

Application of Fourier Transform Near-Infrared (FT-NIR) and Fourier Transform Infrared (FT-IR) Spectroscopy Coupled with Wavelength Selection for Fast Discrimination of Similar Color of Tuber Flours

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Abstract: This research aimed at providing a fast and accurate method in discriminating tuber flours having similar color by using Fourier transform near-infrared (FT-NIR) and Fourier transform infrared (FT-IR) spectroscopy in order to minimize misclassification if using human eye, or to avoid adulteration. Reflectance spectra of three types of tubers (consisted of *Canna edulis*, modified cassava, and white sweet potato) were collected to develop a multivariate model of partial least-squares discriminant analysis (PLS-DA). Several spectra preprocessing methods were applied to obtain the best calibration and prediction model, while variable importance in the projection (VIP) wavelength selection method was used to reduce variables in developing the model. The PLS-DA model achieved 100% accuracy in predicting all types of flours, both for FT-NIR and FT-IR. The model was also able to discriminate all flours with coefficient of determination (R^2) of 0.99 and a standard error of prediction (SEP) of 0.03% by using 1st Savitzky Golay (SG) derivative method for the FT-NIR data, as well as R^2 of 0.99 and SEP of 0.08% by using 1st Savitzky Golay (SG) derivative method for the FT-IR data. By applying the VIP method, the variables were reduced from 1738 to 608 variables with R^2 of 0.99 and SEP of 0.09% for FT IR and from 1557 to 385 variables with R^2 of 0.99 and SEP of 0.05% for FT NIR.

Keywords: FT-NIR; FT-IR; VIP; PLS-DA; tuber flour

■ INTRODUCTION

Tubers, such as cassava, sweet potato, arrowroot, taro, and *Canna edulis*, are abundantly cultivated in several regions in Indonesia and usually consumed as a staple food to alternate rice. Those crops are rich in carbohydrate, providing about 1/3 of that of an equivalent weight of rice or wheat due to their high moisture content, and also sources of a number of compounds such as saponins, phenolic compounds, glycoalkaloids, phytic acids, carotenoids, and ascorbic acid [1]. Tubers have a high metabolic activity after harvest; therefore, they are more perishable than grains [2]. One method to prolong the tuber self-life is by making them into flours. In flour form, the crops can be utilized for several food

productions such as for noodles, biscuits, snacks, or bread.

Among the tubers, *Canna edulis*, modified cassava, and white sweet potato have white color in flour form. Their colors are similar, making them difficult to be differentiated by the human eye. Although similar in color, those flours are different in composition and also in price. Chemical compositions are required to determine the method in food processing as well as to provide nutrition information for people susceptible to certain compounds. Due to the difference in price, adulteration of flours is sometimes inevitable. Low quality and price products are added to other products for economic reasons [3]. Based on seller price in

Indonesia, white sweet potato has the most expensive price, followed by *Canna edulis* and modified cassava flours. Therefore, an incorrect judgment of the type of flours may bring about health or economic consequences.

Quality determination of flours is usually done by sensory analysis using trained panelists [4], GC-MS for aroma [5], colorimeter, and spectrophotometer for color [6], as well as quantitative analysis in the laboratory [7]. Those methods require intense sample preparation, time-consuming, and skilled labors, especially for sensory analysis. For massive and large products, fast and rapid discrimination methods are needed.

Spectroscopy is now becoming popular as a fast and rapid method for qualitative and quantitative food analysis. Infrared spectroscopy covers wide range of electromagnetic regions consisting of near-infrared (NIR) at 14000–4000 cm^{-1} , mid-infrared (MIR) at 4000–400 cm^{-1} and far infrared at 400–50 cm^{-1} ; however, MIR and NIR regions are commonly used for food quality analysis [8]. Whereas spectra in the MIR region contain information on the fundamental molecular vibrations, the absorption spectra in the NIR region contain information on the overtones and combinations of fundamental vibrations [9]. MIR spectroscopy is able to identify very similar and complex molecular structures, so it is useful for compound identification, while NIR spectroscopy is able to identify molecular interactions and chemical groups [10].

Both NIR and IR spectroscopy have been applied for quality identification of flour from wheat [11], rice [12], cassava, taro, and yam [13], and sweet potato [14]. Other applications combine chemometrics analysis with NIR and IR spectroscopy for detecting adulteration of flour products [15-16]. Classification of products using NIR and IR spectroscopy are also studied [17-18], but study about distinguishing flours that have a similar color has not been conducted. Therefore, this paper aims at discriminating flours from tuber crops that have similar color by applying Fourier transform near-infrared (FT-NIR) and Fourier transform infrared (FT-IR) spectroscopy. This study also applies variable importance in the projection (VIP) wavelength selection method in order to reduce processing time.

■ EXPERIMENTAL SECTION

Materials

Canna edulis, modified cassava, and white sweet potato flours were purchased from ten different sellers to obtain large varieties of samples. The sample of this study was *Canna edulis*, modified cassava, and white sweet potato flours obtained from several farmers in Indonesia to provide a wide range of variety shown from different brands. There were ten brands for each flour, making in a total of 30 batches of flour. For every batch, 3 samples were taken for spectra analysis, making a total of 90 spectra data.

Instrumentation

FT-NIR spectrophotometer (Antaris II FT-NIR analyzer, Thermo Scientific Co., Waltham, MA, USA) assembled with an InGaAs detector module, beam splitter, sample holder, moving mirror, laser diode, and halogen NIR light source, as well as FT-IR spectrometer (Nicolet 6700, Thermo Scientific Co., Waltham, MA, USA) using an attenuated total reflectance (ATR) sampling technique, a deuterated triglycine sulfate (DTGS) detector, and a KBr beam splitter, were used for spectra measurement.

Procedure

FT-NIR spectra acquisition

The reflectance spectra of 90 flours were acquired using the FT-NIR spectrophotometer (Antaris II FT-NIR analyzer, Thermo Scientific Co., Waltham, MA, USA) assembled with an InGaAs detector module, beam splitter, sample holder, moving mirror, laser diode, and halogen NIR light source. Each sample was scanned for 32 scans at the wavelength range of 4000–10,000 cm^{-1} at 4 cm^{-1} spectral resolution. The background scan was conducted with a golden slit frequently before acquiring the spectrum from each flour. In total, there were 1557 variables for FT-NIR.

FT-IR spectra acquisition

The spectra of 90 flours were obtained using the Nicolet 6700 FT-IR spectrometer with a range of 650–4000 cm^{-1} , using an attenuated total reflectance (ATR)

sampling technique, a highly sensitive deuterated triglycine sulfate (DTGS) detector, and a KBr beam splitter. A total of 32 successive scans of each sample with a spectral resolution of 3 cm^{-1} was recorded from the bare diamond ATR crystal. A background was recorded before every group of samples scanned with a clean ATR crystal. In total, there were 1738 variables for FT-IR.

Spectra pre-treatment and analysis

All spectra collections were done using Thermo Scientific™ OMNIC™ Series Software. The spectra data were transformed to MS Excel® 2013 and then imported to the Matlab version R2018a (The MathWorks, Inc., Natick, MA, USA) for spectra preprocessing and chemometrics analysis. Two multivariate data analysis techniques were applied, namely principal component analysis (PCA) and partial least-squares discriminant analysis (PLS-DA), to develop a classification model for *Canna edulis*, modified cassava, and white sweet potato flours. PCA was used for reducing dimensions and visualizing data distribution concerning discrimination of samples. For developing the PLS-DA model, the FT-NIR and FT-IR spectra were preprocessed through normalization methods (minimum, maximum, and range), standard normal variate transformation (SNV), multiple scatter correlation (MSC), and Savitzky-Golay (SG) smoothing (1^{st} and 2^{nd} derivatives). The 3^{rd} order of polynomial fit and 5 smoothing points were used for SG smoothing. Variable importance in the projection (VIP) wavelength selection method was used to reduce variables

in developing the model. Of 90 spectra data, 60% and 40% of the data were used for calibration and prediction, respectively. A full-cross validation method (leave-one-out) was used in developing a calibration model using the PLS-DA method. The coefficient of determination (R^2) and a standard error of prediction (SEP) were used to justify the accuracy of the model.

RESULTS AND DISCUSSION

The analysis results from the spectra obtained using FT-NIR and FT-IR were used to compare the performance accuracy of the two spectroscopic techniques in distinguishing *Canna edulis*, modified cassava, and white sweet potato flours.

Spectra Data Exploration

Original spectra of all flours collected from FT-NIR and FT-IR systems are presented in Fig. 1. Fig. 1(a) shows the FT-NIR in the wavenumber range of $4000\text{--}10000\text{ cm}^{-1}$ in which all spectra are widely distributed between samples and have a similar pattern. However, the relative absorbance of *Canna edulis* flour is characterized by higher relative absorbance compared to other flours. Although not too distinct, several peaks on FT-NIR spectra can be observed, which may reflect particular chemical compounds. Original spectra of flours acquired from FT-IR at a wavenumber of $650\text{--}4000\text{ cm}^{-1}$ (Fig. 1(b)) shows sharper fundamental absorptions; therefore, they can be easily assigned to specific chemical compounds [19].

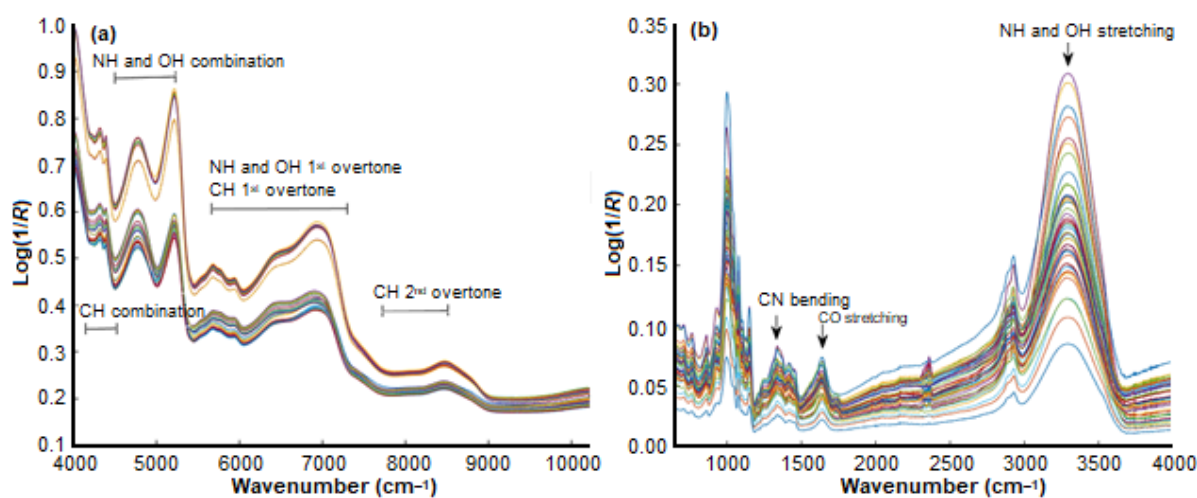


Fig 1. Original spectra of (a) FT-NIR and (b) FT-IR

The typical absorptions in the NIR region (Fig. 1(a)) are dominated by CH second overtone bands (7692–8695 cm^{-1}), NH and OH first overtone bands (5882–7142 cm^{-1}), CH first overtone bands (5882–7142 cm^{-1}), NH, and OH combination bands (4444–5263 cm^{-1}) and CH combination bands (4166–4444 cm^{-1}) [17]. Fig. 1(b) shows the FT-IR spectra of *Canna edulis*, modified cassava, and white sweet potato. In general, FT-IR spectra can be classified into two regions: below 1500 cm^{-1} , which are the fingerprint region, and 1500–4000 cm^{-1} , known as the functional group region [20]. Absorption peaks at a range of 3000–3500 cm^{-1} show NH and OH stretching, while at 1456 and 1643 cm^{-1} show CN bending and CO stretching, respectively [21].

Principle Component Analysis

The Principal Component Analysis (PCA) is applied for dimensional reduction and data exploration of the three tuber flours. By using original spectra for both FT-NIR and FT-IR data, the flours are clearly classified, as shown in Fig. 2(a) and Fig. 3(b). The loading plots (Fig. 2(b) and Fig. 3(b)) provide information about absorption bands, which largely contribute to the discrimination of flours according to the PC values.

As illustrated in Fig. 2(a), the plot of PC-1 and PC-2 provides better visualization of discrimination among the groups of samples for FT-NIR data. PC-1 and PC-2 altogether account for 99.5% the total variability. The PC

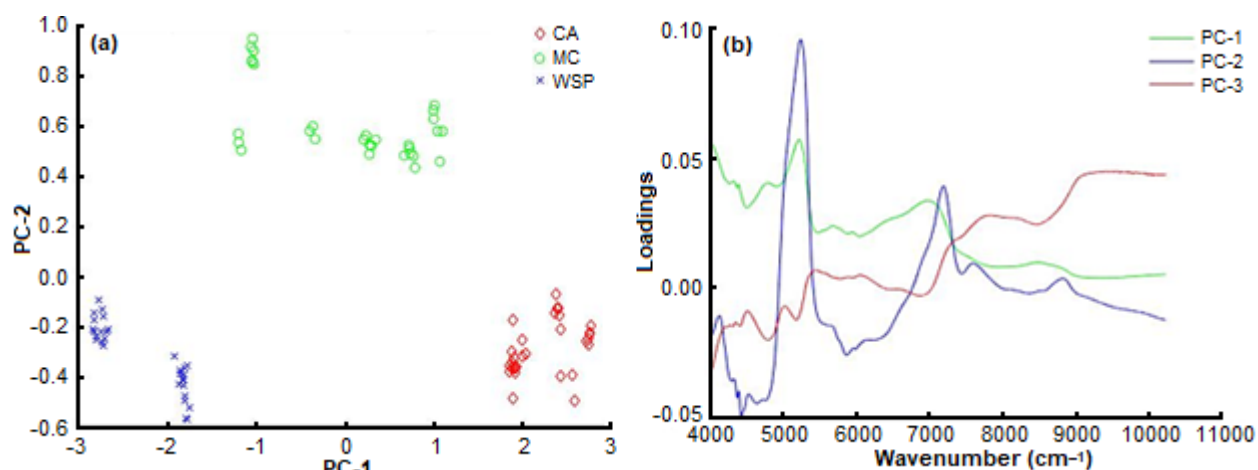


Fig 2. PCA of FT-NIR spectra of CA (*Canna edulis*), MC (modified cassava), and WSP (white sweet potato): (a) score plot and (b) loadings plot of PC-1 and PC-2

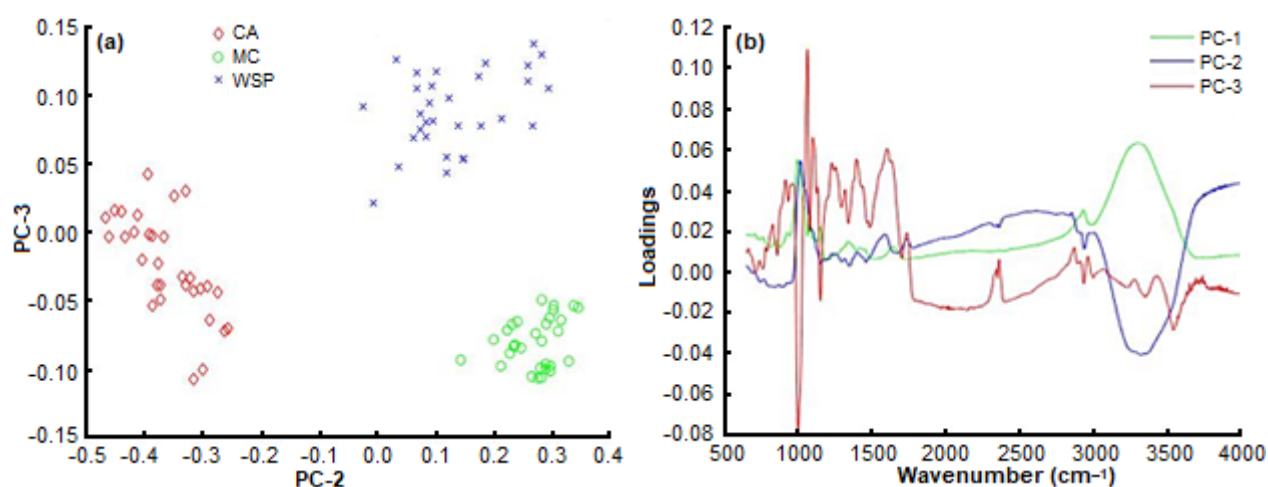


Fig 3. PCA of FT-IR spectra of CA (*Canna edulis*), MC (modified cassava), and WSP (white sweet potato): (a) score plot and (b) loadings profile of PC-2 and PC-3

loading plot (Fig. 2(b)) shows the highest value for PC-1 at 5208 cm^{-1} corresponding to CO stretch second overtone assigned to CONH structure and 6944 cm^{-1} CH combination corresponding to CH_2 . On the other hand, PC-2 shows the peaks at 5208 cm^{-1} similar to that of PC-1, at which 7184 cm^{-1} is CH combination of CH_2 [22].

Fig. 3(b) shows a clear separation of three types of flour indicated by PC-2 and PC-3 for FT-IR data, which account for 13% of the total variability, but in total, the first three principal components account for 99.7% the total variability. The loadings of PC-2 (Fig. 3(b)) showed a negative influence of the bands at 3304 cm^{-1} associated with NH of amines and OH of alcohols, phenols, carboxylic acids, and water, as well as at 1018 cm^{-1} associated to CO of alcohols. The PC-3 shows several peaks on the fingerprint region, which shows several absorption peaks between $1000\text{--}1300\text{ cm}^{-1}$, which are assigned to CO stretch of esters, ethers, alcohols, and carboxylic acids, as well as at 1600 cm^{-1} assigned to CC of the aromatic bond.

Partial Least Square Discriminant Analysis Model

A PLS-DA model is used to distinguish three types of tuber flour that have a similar color. The PLS-DA models are developed using the preprocessed spectra of samples from FT-NIR and FT-IR spectroscopy. The PLS-DA calibration model classified *Canna edulis*, modified cassava, and white sweet potato flour with 100% accuracy for calibration and predictive model for both FT-NIR and

FT-IR spectroscopy (data not shown), by using original spectra and applying all preprocessed methods, from normalization to derivatives. The high classification accuracy demonstrates that tuber flours having a similar color can be correctly identified by FT-NIR and FT-IR instruments.

The highest coefficient determination and standard error of prediction (SEP) of prediction, which are R^2 of 0.99 and 0.012, are obtained by applying the Savitzky-Golay 1st derivative preprocessed for FT-NIR spectra. For FT-IR, the coefficient determination and SEP of prediction, which are R^2 of 0.99 and 0.042, are obtained by also applying the Savitzky-Golay 1st derivative preprocessed. The 1st derivative provided the best PLS model since it removed the baseline offset and provided lesser peaks compared to other derivatives but was able to be distinctly observed. The PLS-DA results are listed in Table 1 for the FT-NIR and FT-IR spectral data.

Fig. 4 shows the beta coefficient of the PLS-DA model resulted from the Savitzky-Golay 1st derivative of FT-NIR and FT-IR spectra, which give the best calibration and prediction model for discriminating *Canna edulis*, modified cassava, and sweet potato flour. Several distinct peaks can be observed on FT-NIR spectra (Fig. 4(a)) at 4048 cm^{-1} symmetrical CNC stretch first overtone relating to protein, 4404 cm^{-1} OH stretch or CO stretch combination relating to cellulose, 5172 cm^{-1} OH stretch or HOH deformation combination relating to starch [22],

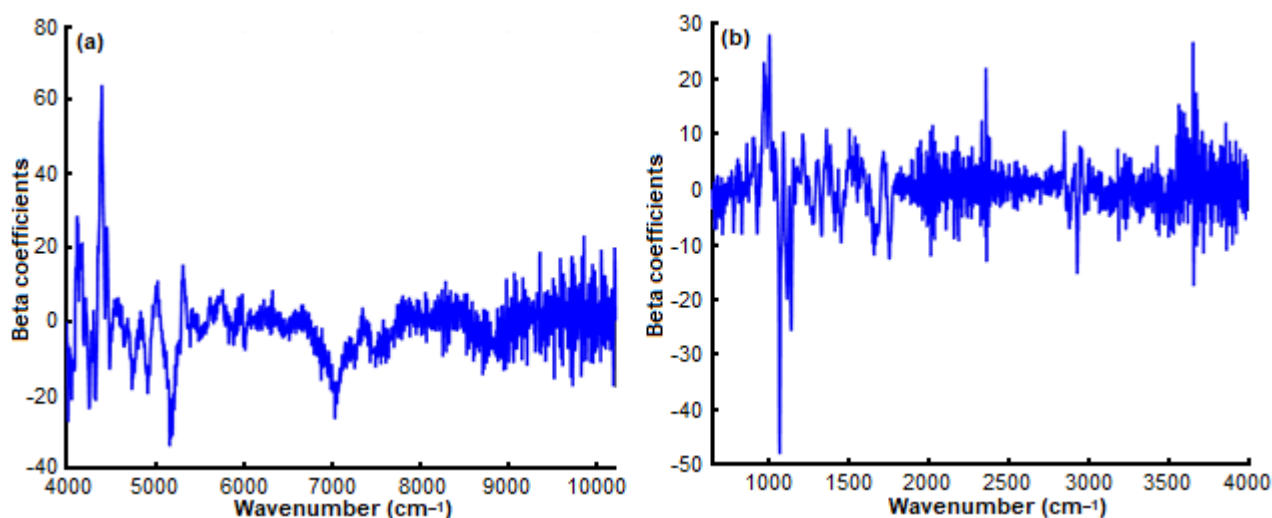


Fig 4. Beta coefficients of Savitzky-Golay 1st derivative of (a) FT-NIR spectra and (b) FT-IR spectra

Table 1. Comparison of original PLS-DA model versus VIP model with various preprocessing methods on FT-NIR and FT-IR spectra

Spectroscopy	Preprocessing	PLS-DA					PLS-DA VIP				
		Calibration		Prediction		LV	Calibration		Prediction		LV
		R ²	SEC	R ²	SEP		R ²	SEC	R ²	SEP	
FT-NIR	Mean norm	0.994	0.062	0.994	0.062	5	0.994	0.066	0.988	0.091	4
	Max norm	0.994	0.065	0.994	0.065	5	0.992	0.072	0.987	0.096	4
	Range norm	0.995	0.060	0.995	0.060	5	0.996	0.054	0.991	0.080	6
	MSC	0.998	0.040	0.998	0.040	7	0.997	0.045	0.995	0.060	6
	SNV	0.997	0.043	0.997	0.043	7	0.996	0.051	0.995	0.060	6
	SG1	0.999	0.012	0.999	0.012	5	0.998	0.034	0.996	0.050	5
	SG2	0.999	0.0121	0.999	0.0121	5	0.998	0.033	0.995	0.057	5
	Original	0.998	0.0409	0.998	0.0409	6	0.998	0.039	0.995	0.060	5
	Variables					1557					385
FT-IR	Mean norm	0.995	0.059	0.995	0.059	5	0.99	0.08	0.98	0.11	5
	Max norm	0.994	0.066	0.994	0.066	5	0.99	0.07	0.99	0.09	6
	Range norm	0.987	0.097	0.987	0.097	3	0.97	0.14	0.96	0.18	3
	MSC	0.995	0.061	0.995	0.061	5	0.99	0.08	0.99	0.10	5
	SNV	0.995	0.059	0.995	0.059	5	0.99	0.07	0.99	0.09	5
	SG1	0.998	0.042	0.998	0.042	5	0.99	0.06	0.96	0.17	6
	SG2	0.995	0.057	0.995	0.057	5	0.99	0.06	0.95	0.19	6
	Original	0.986	0.100	0.986	0.100	5	0.98	0.11	0.95	0.19	5
	Variables					1738					608

Note: R² = coefficient of determination; SEC = standard error of calibration; SEP = standard error of prediction; LV = latent variable; Mean norm = mean normalization; Max norm = maximum normalization; Range norm = range normalization; MSC = multiplicative scatter correction; SNV = standard normal variate, SG1 = Savitzky-Golay 1st derivative; SG2 = Savitzky-Golay 2nd derivative

and 7040 cm⁻¹ relating to water [23]. Results indicate that starch, protein, cellulose, and water may contribute to flour discrimination based on FT-NIR spectra.

Clear peaks in the FT-IR region (Fig. 4(b)) can be observed at 3330, 2929, and 1641 cm⁻¹, which are related to water and protein absorption bands [24]. Other bands below 1500 cm⁻¹ contain complex spectra, but it can be observed that at 1078 cm⁻¹ are due to CC bond vibrations as well as 1011 and 1144 cm⁻¹ are due to COC stretching bonds relate to the carbohydrate [25]. The distinct peak at 3649 cm⁻¹ indicates the OH stretching bond relates to water. Those imply that carbohydrate and water contents among samples contribute to the discrimination of samples based on FT-IR spectra.

FT-NIR and FT-IR spectra contain lots of variables (in this study, there are 1557 and 1738 variables), although only parts of the variables are related to the property of interests. Therefore, the variable selection method is used

to select the number of variables that are able to improve the performance of the model and to ease the interpretation [26]. The variable selection used in this study is the variable importance on projection (VIP), which considers all variables for initialization and then filters the unimportant variables based on some criterions [26]. VIP cut off used is 1.0. The new PLS-DA model developed using VIP selection is compared with the original PLS-DA model, as shown in Table 1. VIP selection is able to reduce variables from 1557 to 385 for FT-NIR and 1738 to 608 for FT-IR. The VIP-PLS-DA model achieves R² of 0.99 and SEP of 0.05% for FT NIR with the Savitzky-Golay 1st derivative preprocessed spectra, as well as R² of 0.99 and SEP of 0.09% for FT IR with the maximum normalization data preprocessing methods. The VIP selection will provide a faster process and lesser computer memory required for computation.

■ CONCLUSION

This study aimed to differentiate three types of tuber flours made of *Canna edulis*, modified cassava, and white sweet potato. The PLS-DA model achieved 100% accuracy in predicting all types of flours, both with a coefficient of determination (R^2) of 0.99 and a standard error of prediction (SEP) of 0.03% for FT-NIR and R^2 of 0.99 and SEP of 0.08% for FT-IR. The VIP method is used to develop PLS-DA models, which result in reducing variables from 1738 to 608 variables for FT-IR and from 1557 to 385 variables for FT-NIR. The VIP-PLS-DA also achieves high accuracy models with R^2 of 0.99 and SEP of 0.09% as well as R^2 of 0.99 and SEP of 0.05% for FT-IR and FT-NIR, respectively. Both FT-NIR and FT-IR provide high accuracy and fast methods in the discriminating types of tuber flours that have similar color, which will be beneficial for large samples.

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