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Evaluation of the patchouli essential oil (*Pogostemon cablin* Benth.) aromatic characteristic by near-infrared spectroscopy

Diego Mauricio Cano-Reinoso[1], Yohanes Aris Purwanto[1,*], I Wayan Budiastra[1], Shinichiro Kuroki[2], Sutrisno[1], Slamet Widodo[1]

[1]Department of Mechanical and Biosystem Engineering, IPB University, 16680, Dramaga, Indonesia
[2]Graduate School of Agricultural Science, Kobe University, 1-1 Rokkodai-cho, Nada-ku, 657-8501, Kobe, Japan
*Corresponding author: arispurwanto@apps.ipb.ac.id

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ABSTRACT This study aimed to evaluate the aromatic characteristic of patchouli essential oil (*Pogostemon cablin* Benth.) by near-infrared spectroscopy combined with chemometric treatments. The study used 84 oil samples collected from around Indonesia, namely in Konawe, Kolaka, Bogor, Garut, Aceh, Jambi, and Masamba. Several pretreatments were used to process the spectral data, together with the application of partial least squares. The spectrum wavelength applied was between 1000 and 2500 nm. The spectra data were separated to develop two models based on their physical and chemical properties (Bogor, Garut, Konawe, and Kolaka in the first model; Aceh, Jambi, and Masamba in the second one). Liquid chromatography-mass spectrometry (LC-MS) was used as a reference method. Patchouli alcohol was established as the main chemical compound of this aromatic oil. The best calibration for the first model was that with mean center normalization as a data pretreatment, while for the second model, it was the one using the second derivative. Both models had a correlation coefficient higher than 0.90 and a coefficient of variation lower than 2.98%. In conclusion, near-infrared spectroscopy can be employed as an accurate tool to determine the characteristic of patchouli oil.

KEYWORDS Non-destructive; Patchouli alcohol; PCA; PLS; Quality

1. Introduction

Aromatic plants are abundant in Indonesia. Those plants are easy to maintain and harvest, creating a preference for small farmers (Ramya et al. 2013; Diego et al. 2018; Cano-Reinoso et al. 2021). Aromatic plants typically are used in fragrances, medicine and culinary, with the perfume industry as one of the largest consumers. Patchouli (*Pogostemon cablin* Benth.), from the family of Lamiaceae, is cultivated mainly for its essential oil, used principally in aromatherapy, perfumery, and cosmetics (Ramya et al. 2013; Diego et al. 2018; Cano-Reinoso et al. 2021).

In Indonesia, patchouli plant is cultivated in the last 100 years ago. The biggest areas with the best production are Sumatra, Bengkulu, Lampung and east of Java (Diego et al. 2018; Cano-Reinoso et al. 2021). Indonesia produces around 80% of all world market; meanwhile, the remaining 20% comes from countries like Malaysia, the Philippines, China, India and Brazil (Sandes et al. 2016; Diego et al. 2018; Cano-Reinoso et al. 2021).

The industry considers Indonesian patchouli oil as one of the best qualities. However, this oil suffers irregularities due to the origin of its raw material implemented in the production (Diego et al. 2018; Dantas et al. 2020; Cano-Reinoso et al. 2021). Usually this situation is associated with problems in the postharvest process of the patchouli plant, making necessary the study of its properties by the chemical composition of the final oil product.

Chemical composition of an oil can be detected employing destructive methods like gas chromatography (GC), and gas chromatography-sniffing (Daferera et al. 2002; Cseháti et al. 2005; Nikolić et al. 2014). For example, Silva-Filho et al. (2016) studied the impact of patchouli oil on leukocyte behavior and the inflammatory response, using GC to show the most abundant chemical compounds of the oil. In the same way, Yahya and Yunus (2013) investigated in Malaysia the influence of the oil extraction time required to obtain an ideal chemical content , employing steam distillation derived from patchouli oil; for that, a GC test of patchouli oil was implemented. Besides, previous studies employing also GC demonstrated that the essential compound of this oil is known as patchouli alcohol $C_{15}H_{26}O$, a sesquiterpene responsible for its aroma and pharmaceutical characteristics (Yahya and Yunus 2013; Sandes et al. 2016). Nonetheless, there are issues associated with any destructive method like GC, which are the consumption of time and the com-

plexity of the process (Widoretno 2016; Diego et al. 2018; Cano-Reinoso et al. 2021).

Given this current situation, the development of an appropriate tool to determine the quality of patchouli is becoming a priority. Therefore, methods such as Near-Infrared Spectroscopic (NIRS) applying chemometric treatments can be successfully implemented as an innovative and rapid analysis for a non-destructive determination in patchouli oil production. For example, NIRS has been used for the detection of chemical properties linked to free acidity, peroxide values, fatty acids, together with the determination of possible adulterations and geographical classification in olive, camellia, and peanut oil (Wang et al. 2017; García Martín 2022).

Despite concerning aromatic patchouli oil still there is no enough documentation about the application of NIRS; based on the previous mentioned information this tool has a considerable potential to be promoted in this field in terms of quality assessment. Therefore, the study aims to evaluate the patchouli essential oil aromatic characteristic by NIRS developing a calibration model to predict its main chemical compound.

2. Materials and Methods

2.1. Samples and NIRS machine

Several plastic bottles containing patchouli oil (total of 84) were collected from seven places around Indonesia; Konawe, Kolaka, and Masamba from Sulawesi, Bogor and Garut from West Java, and Aceh and Jambi from Sumatra island. Fifty mL of oil sample were employed, put inside labeled recipients, and organized according to their geographical origin. Oil as a raw material has been proved to provide an ideal response regarding data acquisition and chemometrics analyzing during NIRS applications (Wu et al. 2013; Sandes et al. 2016). It also follows the recommendations of the Indonesia National Standard (INS) for the manipulation and study of these samples. Also, the samples manipulated in this experiment follow the recommendations of the Indonesia National Standard (INS), associated with the quality determination of aromatic oils.

The machine used in this research was an FT-NIR SPECTROMETER (Fourier Transform Type) NIRFlex N-500, which has demonstrated reliable analytical results for quality control, research and development in the pharmaceutical industry, chemical, food, drinks and feeding, which is the same tool employed in the previous studies of Cano-Reinoso (2018) and Diego et al. (2018).

2.2. Collection procedures and data processing

2.2.1 Measuring procedure of near-infrared in laboratory

The spectrum of the samples was analyzed using a transflectance examination; similar method applied in Cayuela and García (2017) and Cano-Reinoso et al. (2021). Figure 1 exposes the arrangement elaborated for the application of NIRS, including an explanatory scheme concerning the methodology applied to obtain the respective transflectance spectra. The device was set to measure liquid samples, taking advantage of its characteristics. Processed transflectance spectra typically works in function of the transmittance and reflectance spectrum (Cano-Reinoso 2018; Diego et al. 2018; Cano-Reinoso et al. 2021)

The oil was arranged in a small bottle of 3 cm of height with 1.5 cm of diameter. In there, the gun was introduced to carry out the measuring. First, the near-infrared (NIR) radiation coming from the optical fiber (gun) goes through the liquid oil sample; the NIR signal is reflected by a white background surface generating contact with a sensor. And after that , the signal backs through the oil sample, heading to the spectrometer detector (Cano-Reinoso 2018; Diego et al. 2018).

2.2.2 Obtainment of patchouli spectra

The transflectance spectra was captured by scanning the samples 3 times at 3 different points, arranging the gun inside the oil recipient. Thereafter, the spectra momentary were converted to absorbance to carry out the respective spectra graphic analysis. The wavelength interval employed was between 1000-2500 nm, as recommended in previous experiments of Ozaki (2012) and Cano-Reinoso et al. (2021).

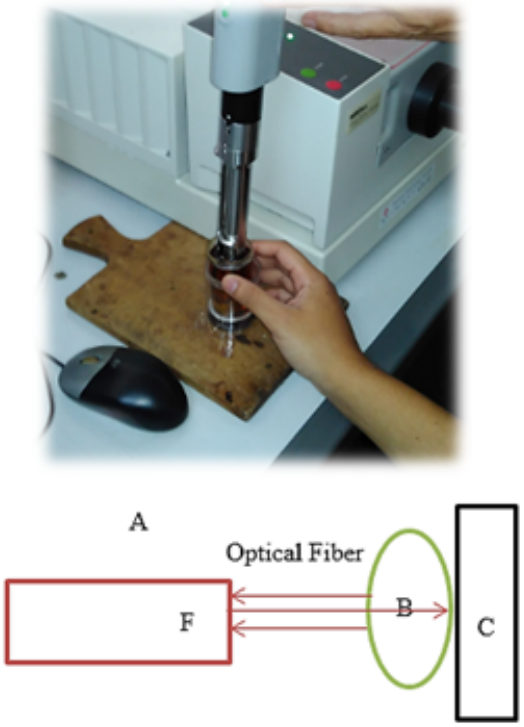

FIGURE 1 Schematic example of the NIRS arrangements and methodology employed in the laboratory to obtain the transflectance spectra. A: Gun with the NIR signal and spectrometer detector, B: Oil sample, C: White background, F: Reflectance Sensor.

2.2.3 Chromatography analysis

The main chemical compound of Patchouli alcohol ($C_{15}H_{26}O$) was determined by liquid chromatography-mass spectrometry (LC/MS). During this process, the oil samples are separated in a mixture of individual components where each component is identified (qualitatively) and measured (quantitatively) (Gokulakrishnan et al. 2013; Murugan and Mallavarapu 2013; Diego et al. 2018). Results were organized according to the percentage of concentration of patchouli alcohol per sample.

2.2.4 Processing and spectra treatment

Partial Least Square (PLS) analysis was carried out with the final transflectance spectra to elaborate a linear correlation between the NIR uptake value and the chemical data employed following the same procedure described in Diego et al. (2018) and Cano-Reinoso et al. (2021). The spectra were not transformed to absorbance to execute the calibration of the model, although absorbance spectra graphic was assessed to select the target wavelength range to determine the essential oil chemical concentration, as mentioned in the previous sections (Kuriakose and Joe 2013; Dupuy et al. 2014). Data pretreatments such Smoothing Savitzky-Golay, normalization mean center, and first and second derivatives were adopted (Polynomial order of two, three smoothing points, left and right sight point of one), as recommended by Lee et al. (2014) and Diego et al. (2018). Due to the liquid characteristics of the samples, there were not detected uneven surface and scattering effects and particle size and multicollinearity changes.

Normally patchouli oil has terpenes, alcohols, aldehydes and esters that interact and provide a unique smell. It has been stablished that patchouli alcohol is the essential chemical component that determines the smell of patchouli oil. In addition, other chemical components such as β-patchoulene and α-patchoulene, have been proved to deliver structural characteristics and physical properties to patchouli oil (Yahya and Yunus 2013; Cano-Reinoso 2018; Cortés et al. 2019).

Yahya and Yunus (2013) explained that there is an improvement of patchouli oil quality associated with an increase on its extraction time. Nevertheless, after a detailed observation, it was detected that some chemical components tend to decrease also with the increase of this extraction time. This phenomenon has been attributed to the side reaction that typically occurs between the carbon double bond and oxygen or hydroxyl ion that converts some chemical species into another form, generating a decrease in the percentage of the chemical content; besides, this described circumstance can cause the rise of other components with the same number of carbons, as mentioned previously in Hu et al. (2006) and Yahya and Yunus (2013). Therefore, taking in account the previous consideration, it is possible to infer that commonly if there is a long extraction time, higher patchouli alcohol content could be obtained. As a result, the most optimal quality of patchouli oil can be detected at ten h, when 47% of patchouli alcohol is extracted employing a steam distillation (Yahya and Yunus 2013).

Consequently, this research divided the calibration models for the PLS analysis into two groups, one for Konawe, Kolaka, Bogor and Garut and the other one for Jambi, Masamba and Aceh samples. The criteria for this process were based on the chemical and physical characteristics of the spectra obtained, and the (LC/MS) results analyzed, similar with the methodology implemented in Diego et al. (2018) and Cano-Reinoso et al. (2021). The chemical composition of the oil manipulated, and physical properties like the odor and color were highly influenced by the extraction time, the extraction method, and the harvest period of the patchouli plant, and the manipulation of the oil before arriving at the laboratory. All these conditions gave an NIR spectra differenced in two groups, especially on the wavelength peaks where literature established the aromatic oil properties (Cano-Reinoso 2018; Cano-Reinoso et al. 2021).

The statistical parameters determined to test the performance of the built calibration model were based on Cano-Reinoso et al. (2021). Those parameters were, correlation coefficient (r), the root mean square error prediction (R_{MSEP}) (Equation 1), coefficient of variation (C_V) (Equation 2), and standard deviation ratio with R_{MSEP} (R_{PD}) (Equation 3). A good calibration model has a near-zero R_{MSEP} values, low C_V, and high r and R_{PD} values.

$$R_{MSE} = \sqrt{\frac{1}{n}\Sigma_{i=1}^{n}(Y_{NIRS} - Y)^2} \quad (1)$$

$$C_V = \left(\frac{R_{MSEP}}{\overline{Y}}\right) \times 100\% \quad (2)$$

$$R_{PD} = \frac{S_{Dp}}{R_{MSEP}} \quad (3)$$

Where n is equal to the number of samples, Y_{NIRS} is the result of the prediction by NIRS, Y is the current valor of the property analyzed, $\overline{Y}$ is the average valor of the analyzed property, and S_{DP} is equal to the stander deviation of the prediction.

3. Results and Discussion

3.1. Analysis of the chemical results and patchouli oil spectra

The differences exhibited are shown in Table 1. The results indicate the valor of patchouli alcohol ($C_{15}H_{26}O$) among the patchouli oil types. The table evidences a difference between the seven types of oil based on its main chemical percentage.

Wu et al. (2013) explained that the essential primary secondary metabolites present in patchouli are essential oil (up to 5%) and tanitos (1.7%). The essential oil consists mainly of sesquiterpenes and alcohol of patchouli. On the other hand, a comparison between essential oil

TABLE 1 Results of the chemical composition of the patchouli oil based on the main chemical component (patchouli alcohol $C_{15}H_{26}O$) by gas chromatography.

Patchouli Oil		
Patchouli Alcohol $C_{15}H_{26}O$		
Samples	**Percentage of the component (Average)**	**Standard Deviation (SD)**
Jambi	33.46	0.79
Kolaka	27.18	0.95
Aceh	29.49	1.04
Konawe	29.81	0.71
Masamba	28.75	0.93
Garut	31.79	1.06
Bogor	24.18	0.18
Range	24 – 34%	0.81

compositions was elaborated between *Pogostemon cablin* and *Agastache rugosa*, founding that the essential components of the patchouli oil were seychellene, bulnesene, β-guaiene, patchouli alcohol, β-longifolene, thujopsene and β-patchoulene (Cano-Reinoso et al. 2021). Similarly, Dũng et al. (1989) has also previously investigated the chemical characteristics of the patchouli oil produced in Vietnam. In this study, patchouli alcohol was exhibited in a range between 32 to 38% from the total patchouli oil content. In addition, ten more chemical compounds were identified, highlighting β-bulnesene and β-guaiene.

The percentage of the level of patchouli's alcohol mean outcomes had representative differences. Jambi obtained the highest one among every type of oil (33.46%) followed by Garut (31.79%), and konawe (29.81%);finally, the lowest results observed were in Bogor and Kolaka, obtaining 24.18% and 27.18%, respectively. Yahya and Yunus (2013) and Diego et al. (2018) mentioned that the usual level of patchouli alcohol can range between 24 to 34%. Moreover, former studies have proved that differences among that range can be generated by the extraction method of the oil in the field, and the quality of its seeds cultivated (Sandes et al. 2016; Cano-Reinoso 2018; Dantas et al. 2020). Due to sample reception conditions of the raw material in the laboratory such information was unknown;

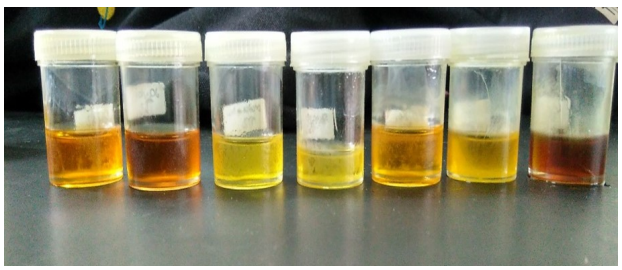

FIGURE 2 Patchouli oil samples used in the experiment with their respective colour. From left to right: Aceh, Jambi, Masamba, Bogor, Kolaka, Konawe and Garut

nevertheless, by observing physically the samples, essentially their colour, it could be possible to infer that those parameters were different from every oil production place. Besides, this particularity can explain why some oils from the same area had different percentages of patchouli oil chemical content.

Furthermore, previous laboratory evaluations noticed that there were samples brighter than others, also that the aroma was highly related to the color. Between darker the color of the samples, the more pungent odor these spreads compare to the brighter ones. The colour of the difference samples employed in this experiment is shown in Figure 2. Based on the physical appearance exposed in this figure, and the previous explanation it is possible to indicate that samples from Garut and Masamba had a higher percentage of patchouli alcohol, and also could have more elevated content of other chemical compounds like α and β-guaiene, seychellene. This physical particularity was also observed by Hasegawa et al. (1992), during its experiment manipulating and collecting patchouli oil aromatic compounds.

Subsequently, Figure 3 was elaborated to expose how the NIR spectra obtained in the laboratory reflect the patchouli oil analysis results by LC/MS. This figure evidences that almost all transflectance spectra are similar; however, by the study of the chemical percentage results, there was evidence of the possible differences among chemical properties of the oil samples.

3.2. Calibration of the model by PLS

Based on Burns and Ciurczak (2002) and Ozaki et al. (2013), in a spectrum graphic of an agricultural based product it is possible to observe that every peak and valley have a meaning and an influence. Usually in a spectrum graphic of this type of products, the wavelength of 1680 and 2230 nm are are considered, water is located at 1940 nm, lignin is 2270 nm, 2336 nm is associated with cellulose, while 2180 nm to protein, and finally carbohydrates are found at 2100 nm. However, diverse studies have determined that generally for an oil the assessment of its main characteristics is located at the wavelength of 2310 nm, close to the combined region of a NIR spectrum (Kuriakose and Joe 2013; Diego et al. 2018; Cano-Reinoso et al. 2021). Williams (2001) and Ozaki (2012) formerly determined the main chemical composition of an oil in the combined region of a typical electromagnetic wave. They mentioned that in the wavelength peak of 2200 nm, the group –CHO (C-H stretch/C==O, stretch combination) could be found, which is highly related to the chemical constitution and structure of patchouli alcohol ($C_{15}H_{26}O$).

Figure 4 shows the trend of the wavelength of the samples organized for the first and second model. The most elevated peak on the spectra graphics was detected among 2220 and 2400 nm; as a result, this peak could represent the patchouli alcohol level of each of the samples manipulated for every model. Therefore, after analyzing this trend on the spectra, and the previous information about the meaning of the oil electromagnetic wave, it was concluded that the wavelength between 2220 until 2400 nm

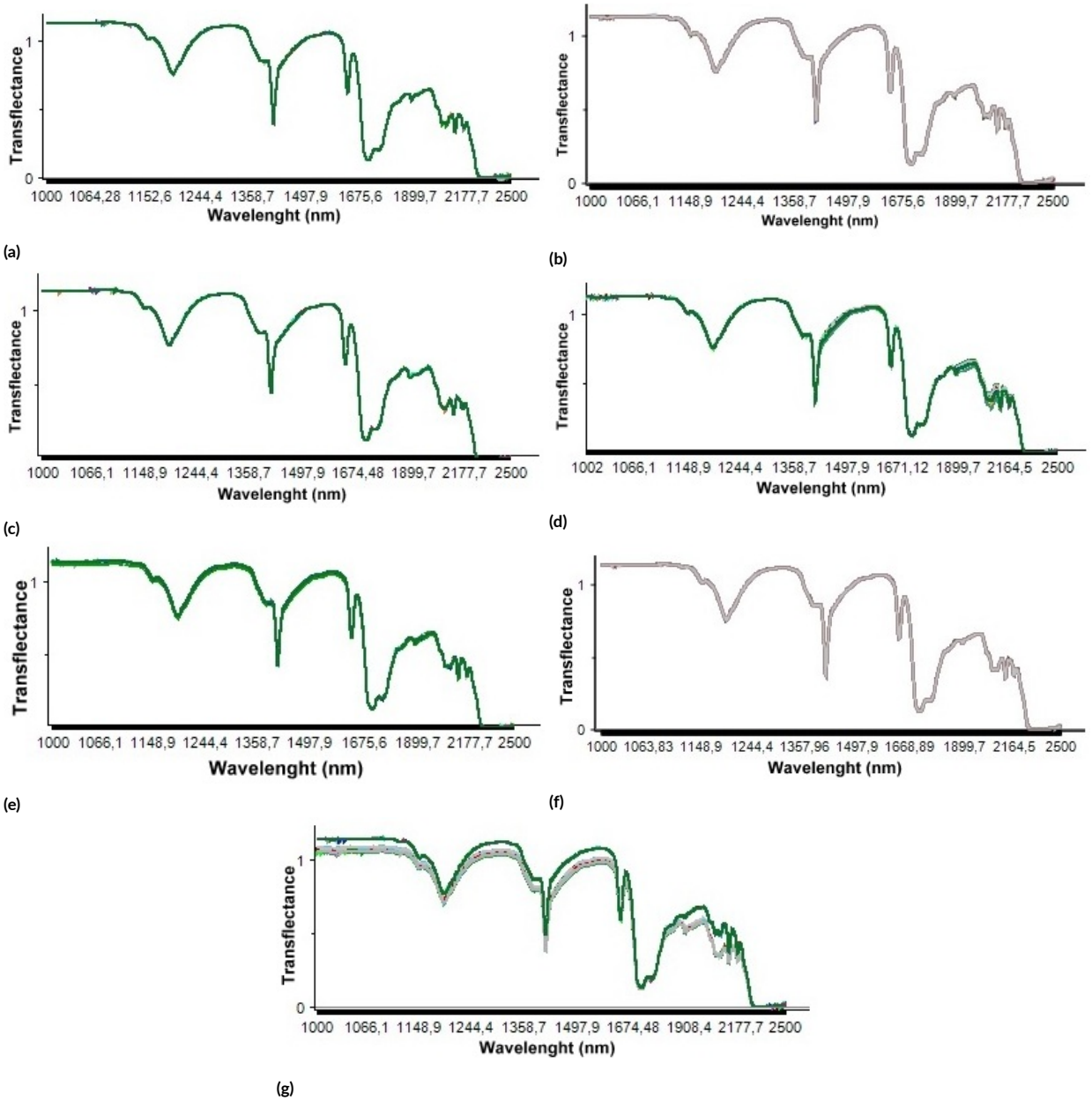

FIGURE 3 Transflectance spectra of different types of patchouli oil tested. Axis X: Wavelength (nm), Axis Y: Transflectance. a: Aceh, b: Bogor, c: Garut, d: Jambi, e: Kolaka, f: Konawe and g: Masamba.

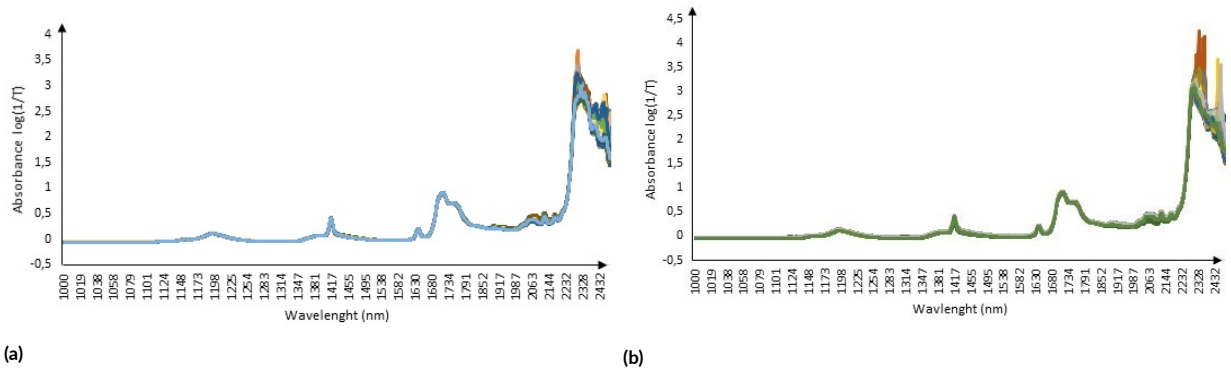

FIGURE 4 Absorbance spectra of the first and second model showing the trend of the wavelength between 2220 to 1800 nm. a: Konawe, Kolaka, Bogor and Garut. b: Masamba, Jambi and Aceh.

should be used to determine the patchouli alcohol content, and to carry out the calibration of the NIR model. In addition, there were other peaks detected, for example,, from 1790 to 1660, 1660 to 1600 and 1440 to 1400 nm, where aromatic properties could be exhibited (Burns and Ciurczak 2002; Cortés et al. 2019).

Pretreatments in the transflectance data were carried out as described in Lafhal et al. (2016) and Cano-Reinoso (2018). The parameters to determine a correct calibration of the model improves after applying some of them. The calibration model is evaluated based on statistical analysis and parameters like r, SEC, SEP, CV, RPD and consistency.

Based on Williams (2001) and Ozaki (2012), optimal predictive models have a r close to 1; consistency values in the range between 80 and 110%, and a SEC and SEP with a value close to 0. Besides, a significant difference between the SEC and SEP values generates an ideal model; otherwise, if this difference is not significant, the calibration set is considered as no representative on the validation set (Lammertyn et al. 2000; Cano-Reinoso et al. 2021). In addition, an RPD value should be greater than 2 (Lebot et al. 2009).

The Table 2 exposes the optimal calibration for the first model with normalization mean center as a data pretreatment; In this case, the factor number 5 provided the best calibration during the process. On the other hand, the optimal calibration for the second model was obtained with

TABLE 2 Result of the calibration and validation of the models by PLS analysis.

First Model							
Treatment	**Factor**	**r**	**SEC(%)**	**SEP(%)**	**CV(%)**	**RPD**	**Consistency**
original	5	0.978	0.684	0.778	2.36	4.85	87.983
Sm	5	0.978	0.689	0.771	2.38	4.81	89.433
D	5	0.965	0.856	0.847	2.96	3.87	101.275
Sm+D	5	0.964	0.871	0.831	3.00	3.81	104.910
N	5	0.980	0.658	0.759	2.27	5.04	86.656
D+N	5	0.975	0.724	0.912	2.50	4.58	79,473
Second Model							
Treatment	**Factor**	**r**	**SEC(%)**	**SEP(%)**	**CV(%)**	**RPD**	**Consistency**
original	4	0.910	0.908	0.920	2.93	2.43	98.845
Sm	4	0.910	0.908	0.920	2.93	2.43	98.824
D	4	0.929	0.811	0.894	2.62	2.72	90.718
Sm+D	4	0.927	0.823	0.870	2.65	2.68	94.624
N	4	0.920	0.858	0.876	2.77	2.58	97.908
D+N	4	0.927	0.821	0.874	2.65	2.69	93.940

*First model: Kolaka, konawe, Bogor and Garut. Second model: Jambi, Masamba and Aceh. D: 2nd derivative, Sm: Smoothing, N: Normalization mean center and Original: Transflectance spectra.

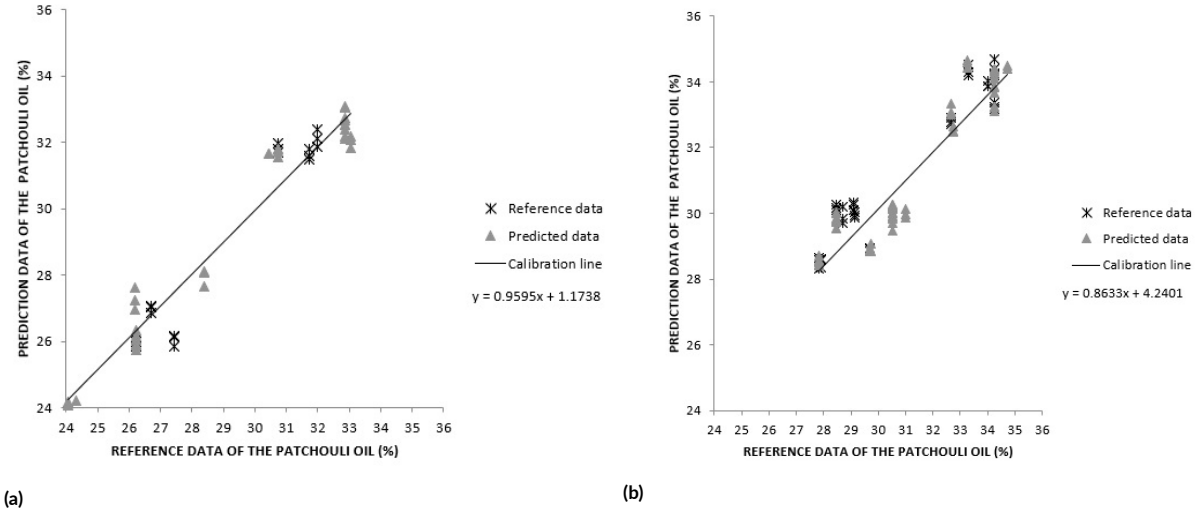

FIGURE 5 Plot of the dispersion data showing the outcomes of the models elaborated using NIRS against the results of the reference method, based on the percentage (%) of patchouli alcohol. a: Second Model, b: First model. V: Validation data, K: Calibration data.

second derivative pretreatment, applying the factor number 4. Indeed, these results are highly related to the chemical transflenctance characteristics of the spectra studied.

Williams (2001) suggest that derivate pretreatment is applied to resolve two basic problems in NIR spectra: the overlapping peaks, and the significant baseline variations. The trend of the graphics spectra demonstrated that the derivate pretreatment in the case of the second model, could decrease the baseline variations permitting a better calibration, based on the chemical characteristics represented among the wavelength peak. Furthermore, the water content of the samples could have influenced the trend of the spectra graphics. Commonly, agricultural products have a considerable water content, which creates spectra graphics shapes almost similar in some cases (Burns and Ciurczak 2002; Cano-Reinoso 2018). Derivate pretreatments avoid that situation, separating the shapes, analyzing it, and helping calibrate a model in function of the chemical composition. In conclusion, samples of Masamba, Aceh and Garut of the second model had a higher water content than samples of the first model, making necessary the application of the derivative pretreatment.

In the case of the normalization mean center pretreatment, Williams (2001) and Ozaki (2012) sustain that the normalization can spread the range or gap between one baseline shape to another and correct it. This procedure means that for example, in the area of the graphic analyzed, wavelength between 2220 to 2400 nm, there were some baseline spectra with a small gap; afterward, these gaps were extended by the application of the normalization pretreatment, displaying as a result better outcomes of the calibration parameters, helping to determine in detail the patchouli alcohol level.

Overall, the chemical content outcomes of the patchouli alcohol have more overfitting in the samples obtained from Konawe, Kolaka, Bogor and Garut than those of the second model; for that reason, the normalization pretreatment was a more ideal option for the first model. Additionally, pretreatments like, smoothing Savitzky-Golay did not produce a meaningful change on the spectra of both models, based on the results of the parameters evaluated in the calibration.

In Figure 5 shown the dispersion graphic of the results for the calibration models developed. there were used 54 data of the spectra wavelength; meanwhile, in the case of the second model, there were implemented 114. Besides, the model's CV was intended to decrease as much as possible the result obtained in function of the standard deviation of the reference method.

4. Conclusions

The results of this experiment demonstrated that NIRS is adequate to determine the patchouli essential oil aromatic characteristic. With the employment of a PLS analysis was possible to calibrate a model that determine the patchouli alcohol, the primordial chemical compound of this oil. The best calibration obtained for the first model was the one using normalization mean center as a pretreatment (r= 0.980, SEC (%) = 0.658, SEP (%) = 0.759, CV (%) = 2.27, RPD = 5.04 and Consistency (%) = 86.656); while for the second model, it was the one using second derivate (r= 0.929, SEC (%) = 0.811, SEP (%) = 0.894, CV (%) = 2.62, RPD = 2.72 and Consistency (%) = 90.718).

Acknowledgments

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Authors' contributions

DMCR, YHP, IWB, S designed the study. DMCR, carried out the laboratory work. DMCR, YHP, IWB, SK, S, SW analyzed the data. DMCR wrote the manuscript. All authors read and approved the final version of the manuscript.

Competing interests

The authors attested that there were no conflicts of interest concerning this paper.

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