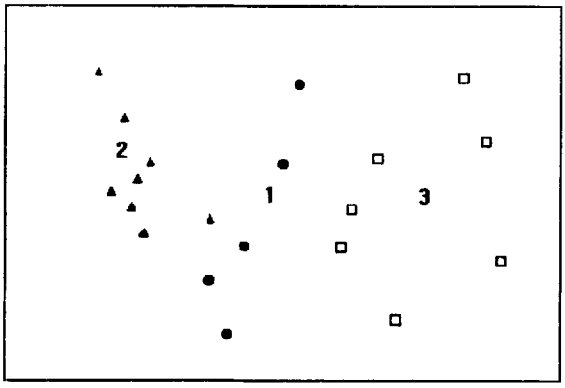

FIGURE 1 Two-dimensional display of three Chinese herbal medicines from the genus *Stephania* Lour. by NLM Class 1: *S. kwangsiensis* (●), Class 2: *S. viridiflavens* (▲), (▲) indicated the stem and leaf sample, Class 3: *S. mashanica* (□).

stem and leaf of *S. viridiflavens* were different from those of root of the plant. Based on the results mentioned above, we think the prediction accuracy was 100%.

NLM (Nonliner Mapping) [1,2]

Classification was also attempted using NLM, a type of display method. The method synthesized a specified number of new features, each of which is a nonlinear function of the old features. It can project the data from high-dimensional space to a space of low-dimension, usually two-dimensional space, which is familiar to people's visual sense. With the two-space projection, significant clustering was observable (Fig. 1). The samples of three Chinese herbal medicines from the genus *Stephania* Lour. were distributed to three different clusters and the stem and leaf of *S. viridiflavens* somewhat deviated from the cluster of its class. So the classification by NLM was the same as that by SIMCA.

EXPERIMENTAL

Chemicals and Reagents

Stepholidine, sinoacutine, crebanine and tetrandrine were isolated and identified by Lao Aina and Chen Yan (Shanghai Institute of Materia

Medica, Academia Sinica). Isocorydine and *l*-tetrahydropalmatine were obtained from Yang Heming (Shanghai Jinshan County Institute for Drug Control), and crebanine from Min Zhida (China Pharmaceutical University). Methanol was of HPLC grade, obtained from Tianjin Shield Company. Triethylamine was of analytical reagent grade, obtained from Shanghai No. 3 Chemical Reagent Factory. Water was distilled in the lab.

Plant Samples

Plant samples were collected (see Table III). Each sample was pulverized to fine powder, dried at 50–60°C for 1 h, cooled, and put into the desiccator.

Apparatus and Chromatographic Conditions

The HPLC determinations were performed on a Gilson chromatography system, equipped with two 302/5s elution pumps, a Holochrome UV detector, a Rheodyne 7125/20 μl six-way injection, a 802 manometric module and a 811 dynamic mixer. Data analysis was performed with AppleII controller and 704 software.

TABLE III Plant samples

Name of plant	*Sources*	*Part of plant*
S. kwangsiensis	(1) Tiandong, Guangxi (Y7029)	root
	(2) Jingxi, Guangxi (Y6968)	root
	(3) Napo, Guangxi (Y7000)	root
	(4) Napo, Guangxi (Y7002)	root
	(5) Napo, Guangxi (Y7003)	root
S. viridiflavens	(1) Du-an, Guangxi	root
	(2) Du-an, Guangxi (Y6959)	root
	(3) Du-an, Guangxi (Y7013)	root
	(4) Du-an, Guangxi (Y7004)	root
	(5) Du-an, Guangxi (Y6961)	root
	(6) Bama, Guangxi (Y7005)	root
	(7) Du-an, Guangxi (Y7016)	root
	(8) Bama, Guangxi	stem and leaf
S. mashanica	(1) Du-an, Guangxi (Y7018)	root
	(2) Mashan, Guangxi (Y7009)	root
	(3) Mashan, Guangxi (Y7010)	root
	(4) Yishan, Guangxi (Y7023)	root
	(5) Du-an, Guangxi (Y7012)	root
	(6) Du-an, Guangxi (Y7022)	root
	(7) Mashan, Guangxi (Y7008)	root

Y indicated Yang Heming's collection number.

The reversed-phase system consisted of ODS column and methanol–water–triethylamine as mobile phase. The gradient eluent involved A: methanol : water : 10%triethylamine (methanol) = 50 : 50 : 0.5, and B: methanol: 10%triethylamine (methanol) = 100 : 0.5. The eluent started at 5%B, increased linearly to 15%B at 8 min and to 75% at 28 min, and later remained at 75%B for 4 min, returned to the original eluent.

Methods

Put the sample powder of 120 mg (precise weight) into a tube, add 5 ml methanol, degas it in an ultrasonic bath (180 mA) for 30 min, set it quietly for 50 min and get the upper solution. The solution was filtered through a 0.45 μm filter and then injected 20 μl to the chromatographic system.

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