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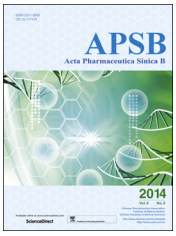

REVIEW

Application of near infrared spectroscopy to the analysis and fast quality assessment of traditional Chinese medicinal products

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Abstract Near infrared spectroscopy (NIRS) has been widely applied in both qualitative and quantitative analysis. There is growing interest in its application to traditional Chinese medicine (TCM) and a review of recent developments in the field is timely. To present an overview of recent applications of NIRS to the identification, classification and analysis of TCM products, studies describing the application of NIRS to TCM products are classified into those involving qualitative and quantitative analysis. In addition, the application of NIRS to the detection of illegal additives and the rapid assessment of quality of TCMs by fast inspection are also described. This review covers over 100 studies emphasizing the application of NIRS in different fields. Furthermore, basic analytical principles and specific examples are used to illustrate the feasibility and effectiveness of NIRS in pattern identification. NIRS provides an effective and powerful tool for the qualitative and quantitative analysis of TCM products.

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1. Introduction

Chinese herbs and patent drugs are important parts of traditional Chinese medicine (TCM), the use of which is considerable not only in China but all over the world. Despite this widespread use, there are many confusing aspects related to TCM such as the fact that many similar TCMs produce different pharmacodynamic effects, one TCM can have two or more names and one name can apply to more than one TCM. These problems lead to difficulty in the quality control (QC) of TCM and call for urgent attention[1].

In comparison with the Chinese Pharmacopoeia 2005 (ChP2005), drug standards and test methods for TCM have been considerably improved and extended in the Chinese Pharmacopoeia 2010 (ChP2010). Common methods now include histological and morphological examination, thin layer chromatography (TLC), high-performance liquid chromatography (HPLC), gas chromatography (GC), liquid chromatography–mass spectrometry (LC–MS) and gas chromatography–mass spectrometry (GC–MS)[2–4]. This more authoritative and comprehensiveness coverage of TCM in the ChP is critical for improving the QC of TCM. However, there are still deficiencies such as the time period of inspection in the ChP is longer than the 28 days recommended by the Institute for Drug Control (IDC) in China.

Another problem is that TCM components are often pretreated by physical or chemical processes before being tested. These procedures are complex and multifarious and some of them such as morphological identification lack accuracy since the results depend on the experience and expertise of the TCM pharmacist undertaking the test[5]. Thus, for objectivity, rapidity and accuracy of testing, more rational methods are needed.

Since the 1990s, the application of near infrared spectroscopy (NIRS) in fields involving drugs, food, agriculture, the petroleum industry and environmental protection has developed rapidly[6,7]. NIRS has many advantages in relation to QC and inspection[8] and allows classification, qualitative analysis and quantitative analysis of TCM products. The further development of NIRS will serve to strengthen quality supervision and control of TCM products and regulate markets[9].

2. Advantages of NIRS technology

The advantages of NIRS are many with rapidity of analysis being one of the most important[10]. Thus NIRS combined with appropriate mathematical models and pattern recognition techniques allows analysis of a wide variety of sample types rapidly. Second, NIRS is a non-destructive technique which avoids complex sample preparation by chemical or physical processes. In fact, both solid and liquid samples in different types of packaging stored under different conditions can all be tested without complex pretreatment[11] because of the better penetrability of fiber optics used in NIRS. Third, it provides acceptable accuracy in both qualitative and quantitative analysis to meet the requirements of QC and preliminary screening[12].

3. Identification of TCM by NIRS

3.1. Qualitative identification

TCM herbs and animal products are subject to numerous complex problems in clinical use. For example, herbs are often adulterated with or replaced by non-therapeutic plants of similar appearance[13–15] because the ability to identify a particular herb is very dependent on the experience of the TCM pharmacist.

Identification based on microscopic examination is frequently applied to TCM powders by looking for the presence of microstructures[16–18]. In addition, it is used to examine slices of TCM plant cells. The ChP2005 recorded 620 items requiring identification by microscopy and the number increased to 1253 in the ChP2010[19]. However, identification using microscopy still depends on the experience of the TCM pharmacist whereas NIRS provides a more reliable non-subjective method to identify TCM products. For example, 269 samples of Bai-Zhi (Radix Angelicae Dahuricae) and 350 samples of wild or cultivated Dan-Shen (Radix et Rhizoma Salviae Miltiorrhizae) were identified and classified by NIRS with a accuracy rates of 99% and 95%, respectively[20].

Some species of TCM are grown in different regions of China where differences in weather conditions and soil environments lead to variations in quality[21]. NIRS can then be used to locate the source of a particular sample. For example, Jin-Yin-Hua (Flos Lonicerae Japonicae) is widely planted in the provinces of Henan, Hebei, Hunan, Shandong and Guangxi. Qualitative analysis by NIRS not only identified 22 samples as coming from Henan province with 100% accuracy but also correctly sourced 68 samples from other provinces and sourced only 9 samples incorrectly[22].

The use of genuine medicinal materials is very important to the integrity of TCM (Table 1). However, many rare and expensive TCM herbs are often adulterated[23]. For example, the adulteration of Dong-Chong-Xia-Cao (Cordyceps), one of most important and precious TCM herbs, is a serious problem. Fortunately, NIRS provides a rapid and convenient method to identify Dong-Chong-Xia-Cao with an accuracy rate greater than 95%[24]. In contrast, Hong-Qu (Rubrum Fermentum) is not a rare material but a commonly used food additive in China and many Asian countries[25]. The problem here is that many substances are similar in appearance to Hong-Qu making identification by microscopy difficult. In this case, NIRS in combination with cluster analysis was successful in classifying Hong-Qu effectively[26,27].

Grinding is frequently used in the preparation of TCM as part of the extraction and purification of desired components from crude materials. As a result, TCM herbs and animal products in the form of powders lose their significant characteristics making identification difficult. In addition, different TCM herbs have similar shape, color and microscopic features[28]. For example, Bai-Zhi (Radix Angelicae Dahuricae), Ye-Ge (*Puerariae Lobatae*), Cang-Zhu (Rhizoma Atractylodis), Bai-Shao (Radix Paeoniae Alba) and Dang-Gui (Radix Angelicae Sinensis) display only subtle differences in appearance[29] and, after grinding, become even more difficult to distinguish. However, using principal component analysis (PCA) and cluster analysis to classify NIRS data allowed TCM powders with indistinguishable appearance to be identified and classified as accurately as by HPLC. NIRS is now considered the technique of choice for the QC of Chinese patent medicines[30–32].

3.2. Pattern recognition technology

A NIR spectrum incorporates a large amount of information and includes overlapping and interconnected signals. As a result, pattern recognition is an important approach to reduce the number of variables. Pattern recognition is classified as either unsupervised or supervised[33]. Cluster analysis, PCA and discriminant analysis