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## Prediction of chemical content in patchouli oil (*Pogostemon cablin* Benth) by portable NIR spectroscopy

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## Prediction of chemical content in patchouli oil (*Pogostemon cablin* Benth) by portable NIR spectroscopy

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**Abstract.** The objective of this study was to develop the calibration model for predicting the patchouli alcohol in patchouli oil by portable Near Infrared (NIR) spectroscopy. Patchouli oil samples were obtained from different origin in Indonesia. Portable NIR spectrometer with wavelength of 760-1050nm was used to collect the spectra of the patchouli oils. The calibration model was developed by partial least square regression (PLS). The best model for predicting patchouli alcohol content is  $y = 0.7209x + 8.2804$  with  $r = 0.86$ ,  $SEC = 2.04\%$ ,  $SEP = 2.16\%$ ,  $CV = 7.6$ ,  $RPD = 1.8$ .

### 1. Introduction

The essential oil is natural extraction from various certain plants. The part of the plant that could be extracted is leaf, flower, wood, and seeds [1]. Currently, there are 150 plants that produce essential oil. The amount of it that being trade internationally is 70 and 40 of it comes from Indonesia. Due to this amount of it, the essential oil is one of Indonesia's predominant export commodities [2].

Patchouli oil is one of the essential oil that belongs to a high selling value export commodity [3]. This oil obtained through steam or water distillation. The main material used can be stem or leaf of patchouli [4]. The quality of oil produced depends on the distillation time and part of the material used [5]. Patchouli alcohol is the major content of patchouli oil that used as quality and price determination. The assessment of its quality usually uses chemical laboratory analysis. This method is accurate yet takes a long time and high cost. Therefore nondestructive method that efficient in the time and cost is needed in order to determine the quality of patchouli oil rapidly. One of technology that can be used is near-infrared spectroscopy (NIRS).

NIRS is a fast analysis method as well as nondestructive that relate to chemometric. The use of this method is appropriate for solid, liquid and biotechnology analysis. On the other hand, NIRS could be implemented in the production process for process monitoring or used in the laboratory for quality control [6]. NIR is enable to predict virgin olive oils. The information about the composition of olive oil given by NIR through real time [7]. FT NIRS can be used to analyze the mixed of crude palm oil and canola oil from the various vendor [8]. The use if NIRS also can classify extra virgin oils based on cultivar [9]. NIRS succeeded to classify patchouli oil based on the origin precisely and accurately [10]. Currently, Portable NIR has been developed so that it easy to use directly in the field. The portable spectrometer is appropriate to use as a daily scanner for customer due to its simplicity, ability to sync and upload measure data wirelessly, and automatically construct data model [11]. Based on the



explanation above, it is necessary to use NIRS as a method to determine the patchouli oil content that has produced from different region in Indonesia.

## 2. Material and Method

The materials used in this research are 30 samples of patchouli oil that obtained from different regions in Indonesia (Konawe, Kolaka and Masamba from Sulawesi island, Bogor, and Garut from west java and Aceh and Jambi from Sumatra). Instrument used in this study was a portable spectrometer SCiO by Consumer Physics (wave length 760-1050 nm) that used for measuring wave spectrum of patchouli oil samples, *liquid scan accessory* used as a tool for laying the *portable spectrometer* when the measuring in order to avoid the sink of SciO sensor in the oil. GC-MS was utilized to determine the content of clove oil. Furthermore, the software used in this research is *SCiO Lab: Developer Toolkit*, *Octave-4.2.1*, *The Unscrambler X 10.4*, dan *Microsoft Office Excel*. There are five steps of patchouli oil determination nondestructively using *Near Infrared Spectroscopy*; (1) samples preparation, (2) Measurement using GC-MS, (3) wave spectrum data intake using NIR, (4) Pre-treatment data process, and (5) development of calibration and validation model.



**Figure 1.** Spectra acquisition using portable spectrometer

## 3. Results and Discussion

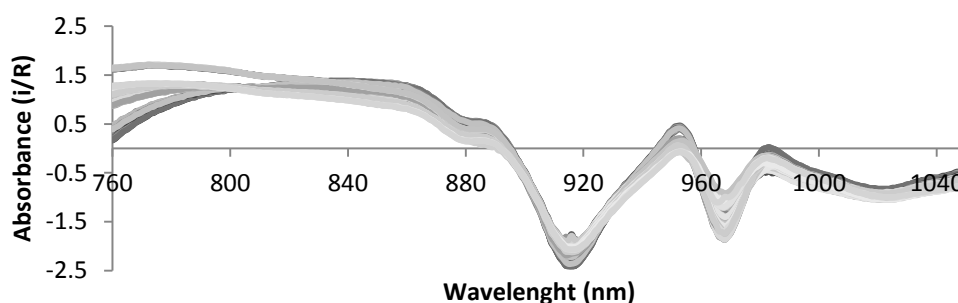
Patchouli oil content was measured using GC-MS method. The results of then used as reference data for prediction model development. The prediction model that was obtained from the correlation between NIR spectrum was shot into patchouli oil with reference data. Hence, the reference data determines the success of predicting quality parameters value of patchouli oil using NIR. GC-MS showed that the content of patchouli oil is patchouli alcohol ( $C_{15}H_{26}O$ ) (Table 1).

**Table 1.** Chemical characteristic of the patchouli oils based on the main chemical component (Patchouli-Alcohol  $C_{15}H_{26}O$ )

Sample	% of the component
Jambi	32.26
Aceh	30.91
Kolaka	26.46
Konawe	29.81
Masamba	24.15
Garut	30.98
Bogor	24.18
average	28.39
Standard deviation	3.40

The collected spectra from portable spectrometer of 760-1050nm was the normalized transfectant spectra data. Spectrum normalized data is a spectrum that already passed through pre-treatment SNV. Pre-treatment SNV is used for minimizing basic variation and deleting multiplicative interferences from scattering effects of spectrum data [12]. Each peak and the valley of the wave on the spectrum could be interpreted that the materials contain different chemical compound [13]. The spectrum peak of the NIR is affected by the chemical compound in the materials as well as physical characteristic in the materials. The absorption of wavelength on the chemical compound of a material on a transfectant spectrum is showed by the peak. The peaks of absorption occurred due to vibration and strain on atomic bond group O–H, N–H, and C–H that are major components as organic compound forming [14]. The high amount of chemical percentage in a material will cause high absorption. This cause the peak on a transfectant spectrum will get deeper.

The absorption peaks on NIR transfectant of patchouli oil occurred on the 915 and 969 nm wavelength. The deepest absorption peaks occurred on the 915 nm wavelength indicated a high percentage of the chemical compound in patchouli oil. However, the lack of information and reference regarding the chemical compound of material on the <1000 nm wavelength make it difficult to determine the kind of detected chemical compound.



**Figure 2.** Original transfectant spectrum of patchouli alcohol

The NIR's transfectant spectrum data of patchouli oil was processed using PLS. PLS used because of the obtained data as numeric data. PLS is a quantitative analysis method that has been a wide reference for evaluating the quality and suitable for linear analysis. PLS could reduce the data dimension in order to find the relevant factors in predicting and interpreting the data. This method produces a better calibration method than PCR [15].

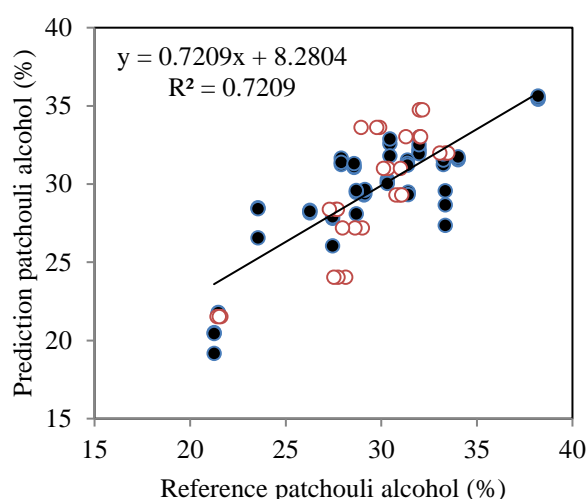
The prediction model of patchouli alcohol content from patchouli oil samples was developed based on the correlation of NIR transfectant spectrum data with data on the chemical content of GC-MS test results. Ideally, all samples should cover a homogeneous calibration range. Two-thirds of the total sample is used for calibration, while 1/3 of the total sample is used for validation. The spectrum of the same sample must be kept together and put in either the calibration set or the validation set. The spectrum with the lowest concentration (minimum) and highest (maximum) must be selected for the calibration set. The purpose of the calibration is to build a mathematical equation model that can be used to predict the chemical content of the material without having to take direct measurements that damage the material [14].

The NIR transfectant spectrum data obtained contained background and noise which caused the prediction model to be less accurate. This is influenced by the nature of scattering and absorption by a material. The disturbance can be reduced or partially eliminated with the help of proper pre-treatment data during processing [12]. Data pre-treatments were carried out with the aim of improving spectra quality and reducing or eliminating unwanted effects on spectrum data without affecting spectroscopic information needed for predictions [16]. Data pre-treatments are applied before calibration and validation are carried out. Pre-treatments carried out in this study were smoothing (SGs) and de-trending (DT). Smoothing Savitzky-Golay (SGs) derives from the idea that around the spectrum measurement points can be installed by low polynomial degrees [17].

**Table 2.** Results of calibration and validation of patchouli alcohol content of patchouli oil with several pre-treatments

Processing	PLS Factor	Calibration			Validation		Consistent (%)
		r	SEC (%)	SEP (%)	RPD	CV (%)	
Original	F4	0,87	2,04	2,16	1,8	2,73	94,56
SGs	F4	0,86	2,05	2,16	1,8	2,94	94,94
DT	F3	0,85	2,15	2,29	1,7	2,62	94,22

The value of RPD 1.86 states that the estimation model is feasible. The value of RPD will be inversely proportional to the value of the CV so that the higher the RPD, the CV value will be smaller. The best model for predicting patchouli alcohol content is  $y = 0.7209x + 8.2804$ , without using pre-treatment ( $r = 0.87$ ,  $SEC = 2.04\%$ ,  $SEP = 2.16\%$ ,  $CV = 2.73\%$ ,  $RPD = 1.8$ ). The results of the prediction of the best calibration model for patchouli alcohol content in patchouli oil can be seen in Figure 3.

**Figure 3.** Calibration model for patchouli alcohol

#### 4. Conclusion

From the results of GC-MS test it can be seen that 30 patchouli oil samples on average contain 28.39% patchouli alcohol as the most dominant chemical content. The absorption peak by the chemical content of patchouli oil occurs at a wavelength of 915 nm as the highest absorption peak and 969 nm. Calibration and validation was done by the Partial Least Squares (PLS) method. The best model for predicting patchouli alcohol content is  $y = 0.7209x + 8.2804$ , without pretreatment ( $r = 0.86$ ,  $SEC = 2.04\%$ ,  $SEP = 2.16\%$ ,  $CV = 2.73$ ,  $RPD = 1.8$ ).

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