Study on the Relationship between the Fingerprint Characteristics of Shatian Pomelo and Its Pharmacodynamics

Shan Cong, Ying Mao, Chunxue Yu

The Second Affiliated Hospital of Qiqihar Medical University, Qiqihar, Heilongjiang, 161006, China

Keywords: Fingerprint characteristics, Pharmacodynamics study, Shatian pomelo

Abstract: With the continuous advancement of modern analytical technology and the continuous deepening of the research on the system of traditional Chinese medicine, the quality control technology of traditional Chinese medicine fingerprints has emerged. The so-called fingerprint atlas refers to a chromatogram that can mark the characteristics of a Chinese medicine after a certain Chinese medicine has been properly processed and a certain analysis method is used. Fingerprint has become a hot spot in the quality research of traditional Chinese medicines. It has become a prairie fire in China and has been widely recognized abroad. However, we must be soberly aware that there are still obvious shortcomings and serious defects in the current research on fingerprints, that is, there is a problem of disconnection between fingerprints and drug effects. This is contrary to the original intention of fingerprint research and limits the development and application of fingerprints. The information reflected by the fingerprint must correspond to the drug effect, or it must have a high degree of relevance to the drug effect. This is the problem that this thesis wants to consider and solve. In this thesis, Shatian pomelo, a citrus genus plant in the Rutaceae family, was used as the object, and the fingerprint of Shatian pomelo was constructed, and the pharmacodynamic test of anti-cough and phlegm was carried out to obtain the quantitative characteristics and pharmacodynamic data of the fingerprint. On this basis, the gray correlation analysis method is used to find the corresponding relationship between the spectral effects of Shatian pomelo.

1. Introduction

In recent years, with the continuous advancement of modern analytical technology and the continuous deepening of the research on traditional Chinese medicine systems, the quality control technology of traditional Chinese medicine fingerprints has emerged at the historic moment. The so-called fingerprint atlas refers to a chromatogram that can mark the characteristics of a Chinese medicine after a certain Chinese medicine has been properly processed and a certain analysis method is used. Fingerprints have become a hot spot in the quality research of traditional Chinese medicines, and they are becoming a prairie fire in China. Internationally, the American FAD, the British Herbal Medicine Code, the Indian Herbal Medicine Code, the German Medicinal Plant Society, and the Canadian Medicinal Plant Society all accept fingerprint quality control methods. However, we must be soberly aware that there are still obvious shortcomings and serious defects in the current research on fingerprints, that is, there is a problem of disconnection between fingerprints and drug effects. This is contrary to the original intention of fingerprint research and limits the development and application of fingerprints. The information reflected by the fingerprint must correspond to the drug effect, or it must have a high degree of relevance to the drug effect. This is the problem that this thesis wants to consider and solve. This dissertation aims to establish a quality control mode of traditional Chinese medicine that “fingerprints are related to their efficacy”, which can make up for a common defect in the current research on fingerprints of traditional Chinese medicines, which is the disconnection between fingerprints and drug effects.

The HPCL method was used to analyze Shatian samples from different sources, and the chromatographic conditions (including mobile phase, elution gradient, chromatographic column, detection wavelength, etc.) were optimized, and the systematic methodological investigation was completed, and the Shatian pumping HPCL was constructed. Fingerprint. The “Computer Aided

  DOI: 10.25236/bmmss.2021.002

Similarity Evaluation System Software for Chromatographic Fingerprints of Traditional Chinese Medicines" was used to evaluate the similarity of HPCL fingerprints from Shatian. The quantified fingerprint characteristics (peak area of chromatogram) were analyzed by computer cluster analysis by systematic clustering analysis; the canonical discriminant function and Fihser's discriminant function were established, and the results were in full agreement with the actual situation, indicating that this method is extremely reliable. In practical application, only need to analyze the sample to be tested according to the chromatographic conditions described in this study, and input the quantitative fingerprint characteristic data into the computer for calculation, and the classification result can be quickly obtained. This research has theoretical significance and practical value.

On the basis of obtaining the fingerprints and pharmacodynamic quantitative data of Shatian extraction, the gray correlation analysis technology is used to find the contribution of the chemical components represented by the fingerprints to the pharmacodynamics. The results showed that the cough-relief and phlegm-relief effects of S. cypress is the result of the joint action of its "chemical component groups". According to the degree of correlation, the order of the contribution of each component to the "cough relieving effect" is determined as follows: peeling smoothie> orange peel internal vinegar hydrate> Citrus citron> Bergamot patina> isohesperidin> Peeling element> New orange peel> Wild sumac. The order of the contribution of each component to the "phlegm-reducing effect" is: wild sumac tree smoothie> new orange peel smoothie> peeling smoothie> citron vinegar> orange peel endocurve hydrate> peeling element> different orange peel vinegar> Bergamot Pavilion. This research establishes a brand-new comprehensive quality control mode that can make the spectrum-efficiency relationship correspond and unify, and fill the gap in this field in China in the study of the quantitative relationship of the fingerprint spectrum-efficiency of traditional Chinese medicine. This is a brand-new research model of traditional Chinese medicine. It links the fingerprint characteristics of the "effective component group" of traditional Chinese medicine with the efficacy, and grasps the synergistic characteristics of the "effective component group" in traditional Chinese medicine as a whole. This research is carried out by searching for the relationship between the fingerprint characteristics of the "effective component group" and the activity effect. It must be pointed out that the fingerprint spectroscopy effect of Chinese medicine is different from the structure-activity relationship of drugs in western medicine research; the overall effect of Chinese medicine can not be expressed by the linear superposition of the individual effects of each component.

2. Study on Pattern Classification of Shatian Pomelo Hplc Fingerprint Features

Cluster analysis is to classify samples or variables with similar characteristics according to the principle of "things are clustered together", so that individuals in the same class have greater similarity, and individuals in different classes have greater differences. The clustering process is to first regard n samples as n classes, and then merge the 2 classes with the closest (or the most similar) properties into a new class, which is divided into n-1 classes. Then find the closest 2 and merge it into n-2 categories, and so on, theoretically all samples can be gathered in-category. As a computer pattern classification method, cluster analysis has a good application prospect in the field of identification and classification of traditional Chinese medicine. In this study, samples No. 1-10 are young fruits from Shatian, No. n-13 are young fruits from Huazhou, and No. 14-18 are mature exocarps of Shatian Pomelo. The author used computer spectrum analysis technology to process the fingerprints of the above samples, and obtained their quantitative fingerprint characteristics (HPCL chromatographic peak area data). The quantified fingerprint features were input into the computer as variables, and the SPSS10.0 statistical software was used for systematic clustering analysis.

On the basis that the systematic cluster analysis can better distinguish the young fruit of Shatian, the young fruit of Huazhou sleeve and the mature exocarp of Shatian Pomelo, the data is further discriminated and analyzed. Discriminant analysis is to establish a discriminant function based on a batch of samples whose classifications are known, so that the error rate of the sample is minimized when the function discriminates the classification of samples. The establishment of the discriminant function will make the judgment of the category of Shatian Pomelos more rapid, accurate and

intuitive, which is beneficial to practical applications.

3. Pharmacodynamic Study of Shatian Pomelo

Take skg of young fruit from Shatian, cut into decoction pieces, add water to decoct 3 times, each time hlr, filter, the filtrate is concentrated to a relative density of 1.10~1.12, add ethanol to make the alcohol concentration reach 8%, let stand for 24hr, filter and take The supernatant and the filtrate recovered ethanol until there was no alcohol taste, concentrated to a relative density of 1.10, placed d7, precipitated out, filtered, and dried to obtain. A total of 10 batches of test drugs were prepared in this experiment (prepared from the young fruit samples of Shatian Pomelos No. 01~10. A mouse model of cough induced by ammonia water was used, and normal saline was used as a blank control to study the antitussive effect of the tested drugs. The principle is: after inhaling the aerosol of irritating chemical drugs, mice stimulate the receptors of the respiratory tract and cause cough reflexively. Any drug that can inhibit the cough center or reduce the sensitivity of the receptors has the effect of relieving cough. If the drugs used are effective, they can suppress the cough caused by ammonia.

The mice were randomly divided into n groups (ie blank control group and No. 01-10 test drug group), each with 20 mice. Before the experiment, the mice were fasted without water for shr, and then each group of mice was given 0.2ml/209 body weight by gavage, 1 time/d, for a total of d7, and the blank control group was given an equal volume of normal saline. After the last gavage of hlr, start to receive spray. Spray into the concentrated ammonia mist at a fixed time. After the spraying is over, the mice are taken out immediately to observe whether there is a cough reaction. Observe the number of coughs within 1 min. If there are more than 3 typical coughing actions (abdominal muscle contraction or chest contraction, while opening the mouth, sometimes coughing), it is counted as “coughing”. Otherwise it is counted as “no cough”. Sequential method (up and down method) was used to determine the spray time (EDTso) that caused half of the mice to cough. Calculate the R value. If the R value is greater than 130%, it indicates that the drug has an antitussive effect. If the R value is greater than 150%, it shows a significant antitussive effect.

A mouse model of phenol red expectorant method was used, and physiological saline was used as a blank control to study the phlegm-resolving effect of the tested drugs. The principle is: using phenol red as an indicator of the expectorant effect, under the influence of the test drug, as the bronchial secretion increases, the more phenol red is discharged from the respiratory mucosa, the more the concentration of phenol red in the tracheal lavage fluid high. The excretion of phenol red is measured with a spectrophotometer, and the strength of the phlegm-resolving effect of the test drug can be judged.

4. Grey Correlation Analysis of Shatian Pomelo Fingerprint Characteristics and Pharmacodynamic Indexes

In the fingerprint of traditional Chinese medicine, each characteristic peak represents a chemical component in it. The medicinal effect of traditional Chinese medicine is the result of the synergistic effect of its internal chemical components, so there must be some correlation between fingerprint characteristics and medicinal effect. How to find the correlation between fingerprint characteristics and drug efficacy is exactly the problem that the domestic pharmacy community must think about and solve. Correlation analysis provides ideas for solving this problem. The so-called correlation degree refers to the measurement of the correlation between two systems or two factors. The degree of relevance describes the relative changes between factors during the development of the system. If the relative changes of the two are basically the same in the development process, then the two are considered to be highly correlated; on the contrary, the correlation between the two is small. There are n traditional Chinese medicine samples, and each sample has m fingerprint feature quantitative indicators, which constitutes m sub-sequences. Taking the sample pharmacodynamic index as the parent sequence, and according to the degree of correlation between the parent sequence and the subsequence, the contribution of the fingerprint features to the drug effect can be determined.

The correlation coefficient and correlation degree between the fingerprint characteristics of the young fruit of Shatian and its antitussive effect. The results show that: tR=10.38, 17.11, 21.74, 23.05, 25.91, 27.95, 35.95, 44.25min and other peaks represented by the chemical components are highly correlated with the antitussive effect (correlation degree>0.95), indicating that the antitussive effect of Shatian pump is among them the result of the joint action of the “chemical composition group”. According to the degree of correlation, the order of the contribution of each component to the “cough relieving effect” is determined as follows: Peeling Camp> Orange Peel Internal Vinegar Hydrate> Citrus Citrus> Bergamot Pavilion> Isocellane Internal Vinegar> Peeling Element> New Orange Peel Camp>Wild Sumac Camp.

The results show that: tR=10.38, 17.11, 21.74, 23.05, 25.91, 27.95, 35.95, 44.2m5ni and other peaks represented by the chemical components are highly correlated with the phlegm resolving effect (correlation degree> 0.95), indicating the phlegm resolving effect of Shatian pumping It is also the result of the “chemical component group” in it. According to the degree of correlation, the order of the contribution of each component to the “phlegm-reducing effect” is determined as follows: wild sumac> new orange peel camp> peanut camp> citronella citron> orange peel hydrate> pectin> Different orange peels are cool inside> Bergamot Pavilion.

In this section, on the basis of obtaining the fingerprint spectrum and pharmacodynamic quantitative data of Shatian Pomelo, the gray correlation analysis technology is used to find the contribution of the chemical components represented by the fingerprint spectrum characteristics to the drug efficacy. This research has established a new comprehensive quality control model that can correspond and unify the spectrum-effect relationship. This is a frontier topic in the modernization of traditional Chinese medicine. It has positive significance for the development of traditional Chinese medicine and has a wide range of application values.

5. Conclusion

Fingerprint and computer identification of traditional Chinese medicines are currently a hot spot in the quality research of traditional Chinese medicines, and they are becoming a prairie fire in China. The fingerprint of traditional Chinese medicine has obvious advantages in realizing the overall control of the substance group, and it has also been recognized by the international community. The US FDA, the British Herbal Medicine Code, the Indian Herbal Medicine Code, the German Society of Medicinal Plants, and the Canadian Society of Medicinal Plants all accept fingerprint quality control methods. However, we must be soberly aware that the current research on fingerprints is flawed, that is, there is a problem of disconnection between fingerprints and drug efficacy. Many insightful people in the domestic academic circles are looking for ways to solve this problem. This dissertation is aimed at this problem.

References

[1] Qiu Xiuzhen. Study on Fingerprint of Shatian Pomelo Pulp Extract. Journal of Shaoguan University, 2009, 30(006):61-64.

[2] Li Yi, Ma Xianfeng, Tang Hao, et al. Development of SSR markers and construction of fingerprint library for identification of citrus varieties. China Agricultural Sciences, 2018, v.51(15):149-159.

[3] Wang Huijuan, Hou Daping, Wang Huili. Identification of several groups of miscible Chinese herbal medicines using electrochemical fingerprinting technique. Liaoning Journal of Traditional Chinese Medicine, 2010, 037(004):703-705.

[4] Xie Wei, Yang Ni, Jiang Shoujun. HPLC characteristic fingerprint and pattern recognition of Baibei leaves. Chinese Journal of Experimental Formulas, 2017(18):61-66.

[5] Tang Xianhong. Comparison of characteristic fingerprints of Huanglian Shangqing tablets from different manufacturers. Chinese Journal of Experimental Formulas, 2011(24):77-81.