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Identification of Geothermal and Non-Geothermal Laban Plant (Vitex Pinnata) With a Combination of Infrared Spectroscopy – Principal Component Analysis Methods

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ABSTRACT
The purpose of this study is to identify laban leaf which originates from Ie Seu'um, Gunung Paro, and Lambaro, with a combination of Spectroscopy Fourier Transform Infrared (FTIR) and Principal Component Analysis (PCA) methods. FITR spectrum pattern from each sample was identified as multivariate using PCA and classified based on similarity or variety of the spectrum. The PCA analysis results of laban leaf samples are separated and forming both good groups as well as diversity percentage which is 96%. The extracted groups can be used to identify the difference between geothermal and nongeothermal location compared to the fresh sample

Keywords: *Laban leaf, FTIR Spectroscopy, Chemometric, PCA*

1. INTRODUCTION

As a mega biodiversity country, Indonesia is rich in medicinal plants. This plants can be used in many medical purposes, such as antibacterial [1] [2] dental therapeutic treatment [3] antimicrobial [4], antibiofilm [5], eczema treatment [6] and so on. Laban (*Vitex Pinnata*) or in Acehnese called "Mane" is a tropical plant in Asia with potential medicinal properties. Almost all of its parts can be used as traditional medicine. The leaves are used as a remedy for fever, loss of appetite, and wound. The bark is reported to able to cure stomach aches and wounds and to be used as a coloring agent. While the roots are used as stomach ache remedies [7]. According to Goh et.al (2017) [8], *Vitex pinnata* contains a variety of secondary metabolic compounds as alkaloid, anthocyanidin, aucubin, coumarin, flavonoid, flavanol, tannin, gallic, iridoid, protein, redactor, steroid, triterpenoid, glycoside. Secondary metabolites in plants are highly depend on the geographical location. Plants that grow in the place with a high mineral level, such as geothermal [9] [10] [11] and coastal [12] areas, are suggested to contain higher secondary metabolites, such as phenol and terpene, than a low mineral area.

A popular method that is often used to identify organic substances, such as coal [13], char [14], protein [15], metabolite [16] and even inorganic one like bone [17], is FTIR. FTIR spectra are the result of interaction among the chemical compounds in the complex sample matrixes. FTIR spectra have rich information of

molecular structure with a series of specific absorption bands for each molecule so that it can be used to differentiate a similar raw material [18]. The advantages of FTIR include fast and simple analysis without prior separation stage [19]. The drawback of FTIR is the direct visual interpretation that is hard to do because of the overlapping absorption spectrum from the molecules in samples. In order to overcome that problem the FTIR analysis result need to be followed by chemometric technique [20]. One of the technique is multivariate analysis that can be used for complex spectrum pattern recognition such as Principal Component Analysis (PCA) [21].

A combination of FTIR and Chemometric methods can be used to identify the variety of plants metabolite contents from different geographical locations. This methods have been used to identify various samples, some of them are Arabica coffee's leaf [22] and wheat samples [23]. The result showed the different pattern of FTIR spectra from the same samples that were collected from different location.

In this research, laban leaves that were obtained from different location, that are residential area of Lambaro, coastal area of Gunong Paro, and geothermal area of Ie Su'um, were identified by FTIR. The FTIR spectra patterns were analyzed by PCA.

2. RESEARCH METHODOLOGY

2.1 Tools and Materials

The tools used in this study is a set of extraction tools, jar, scissors, filter, separating funnel, rotary evaporator, measuring cylinder, and FT-IR spectroscopy device. As for materials, ethanol solvent 70%, and laban leaf obtained from 3 different regions in the Aceh Besar district, which is Ie Seu'um, Lambaro Village and Gunung Paro are used (Table 1).

2.2 Samples Preparation

Samples used in this research include fresh leaves (without preparation), macerated fresh leaves and macerated dried leaves. Fresh leaves are macerated after grinded with mortar and pestle, where the obtained powder is extracted using ethanol 70% for 48 h and concentrated with Rotary Evaporator. For the other kind of sample, the leaves are dried at room temperature for five days. They are then grinded with mortar and pestle. Next, the obtained powder is macerated with ethanol 70% for 48 h and concentrated Rotary Evaporator. All samples are analyzed with FTIR.

Table 1. Samples' labels according to their preparation methods and sampling locations.

Label	Preparation Method	Location
S Ie Seu'um	Maceration (dry sample)	Ie Seu'um
E Ie Seu'um	Maceration (fresh sample)	
D Ie Seu'um	Fresh leaf (fresh)	
S Lambaro	Maseration (dry sample)	Lambaro
E Lambaro	Maceration (fresh sample)	
D Lambaro	Fresh leaf (fresh)	
S Gunung Paro	Maseration (dry sample)	Gunung Paro
E Gunung Paro	Maceration (fresh sample)	
D Gunung Paro	Fresh leaf (fresh)	

2.3. Measurement

The analysis is carried out with FTIR spectroscopy on a wavelength of 400-4500 cm^{-1}. Results of spectra measurement are saved in *Microsoft Excel* format for PCA analysis.

2.4. Statistical Analysis

Before PCA analysis, the obtained data must be preprocessed to minimalize the light scattering effect and relieve noise. Signal processing is done using baseline, smoothing dan SNV. Multivariate analysis from FTIR uptake data (excel file) is done with the PCA method using ***XLSTAT***.

3. RESULTS AND REVIEW

3.1. Laban Leaf (Vitex Pinnata) FTIR Spectrum

The FTIR analysis of laban samples showed similar functional groups absorption for all samples, with the intensity as the exception (Figure 1). Those similarities suggested that the chemical compound in all samples was probably almost similar, however different in concentration level.

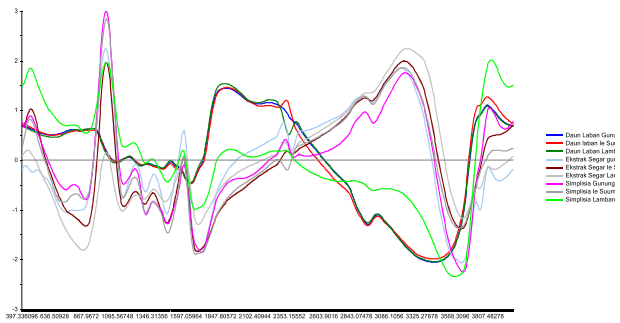

Figure 1. FTIR Spectra of fresh laban leaves, macerated fresh laban leaves, and macerated dried laban leaves obtained from Ie Seu'um, Gunung Paro, and Lambaro areas.

Functional groups that were identified by all of the laban leaves (*Vitex Pinnata*) FTIR spectra are acid O-H (3340 cm^{-1}), C-H stretching (2927 cm^{-1}), C=O (1631 cm^{-1}), C-H bending (1431 cm^{-1}), and C-O (1076 cm^{-1}). Based on the band characteristic from the functional unit detected by FTIR, it was predicted that the compounds contained inside the samples were carboxylic acids and esters.

3.2 Principal Component Analysis (PCA)

The main objective of PCA is to find a pattern, similarity, or difference among samples in variables of data [24]. In PCA procedures, FTIR spectrum signal processing needs to be done to increase PCA ability in grouping samples without losing major information in the total variation calculation process. The processing is done using baseline, smoothing dan SNV.

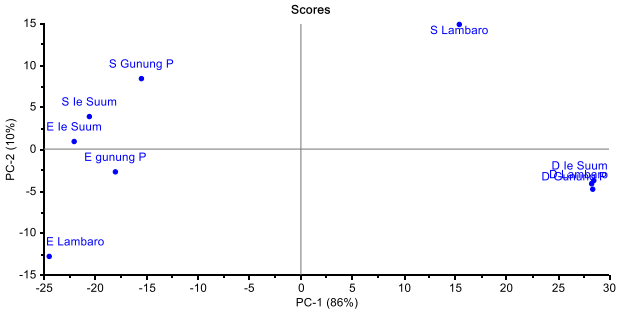

Figure 2. PCA plot of the fresh laban leaves, macerated fresh laban leaves, macerated dried laban leaves obtained from Ie Seu'um, Gunung Paro, dan Lambaro areas.

The PCA results showed that there was a similarity from the leaf FTIR spectra. All three fresh leaf spectra from three sampling locations formed one group. Meanwhile, the macerated samples form another three separated groups.

The variety level that can be explained from the PCA, where for PC1 is 86% and PC2 is 10%. Therefore, the total variety level reached 96%, where statistically the value was considered good enough to determine the correlation among variables.

Based on the analysis description of the PCA spectrum of the fresh laban leaves from three sampling locations description sampling (D Ie Seu'um, D Gunung Paro, dan D Lambaro), it showed a very identical pattern. Differences of spectrum pattern against the sampling locations can only be observed after samples are extracted with maceration. This is due to the fact that those samples form their own groups respectively according to their collected locations. Nevertheless, Gunung Paro and Ie Seu'um still formed the same group. This can be ascribed by the similarity of ground mineral contents in both locations. Ie Seu'um and Gunung Paro regions have a high concentration of ground chloride. Ie Seu'um is a geothermal region, therefore the chloride is originated from the geothermal manifestation [25]. Meanwhile for Gunung Paro, since it is a coastal region, the chloride is originated from the seawater.

4. CONCLUSION

A combination of FTIR and Chemometric methods can be used to identify and differentiate the types of laban plant which collected from Ie Seu'um, Gunung Paro, dan Lambaro. The PCA results show a good variety level, which is 96%. More specifically, the PCA from extracted samples can be used to identify the difference between geothermal and non-geothermal location compared to fresh samples.

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