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REVIEW PAPER

Chemometrics: A new scenario in herbal drug standardization

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Abstract Chromatography and spectroscopy techniques are the most commonly used methods in standardization of herbal medicines but the herbal system is not easy to analyze because of their complexity of chemical composition. Many cutting-edge analytical technologies have been introduced to evaluate the quality of medicinal plants and significant amount of measurement data has been produced. Chemometric techniques provide a good opportunity for mining more useful chemical information from the original data. Then, the application of chemometrics in the field of medicinal plants is spontaneous and necessary. Comprehensive methods and hyphenated techniques associated with chemometrics used for extracting useful information and supplying various methods of data processing are now more and more widely used in medicinal plants, among which chemometrics resolution methods and principal component analysis (PCA) are most commonly used techniques. This review focuses on the recent various important analytical techniques, important chemometrics tools and interpretation of results by PCA, and applications of chemometrics in quality evaluation of medicinal plants in the authenticity, efficacy and consistency.

1. Introduction

Herbal medicines (HMs) including Chinese medicine (CM) and other folk medicines are getting more and more popular nowadays globally for improving health condition of human beings as well as preventing and curing diseases. They have played an important role in the clinical therapy in many oriental countries for thousands of years. During the past two decades, they attracted attention to a greater extent in western countries because of their high pharmacological activities with low toxicity and rare complications. However, HMs have not been officially recognized worldwide because the quantity and quality of the safety and efficacy data on traditional medicine are far from sufficient to meet the criteria needed to support their use everywhere. Therefore, the World Health Organization (WHO) provides guidelines for the assessment of the quality of HMs [1].

Now, one or two markers or pharmacologically active components in herbs or herbal mixtures are currently employed for evaluating the quality and authenticity of herbal medicines. However, this kind of determination does not give a complete overview of an herbal product, because multiple constituents are

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usually accountable for its therapeutic actions and effectiveness. These multiple constituents may work 'synergistically' and could hardly be separated into active parts [2,3].

There are various techniques that are used for this sort of determination like high-performance liquid chromatography (HPLC), gas chromatography (GC), ultra-high performance liquid chromatography (UHPLC) and thin layer chromatography (TLC). Moreover, the recent approaches including hyphenated chromatography and spectroscopy like high-performance liquid chromatography-diode array detection (HPLC-DAD), gas chromatography–mass spectrum analysis (GC–MS), capillary electrophoresis-diode array detection (CE-DAD), HPLC–MS and HPLC–nuclear magnetic resonance (NMR) might give the additional spectral information which may be helpful for the qualitative and quantitative analysis and even for the structural elucidation. With spectral information, the hyphenated instruments show greatly improved performances in terms of the elimination of the instrumental interferences, retention time shift correction, selectivity, chromatographic separation abilities, measurement and precision.

Since complicated data from these techniques cannot be evaluated easily, we need data processing techniques for this purpose. These techniques provide a good opportunity for mining more useful chemical information from original information-rich data.

Chemometrics is the application of mathematical and statistical techniques to retrieve more information from the chromatographic data [4–6]. The International Chemometrics Society (ICS) defines chemometrics as the science of relating measurements made on a chemical system or process to the state of the system via application of mathematical or statistical methods [7].

It promotes equipment intellectualization and offers new ideas and methods for the construction of new and high-dimensional and hyphenated equipments. Furthermore, with the rapid development of the microcomputer and retrieval of the analysis of high-dimensional data, artificial neural networks, research of artificial intelligence of chemistry and expert systems have made great progress. With the development of analytical chemistry, chemometrics is also being developed vigorously [8,9].

With the advance of computer technology, chemometrics methods have become a leading tool among the scientific communities towards faster analysis results and shorter product development time. Among others, an unsupervised pattern recognition technique such as principal component analysis (PCA) is the most often used method for handling multivariate data without prior knowledge about the studied samples. While the supervised classification procedure using soft independent modeling of class analogy (SIMCA) based on making a PCA model to assign unknown samples into the predefine class model has also been applied to the analysis. Thus, the application of chemometrics techniques will greatly improve the quality of the fingerprint obtained (Fig. 1) [4,9,10].

In this review, we have discussed the origin and development of chemometrics in the first part and further stressed various important chromatographic techniques for HDs fingerprint development. Furthermore, multivariate methods that are used to extract the information from the chromatographic data like pretreatment of chromatogram, multivariate resolution methods and various classification and discrimination methods applied in the chemical analysis of herbal drugs have been discussed. In the final part, we have discussed its application in herbal drug standardization with respect to authenticity and determination of chemical components by analytical techniques, especially on the use of chemometrics in combination with chromatographic fingerprint for quality evaluation based on active ingredients.

2. Origin and development of chemometrics

A Swedish scientist Svante Wold in 1971 coined term "kemometri" in Swedish form and its English equivalent is "chemometrics" [11]. In year 1986 and 1987 two journals were started named as "Chemometrics and Intelligent Laboratory Systems" and "Journal of Chemometrics", which promoted equipment intellectualization and offered new methods for the construction of new and high-dimensional hyphenated equipment. These hyphenated equipments have opened many new options for data analytical method improvement. Now, chemometrics has emerged to have a major role within the analytical chemistry [12].

3. Herbal drugs chromatographic fingerprinting

Herbal drugs may contain a large number of compounds even though many of them are present in low concentrations but they may be important in terms of quality, safety and efficacy of the herbal medicines because they show synergetic effects and their therapeutic actions are based on interaction between numerous constituents. In order to evaluate the complete pattern of herbal medicine, chromatography offers a powerful tool for separating the individual components and developing a characteristic profile of the sample, called a fingerprint. This section basically deals with different chromatographic techniques used for herbal fingerprinting and their advantages and disadvantages.

3.1. *Thin layer chromatography (TLC)*

TLC is a technique used for fast screening of samples to identify herbal products and to differentiate between herbal species [13–16]. One of the major advantages of TLC is its tractability to optimize operational parameters, such as the sample application, plate

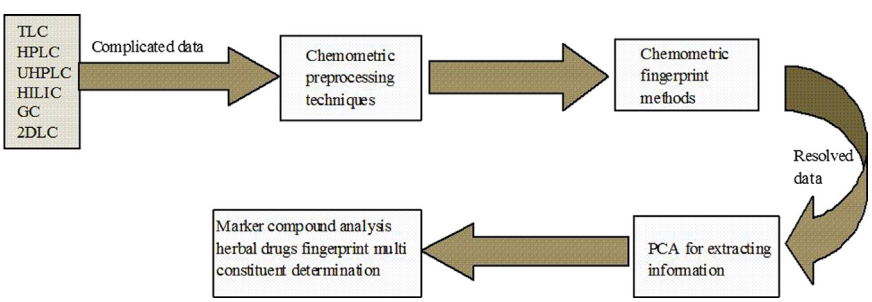

Fig. 1 Schematic interpretation of complicated data comes from various hyphenated instruments by various chemometrics techniques.