Posterbeitrag Themenkreis D: Qualitätsmanagement und Pflanzenanalytik

P 7 Cluster analysis of component composition of essential oil taken from plants of *FIlipendula* genus

Die Clusteranalyse der Zusammensetzung der Öle, die in den Pflanzen der Gattung Filipendula vorkommen

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Zusammenfassung

Die verschiedenen Pflanzen der Gattung von *Filipendula* sind Quellen von ätherisches Öl und werden im wissenschaftlichen oder der Volksmedizin sehr häufig verwendet. Infolge der geführten Forschung wurde gegründet die Zusammensetzung von im ätherisches Öl ist methylsalycylate und salicylic Aldehyd und mono - und sesquiterpenes hauptsächlich. Zur gleichen Zeit wurde der quantitative Inhalt von getrennten Bestandteilen von ätherisches Öl bedeutsam unterschieden. Weiter sind die Mittel des Clusteranalyse angewandt worden, der erlaubt hat, den Satz aller experimentellen Angaben gleichzeitig zu analysieren. Die Analyse des gebauten hierarchischen Baums hat gezeigt, dass die erforschten Pflanzen in 3 Gruppen in Übereinstimmung mit dem Grad des Unterschieds integriert werden können: 1 - *F. camtschatica*, *F. glaberrima*, *F. palmata*; 2 - *F. ulmaria, F. denudata, F.picbaueri*; 3 - *F. vulgaris*. Solcher Vertrieb entspricht Taxonomiepositionen dieser Pflanzen der Gattung von *Filipendula*. So, der vorgeschlagene Ansatz zur Analyse der Teilzusammensetzung des Öl, als ein zusätzliches Zeichen im Lösen von Taxonomieaufgaben verwendet werden, um verschiedene Spezies zu teilen. Außer der Clusteranalyse der Zusammensetzung von ätherisches Ölen kann als eine methodische Grundlage der Durchführung eine "Fingerabdruck"-Technologie sein, die für die Identifizierung nicht qualitative Kräutrohstoffe verwendet werden kann, die andere Pflanzen enthalten.

Stichwörter: *Filipendula*, ätherisches Öl, Clusteranalyse, Fingerabdruck

Abstract

The different plants of *Filipendula* genus are sources of essential oil and are used in scientific or folk medicine very often. As a result of conducted research, it was established that the component composition of essentially oil are methylsalycylate and salicylic aldehyde and mono- and sesquiterpenes mainly. At the same time the quantitative content of separate components of essential oil were significantly differed. Further the means of data clustering have been applied which allowed to analyze the set of all experimental data simultaneously. Analysis of built hierarchical tree showed the researched plants can be integrated into 3 groups in accordance with degree of difference: 1 - *F. camtschatica*, *F. glaberrima*, *F. palmata*; 2 - *F. ulmaria*, *F. denudata*, *F.picbaueri*; 3 - *F. vulgaris*. Such distribution corresponds to taxonomy positions of these spesies of *Filipendula* genus. Thus, the proposed approach to analysis of the components composition of essential oil can be used as an additional sign in solving taxonomy tasks for dividing various species. Besides the cluster analysis of component composition of essential oils can be as a methodical basis of implementation of technology a "fingerprint" technology, which can be used for identification of not qualitative herb raw materials containing other plants.

Keywords: *Filipendula*, essential oil, cluster analysis, fingerprint

Introduction

Essential oils which can be taken from herbs are used in scientific or folk medicine very often. They are complex chemical compounds which include a lot of different terpenoid substances. We should note that the pharmacological activity of such remedies depends on not only the main

compound which prevails but also on that can be determined by minor compounds often enough. The complexity of such mixes allows to enter a concept of a component spectrum or profile of essential oil. Naturally, quality of the phytomedicines made by using such essential oils will depend on it component spectrum. Due to this the goal of this work is that it's necessary to provide constancy of component spectrum of essential oil taken from herb raw material.

In this case we must determine the component spectrum of essential oil contained in herb as a "fingerprint" and then compare this spectrum with reference-standard using any procedure.

At the same time biosynthesis of the individual chemical compounds which are a part of essential oil is species-specific and is defined by a gene pool of the plant. Nowadays, separate chemical compounds of essential oil composition are used as a species-specific marker for solving taxonomical tasks. However, such approach can be realized if it is possible to determine a dominant chemical compound. Most often this is impossible to do, and the prevailed compound is unknown, so the ways for analysis of such multicomponent mixes aren't available in a hemotaxonomy.

Approaching formal positions, a problem of comparison of objects which have a lot of parameters is a typical problem of one of sections of mathematical statistics—the multiple-factor analysis. One of methods to solve similar tasks is the method of the cluster analysis. In this case we use a concept of a certain multidimensional space the ordinates of which are the content of each component in essential oil. Each studied sample of the essential oil emitted from the analyzed herb raw materials is characterized by a certain situation in this space or the cluster depending on a component spectrum of oil.

Comparing distances between clusters in this space which concerns a certain standard it is possible to make a conclusion about the importance of differences in a component range of the research samples.

The very interesting plant from this point of view is the different plants of *Filipendula* genus. The unique feature of these plants – the ability to accumulate volatile derivatives of salicylic acid - is the reason of it [Lindeman,1983]. Systematic researches of this group of chemical compounds and comparative researches of essential oils taken from different species of the *Filipendula* genus weren't conducted.

The aim of this work was a comparative research of component spectrum of various plants of *Filipendula* species with using cluster analysis.

Materials and Methods

The inflorescences of following plants - *F. camtschatica* Maxim., *F. glaberrima* Nakai, *F. palmata* Maxim., *F. ulmaria* Maxim., *F. denudata* Fritsch., *F.picbaueri* Smejkal. and *F. vulgaris* Moench. -which were collected in stage of flowering, were used as the research objects. The collected inflorescences were dried up and crushed. The essential oil was taken by using solid state extraction. The ingredient composition of essential oil taken from researched raw material was defined by Gas Chromatography/Mass Spectroscopy with using Agilent Technologies. Identification of components is determined by using comparison of the measured retention time with appropriate retention time for standard sample.

Results

As a result, 19 components were defined in essential oil composition taken from every herb and their total content accounts for significant fraction (more than 96%) in all volume researched oil.

The existence of phenolic compounds was established with methylsalycylate and salicylic aldehyde were the dominant ingredients. The terpenoids were the second main group with mono- and sesquiterpenes prevailed.

Further the means of data clustering have been applied which allowed to analyze the set of all experimental data simultaneously [Kruglov,2012]. The chosen method of cluster analysis involves hierarchical agglomerative clustering, in which two groups, chosen to optimize some criterion, are merged at each stage of the algorithm. The Ward's criterion was taken as a rule for association or communication of two groups into one cluster. The sum of root-mean-square deviations for any two (hypothetical) clusters which can be generated on each step must be minimized by this method. The distance between different clusters must be not less than a limit of variability of amount of the component spectrum of essential oil, the value of which was taken as 20%.

The hierarchical tree which was built because of such analysis is presented on fig 1.

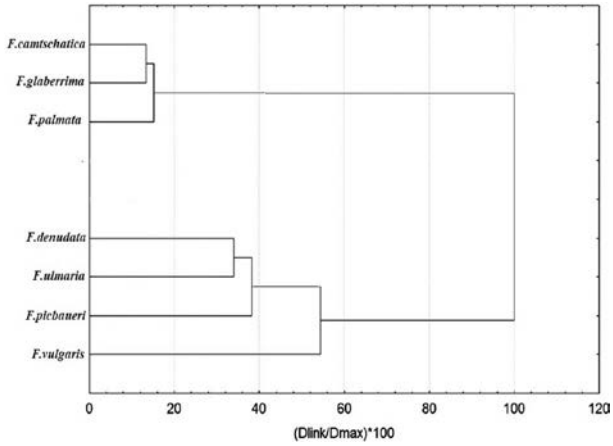

Fig 1 The hierarchical tree of different species of *Filipendula* genus

It is visible from the presented data that there are practically no crossed clusters except two close species *F. camtschatica* and *F. glaberrima* which are sometimes rating as varieties. At the same time, the researched plants can be integrated into 3 groups in accordance with degree of difference: 1 - *F. camtschatica*, *F. glaberrima*, *F. palmata*;

2 - *F. ulmaria, F. denudata, F.picbaueri*;

3 - *F. vulgaris*.

Such distribution on above described groups corresponds to distribution of these species of *Filipendula* genus according to their taxonomy positions. The obtained data demonstrates that the researched species on proximity can be divided into 3 groups: group 1 – the subgenus *Aceraria*, group 2 – subgenus *Ulmaria* and group 3 - subgenus *Filipendula*. In groups accurate division of species is observed according to taxonomical positions. These results correlate with taxonomical picture which is based on morphological features.

It is known that components of essential oil are secondary metabolites which are necessary for adaptation to growth conditions of plants. In this case the position of created cluster in space of the components of essential must depend on the species position of each plant. Thus, the proposed approach which is based on using cluster analysis can be used in solving taxonomy tasks for dividing various species.

On the other hand, herb raw materials can contain other plants. Such raw materials can't be used, and they must be identified and isolated. In this connection the application of cluster analysis of component composition of essential oils can be a methodical basis of implementation of a "fingerprint" technology, which can solve similar tasks enough successfully.

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