

University of Macau

Abstract

**Chemical Analysis Studies on the Volatile Components  
of Herba Pogostemonis**

by Linfeng Hu

Thesis Supervisor: Dr. Zhiling Yu & Professor Yitao Wang

Chinese Medicinal Science

Cablin Patchouli Herb is the dried aerial part of *Pogostemon cablin* (Blanco) Benth. (Fam. Labiatae). The tastes: pungent, warm. Meridian tropism: spleen, stomach, and lung. The plant has been used as Chinese herbal medicine to remove dampness, stop vomiting and stimulate the appetite, and relieve summer-heat. It is used for the treatment of dampness obstruction, stomach distension and vomit, fatigue caused by summerheat-damp, uncomfortable chest depression, cold-damp closing summerheat, vomit and diarrhea accompanying abdominal pain, headache caused by nasal obstruction. It is a common herb that widely used in digestive system diseases.

Herba Pogostemonis contains about 2-2.8% volatile oil which is the main effective part of the plant. In this study, two active components (patchouli alcohol and pogostone) were separated and isolated from patchouli oil. The purity of each compound is up to 98%. The quality control system (GC/MS) of Herba Pogostemonis was studied based on patchouli alcohol and pogostone. And 18 samples of Herba Pogostemonis, obtained from different places, and *Agastache rugosa*, were compared by using GC-MS.

This thesis is divided into five chapters:

Chapter 1 is the literature review of the studies on volatile components of *Pogostemon cablin* containing the following parts: chemical constituents, extraction and separation skills, quality control methods and pharmacology.

Chapter 2 is about the preparation and identification of reference compounds. Two crystals were obtained from patchouli oil with silica gel column chromatography, extracting and preparative HPLC. The purity of each compound was checked by TLC and HPLC and was found to be over 98%. By comparing the UV, MS, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra, the two crystals were identified as patchouli alcohol and pogostone, respectively. It is reported that patchouli alcohol has a regulatory action on enteron and spasmolysis of smooth muscle, and pogostone has an antifungal action. These compounds were used as standards for both qualitative and quantitative analyses, which are very important to the establishment of multi-marker quality control system for Herba Pogostemonis.

Chapter 3 focuses on the establishment of GC/MS analytical methods for the quantification of these two components in Herba Pogostemonis. In GC/MS method, target ion quantification was used after the separation by temperature gradient program. 18 Chinese Guang Huoxiang samples (Herba Pogostemonis) were obtained and used in the studies. The comparisons among different kinds of Herba Pogostemonis from different habitats and *Agastache rugosa* were made by using the GC/MS methods. The GC/MS methods were found to be simple, accurate and reproducible. On the other hand, pressurized liquid extraction (PLE) conditions were optimized. Finally, comparisons were made among PLE, ultrasonic extraction (UE), Soxhelt's extract (SX) and steam distillation (SD) which is a traditional extraction method for patchouli oil.

In chapter 4, hierarchical clustering analysis based on characteristics of 10 investigated peaks in GC profiles showed that 18 samples could be divided into three main clusters, patchouliol-type, pogostone-type and the third one between the two chemotypes. The simulative mean chromatogram for the three types Herba Pogostemonis was generated using the Computer Aided Similarity Evaluation System. The fingerprint can help distinguish the substitute or adulterant, and further assess the differences of Herba Pogostemonis grown in various areas of China.

And Chapter 5 is an overall conclusion.

In conclusion, two pure compounds were isolated from patchouli oil and were identified. Both compounds were previously reported to be pharmacologically active. New GC/MS analytical methods for quantification of the two compounds were also established in this study. The accurate quantification may provide a very useful method for the quality control of Herba Pogostemonis and its related products. The fingerprint can help distinguish the substitute or adulterant, and further assess the differences of Herba Pogostemonis grown in various areas of China

**Keywords:** *Pogostemon cablin*; volatile oil; reference compounds; quality control; GC-MS fingerprint