

Abstract

Chemical standards are the key substances for the qualitative and quantitative analysis, which play a key role for controlling the quality of traditional Chinese medicines (TCM). However, the chemical components especially the volatile compounds from TCM are not only difficult to obtain, but also hard to be preserved due to their unstability. Therefore, absence of chemical standards has become a bottleneck for the internationalization of Chinese medicines.

The purpose of present study was focused on the development of digital chemical standard library for qualitative and quantitative analysis of volatile compounds in TCMs. *Ezhu*, one the commonly used Chinese herbal medicine, was selected as the target. Based on the main volatile components separated from *Ezhu* and a series of n-alkane, a digital chemical standard library was established, which can be used for their qualitative and quantitative analysis when there were absence of these volatile chemicals.

There are four chapters for the thesis. **Chapter I** introduced the background and strategy for the present study. As the short of supply of chemical standards on the market, it is urgent to seek for alternative pathway without reference compound for quality control of Chinese medicines.

Chapter II was for the establishment of digital chemical standard library. Firstly, the collection of MS data for the target compounds was obtained by using the Automatic Mass Spectral Deconvolution and Identification System (AMDIS). There were more than 40 compounds' MS data collected in the MS library. Secondly, GC-MS method was developed for the analysis of *Ezhu* spiked with a series of n-alkane. And then the relative retention times to adjacent alkanes as well as the MS data of the compounds can be used for the identification (qualitative analysis) when there were short of chemical standards. Finally, a quantitative method based on corrected factor was developed by using the chemical standards and n-alkanes, while the qualitative and quantitative validity for the developed method were tested. The results showed that the developed digital chemical standard library is feasible for the

qualitative and quantitative analysis of the nine volatile components without or with a reference substance. Furthermore, the characteristics of the developed method were also compared with multi-components quantitation using one marker and chemical analogue methods.

Chapter III was the application of the established digital chemical standard library for the analysis of 19 batches of *Ezhu* samples collected from different hospitals distributed in China. While the quantitative result was compare to that of classic standard curve method; the results indicated that the virtual standard was practical and feasible for quality control of Chinese medicine.

In a word, digital chemical standards were developed and employed for quality control of Chinese medicines, which is helpful to control the quality control of Chinese medicines when there are lack of reference substances.

Key words: Digital chemical standard, volatile components, Chinese medicine, qualitative analysis, quantitative analysis, *Ezhu*