Preliminary Investigation into the Identification of Wood Species from Different Locations by Near Infrared Spectroscopy

Zhong Yang,* Yana Liu, Xiaoyu Pang, and Kang Li

The feasibility of using near-infrared spectroscopy (NIR) to identify wood species was investigated in this study. Case I considers the principal component analysis scores plot of NIR spectra for three wood species. Case II considers whether NIR combined with partial least squares discriminant analyses can be used to identify the three wood species. Three wood species were studied, and each species included five randomly collected wood blocks, 21 samples for each wood block, and 315 total wood samples. In case I, the samples in the PCA analysis were clustered together. In case II, samples in the training set were classified into the correct group, and the accuracy of the test set was up to 90%.

Keywords: Wood; Identification; Different locations; Near-infrared spectroscopy; PLS-DA

*Contact information: Research Institute of Wood Industry, Chinese Academy of Forestry, Beijing 100091, China; *Corresponding author: zyang@caf.ac.cn*

INTRODUCTION

To realize the optimal utilization of wood, different wood species should be treated separately in wood processing and with respect to the final wood products. This is because different wood species have different characteristics and properties, such as the mechanical and machining properties. Therefore, the identification of wood species is of great significance for industrial utilization as well as the quality of the final product.

With a considerable variety of wood species being applied to produce wood flooring (for example, the *Pometia*, *Instia*, and *Couratari* species are commonly used in the field), the market for wood flooring has been quickly expanding. Although the three wood species, with different qualities and price, are liable to be identified by skilled inspectors, the online operators might not know the details of wood identification. The non-destructive and fast separation of these three wood species can improve the speed of production and enable the processes to be more efficient.

The traditional methods for wood identification include the use of physical, anatomical, and visual aspects of wood species, which are time- and labor-consuming. Some advancements have occurred in wood identification technology, such as DNA markers and chemical isotope methods. Based on the specific DNA fragments of different wood species or tree species from different origins, the DNA identification method was used to successfully identify six kinds of poplar wood in 2007 (Degen and Fladung 2008). The chemical isotope method has great potential for identifying the origins of wood species by analyzing stable isotopes in wood species (Keppler *et al.* 2007). While these advanced technologies can be accurate in determining the origin of wood species, they take up unnecessary time in the sample preparation process, which is not practical in industry.

The near-infrared spectrum, which covers the region from 780 to 2500 nm, contains information pertaining to the overtones and combinations of fundamental vibrational transitions, including those of the C-H, O-H, and N-H functional groups. With minimal sample preparation, nondestructive features, and rapid results, near-infrared spectroscopy (NIR) has yielded promising results in the fields of medicine (Conway *et al.* 1984), agriculture (Batten 1998), food (Osborne and Fearn 1998), paper (Birkett and Gambino 1989), and others. Considerable research has demonstrated that NIR has been successfully used in predicting wood properties, such as the physical properties density (Hein *et al.* 2009), moisture content (Adedipe *et al.* 2008), and mechanical strength (Thumm and Meder 2001; Kelley *et al.* 2004); chemical properties (Kelley *et al.* 2004; Poke and Raymond. 2006; Emandi *et al.* 2011); and the anatomical properties fiber length (Inagaki *et al.* 2012) and microfibril angle (Schimleck *et al.* 2002; Hein *et al.* 2010).

The ability of NIR to identify wood species was first reported by Borga *et al.* (1992). Then, Schimleck (1996) successfully classified eucalypt species using NIR combined with principal component analysis. Brunner *et al.* (1996) used NIR to classify wood from 12 species. Currently, the applications of NIR in wood discrimination include the discrimination of wood species with similar appearance (Flaete *et al.* 2006; Haartveit and Flæte 2008), wood samples from different parts of one species (Via *et al.* 2003; Sandberg and Sterley 2009), wood samples of one species, but from different regions (Rana *et al.* 2008; Sandak *et al.* 2011), and wood species after physical or chemical treatments (Hinterstoisser *et al.* 2003; Schwanninger *et al.* 2004; Bächle *et al.* 2012).

In this paper, two cases of wood identification are considered to investigate the applicability of NIR in wood identification. Case one considers the feasibility of NIR to identify the three wood species, and case two considers whether NIR can identify wood block samples from different locations.

EXPERIMENTAL

Sampling Preparation

Three wood species, *Pometia* sp., *Instia* sp., and *Couratari* sp., were collected from Beijing Dongba wood market where hardwoods are imported from all over the world. Each species included five 900×160×18 mm wood blocks randomly collected from 2007 to 2012 years. The collected wood blocks were heartwoods. Since collecting each wood block came from a different year, it was speculated that these 15 wood blocks were from different trees around the world. The wood blocks were processed by saw and planer into cubic shapes with dimensions of 15 mm × 15 mm × 15 mm.

Twenty-one wood samples were processed from each wood block (14 samples were used for the calibration set and seven samples were used for the prediction set). There were 105 samples for each species, and 315 wood samples in total were prepared. The wood samples were equilibrated in a constant temperature and humidity laboratory with a temperature of 20 °C and 65% relative humidity. During absorption of moisture, the wood samples were weighed once every 24 h until the two mass differences were less than 0.5% of the wood samples mass, which is considered to reach equilibrium moisture content.

Measurements of NIR Spectra

The NIR spectra were measured in a diffuse reflectance mode with an ASD Field Spec® spectrometer (Analytical Spectral Devices, Boulder, CO) at 1-nm intervals over the wavelength range of 350 to 2500 nm. A white Teflon® background was used. A fiber-optic probe with an 8-mm light spot was oriented perpendicular to the surface of wood samples.

NIR spectra were obtained from the cross section, radial section, and tangential section of wood samples. Thirty spectra were collected and then averaged to a single spectrum. To reduce the noise of the instrument, the spectral region of 400 to 2500 nm was selected for data analysis.

Chemometric Analysis

To better obtain qualitative information based on the spectra, this study applied an effective chemometric technique to conduct data analysis. Principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA) were performed using the Unscrambler® software (CAMO, Corvallis, OR, USA). These procedures are briefly described next.

Principal component analysis (PCA)

PCA is a method that has been used for the extraction of the systematic variations in a single data set. The objective of PCA is to decompose a linear combination of original variables into a few principal components or variables while preserving the characterization of the original variables.

Principal component scores are the projected locations of each sample onto each corresponding principal component, which represent the latent structures and clusters of samples. The loadings express the contribution of each variable (wavelength) to each principal component.

Partial least squares regression (PLSR)

PLSR is that it simultaneously projects the x and y variables onto the same subspace in such a way that there is a good relationship between the predictor and response data. PLSR can be divided into the partial least squares 1 method and partial least squares 2 method.

The partial least squares 1 method extracts the spectral information and transforms it into PLS components to ensure the maximized covariance to the dependent variable. In the partial least squares 2 method, two or more dependent variables are modeled simultaneously.

Partial least squares discriminant analysis (PLS-DA)

Partial least squares discriminant analysis involves developing a conventional partial least squares regression model, in which the variable is a binary variable. If a variable takes the value of 1, the specimen in question is a member of that group and if a variable takes the value of 0, the specimen in question is not a member of that group.

To evaluate the models, the coefficients of determination (R^2), standard error of calibration (SEC), standard error of validation (SEV), the number of correct classifications, and the accuracy of classification were used in this study.

RESULTS AND DISCUSSION

Case I: Discrimination of Three Wood Species

NIR spectra

Figure 1 displays original near-infrared spectra of the three wood species in three sections. The original spectra demonstrate the existence of the peaks at 1473, 1925, 2092, and 2267 nm. The peak at 1473 nm was primarily attributed to the first overtone O–H stretching of cellulose. The strong peak at approximately 1925 nm was primarily attributed to the O-H asymmetric stretching and O-H deformation from water. The O-H and C-H deformation and O-H stretching vibration of cellulose and xylan were indicated by spectra changes at 2092 nm. Further, the overtone of O-H stretching and C-O stretching from lignin at 2267 nm also showed a change in absorption.

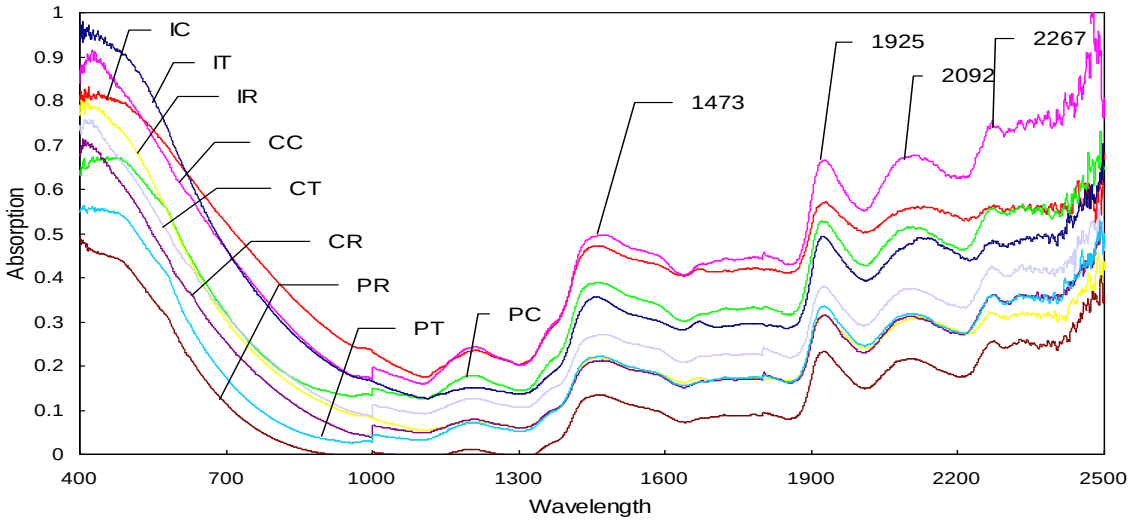

Fig. 1. NIR original spectra of the three wood species in three sections.
Note: The first letter stands for the wood species (I - *Intsia*, C - *Couratari*, P - *Pometia*); The second letter stands for the different sections (C - Cross section, R - Radial section, T - Tangential section)

PCA analysis

To compress the large datasets of these spectra, the spectra of 315 samples were respectively placed into three sections for partial least square analysis, and then the useful information was extracted for identification of the three wood species. Eight principal components were selected for each PCA analysis in case I, which describes the original spectra with high significance. Figure 1 shows the score plot of principal components 1 and 2; they have the proportions of variance of 76% and 11% with respect to the cross-section spectra, respectively. Because the repetitions of each wood species cluster together, it is evident from the PCA scores plot that there is a tendency for the three wood species to be identified.

The result of PCA analysis of the spectra obtained from radial sections is shown in Fig. 2, The first principle component has a proportion of variance of 84%, and the second principle conponent has a proportion of variance of 9%. Figure 3 shows the PCA analysis result of the spectra obtained from the tangential sections of the three wood species, in which the principle components 1 and 2 showed the proportions of variance of 87% and 7% with respect to the original spectra, respectively.

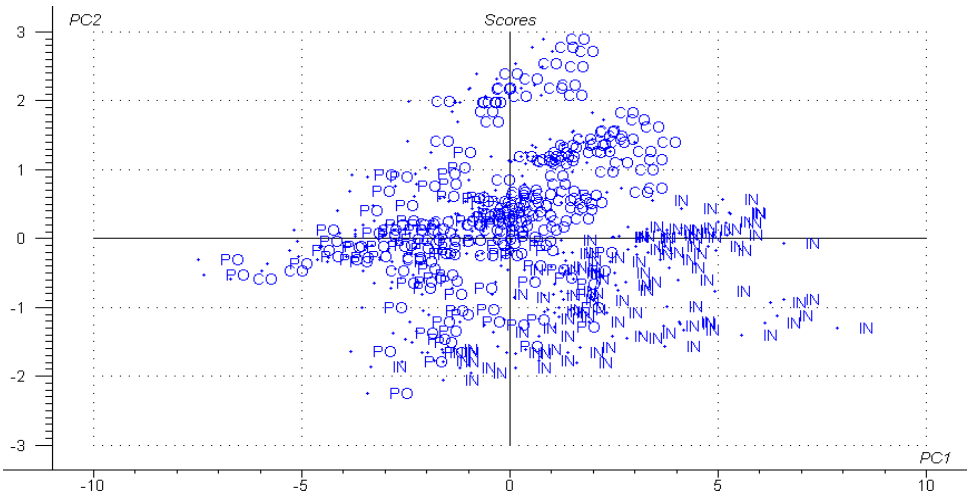

Fig. 2. PCA analysis of the spectra obtained from cross-sections

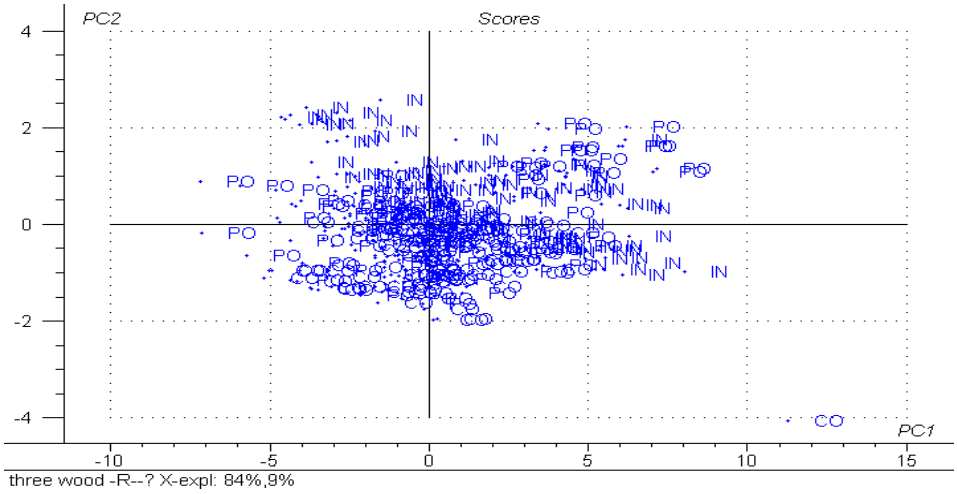

Fig. 3. PCA analysis of the spectra obtained from radial sections

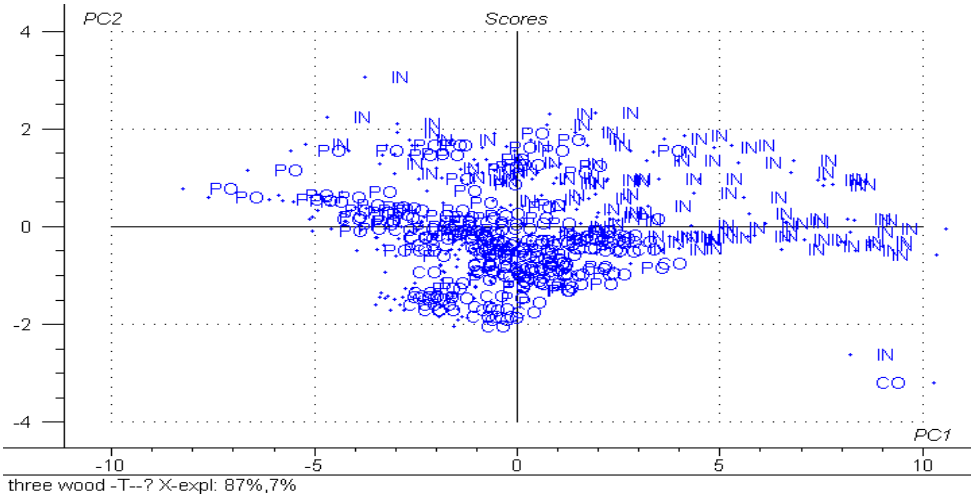

Fig. 4. PCA analysis of the spectra obtained from tangential sections

It was observed from these two PCA scores plots that the *Instia* species can be separated from the *Pometia* and *Couratari* species. Despite some confusion that arose between samples of *Pometia* and *Couratari* species, the two wood species could still be separated to some extent. Combining the three PCA score plots, the three wood species could be separated, to a degree, into the principle components. The spectra obtained from cross-sections performed better regarding the separation of the three wood species, compared with the spectra obtained from the radial and tangential sections. Therefore, we eastablished three PLS-DA identification models based on the cross-section, radial, and tangential spectra of the three wood species, aiming to test the ability and accuracy of the NIR models.

PLS-DA model

Eight fitted principal components were used to develop the three PLS-DA models. The 315 wood samples of the three wood species were divided into calibration (210 samples) and prediction (105 samples) sets for each model. The calibration set included 70 samples of each wood species and was used to establish the PLS-DA model; the prediction set consisted of 35 samples of each wood species, which were used for model testing. The models were validated by the leverage correction method. The model calibration and validation are shown in the following tables.

Figure 5(a) displays regression plot of true and predicted category variables of *Pometia* in tangential section. The two straight lines are the regression lines between the calibration and validation results of model and actual classification, respectively. The two regression lines exhibited a close coincidence, which demonstrates that the PLS-DA model has robust reliability and can be used to detect and discriminate new samples. Figure 5(b) shows the discriminant results of *Pometia* samples in tangential section. All category variables predicted values of *Pometia* samples were more than 0.5, and all deviations were less than 0.5. At same time, category variables predicted values of other two wood species samples were close to 0, and all deviations were less than 0.5. Thus, all the *Pometia* samples were judged as *Pometia* species according to the discriminant rule of PLS-DA.

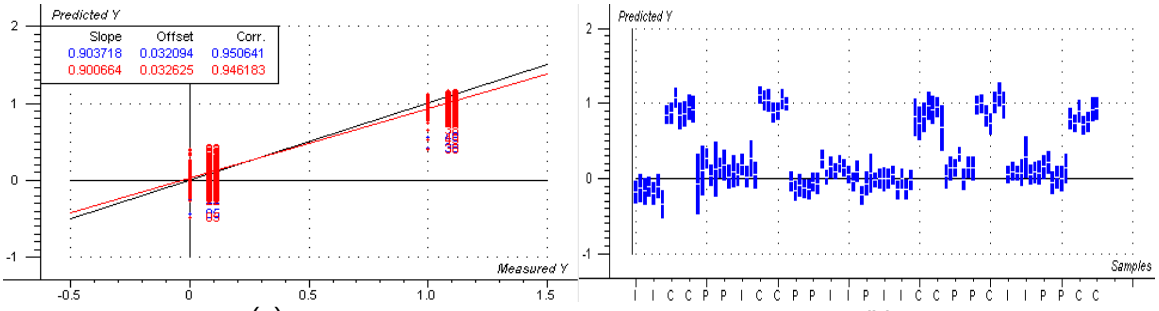

Fig. 5. (a) Relationship between true and predicted category variables of *Pometia* in tangential section. (b) Discriminant results for *Pometia* samples in tangential section.

Table 1 summarizes the efficiency of the three PLS-DA models based on the cross-section, radial, and tangential spectra (400 to 2500 nm) of the three wood species, all of which achieved identification accuracy of 100%, with high coefficients of determination of 0.88 to 0.96, 0.88 to 0.94, and 0.90 to 0.94, respectively, and low SEC or SEV of 0.10 to 0.17, 0.12 to 0.16, and 0.11 to 0.15, respectively. This demonstrates

that the three PLS-DA models have the capacity to identify *Pometia*, *Instia*, and *Couratari* species. Table 2 lists the testing results for the three PLS-DA models regarding the prediction of unknown samples of the three wood species. In the testing sets of models based on cross-section and radial spectra of wood samples, the 35 samples of each wood species were all classified into the correct group; 100% of wood samples were identified correctly. In the testing set of a model based on the tangential spectra of wood samples, two samples of the *Couratari* species were missclassified into other wood species. However, the predictive performance of this model still presented a high total prediction accuracy of 98%.

Because cross-sections provide more comprehensive information about the wood surface, they are the most important sections for wood identification. Models based on the cross-section spectra of wood samples will perform better than the radial and tangential spectra in theory. However, with the identification accuracy of 100% shown in Table 1, all three models performed well in model calibration and validation. It is possible that all three wood species belonged to hardwoods because the line of growth rings is not obvious and the surface structure is consistent in all three sections.

In case one, we have demonstrated that NIR, combined with partial least squares discriminant analysis, can identify different wood species with high accuracy. We further investigated the feasibility of NIR to identify tree samples from different locations in case two.

Table 1. Calibration and Validation Results of NIR Spectra Acquired on the Cross-Section, Radial Section, and Tangential Section of Wood Samples

Sample sets	Samples	Cross-section			Radial section			Tangential section		
		R^2	SEC /SEV	Accur-acy	R^2	SEC /SEV	Accur-acy	R^2	SEC /SEV	Accur-acy
Calibration (n=210)	*Pometia* (n=70)	0.88	0.15	100%	0.90	0.15	100%	0.90	0.15	100%
	Instia (n=70)	0.96	0.10	100%	0.94	0.12	100%	0.94	0.11	100%
	Couratari (n=70)	0.92	0.14	100%	0.90	0.14	100%	0.90	0.15	100%
Validation (n=210)	*Pometia* (n=70)	0.88	0.17	100%	0.88	0.16	100%	0.90	0.15	100%
	Instia (n=70)	0.94	0.11	100%	0.92	0.12	100%	0.94	0.12	100%
	Couratari(n=70)	0.90	0.15	100%	0.90	0.15	100%	0.90	0.15	100%

Table 2. Identification of Unknown Samples from Different Species using the Three PLS-DA Models

Models	*Pometia* (n=35)		*Instia* (n=35)		*Couratari* (n=35)	
	Correct samples	Accuracy	Correct samples	Accuracy	Correct samples	Accuracy
M_{Cross}	35	100%	35	100%	35	100%
M_{Radial}	35	100%	35	100%	35	100%
$M_{Tangential}$	35	100%	35	100%	33	98%

Case II: Discrimination of Wood species from Different Regions

NIR spectra

Figure 6 shows NIR original spectra of the three species in cross section. The spectra of *Couratari* and *Instia* appear overlapping phenomenon. The development of chemometric makes the theory and technology of multi component analysis more mature, and solves the problem of the overlap of the near infrared spectral region.

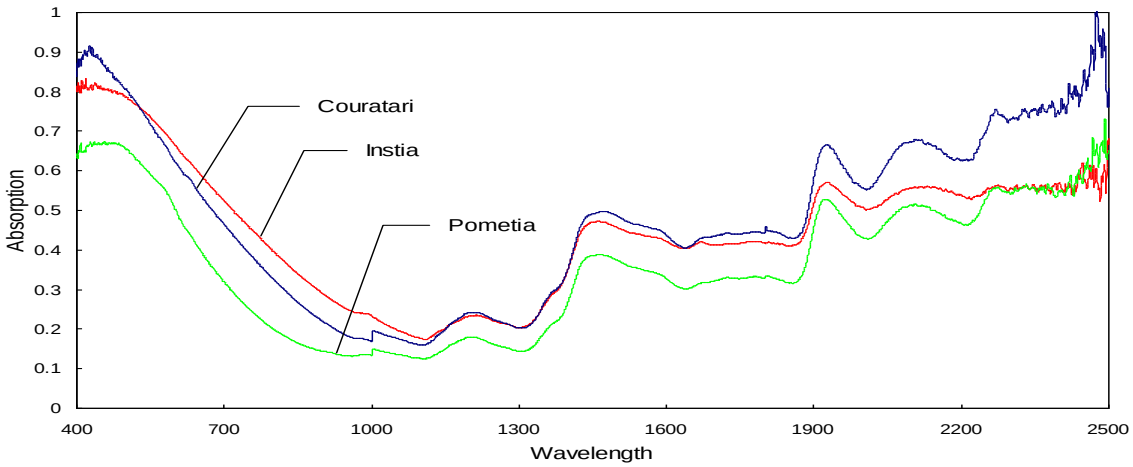

Fig. 6. NIR original spectra of the three species in cross section

PCA analysis

Trees growing in different locations differ in some properties, as trees respond to all environmental factors, including the local climate, soil, wildlife, and forest density. Hence, the identification of wood species from different locations is also required in the forest industry. In this case, three wood species (*Pometia*, *Instia*, and *Couratari*), each with five wood blocks from different locations, were used for the identification. First, using the NIR spectra of each species to conduct PCA, each species included five wood blocks from different locations and 21 samples from each wood block, producing 105 wood samples in total for each species. The PCA analysis for each species is shown in Figs. 4, 5, and 6.

As shown in Fig. 4, the scores plot for principle components 1 and 2 of the five wood blocks of the *Pometia* species had the proportions of variance of 69% and 15%, respectively, with respect to the original spectra. There was a slight tendency for the five wood blocks to be differentiated by PCA scores. For example, wood block numbers 1, 4, and 5 were basically clustered around each other. Wood blocks from numbers 2 and 3 were completely confused with each other. Figures 5 and 6 show the score plot of principle components 1 and 2 of the five wood blocks of the *Instia* and *Couratari* species, which explains the proportions of variance of 83%, 8%, 67%, and 18% compared with the original spectra, respectively. Except for the samples of the fourth wood block, which were confused with other wood blocks samples, the repetitions of other wood blocks of the *Instia* species cluster together. Meanwhile, wood samples of the *Couratari* species can be differentiated entirely using the PCA scores.

PLS-DA model

In case two, based on the partial least squares discriminant analysis, we developed three NIR models for the *Pometia*, *Instia*, and *Couratari* samples. Each model consisted of 105 samples from wood blocks from five different locations. Seventy samples, including 14 samples from each wood block, were used for the calibration set. The remaining 35 samples, including seven samples from each wood block, were used as a prediction set for the model testing. The models were all validated by the leverage correction method, and the results of the model calibration and validation are shown in Table 3.

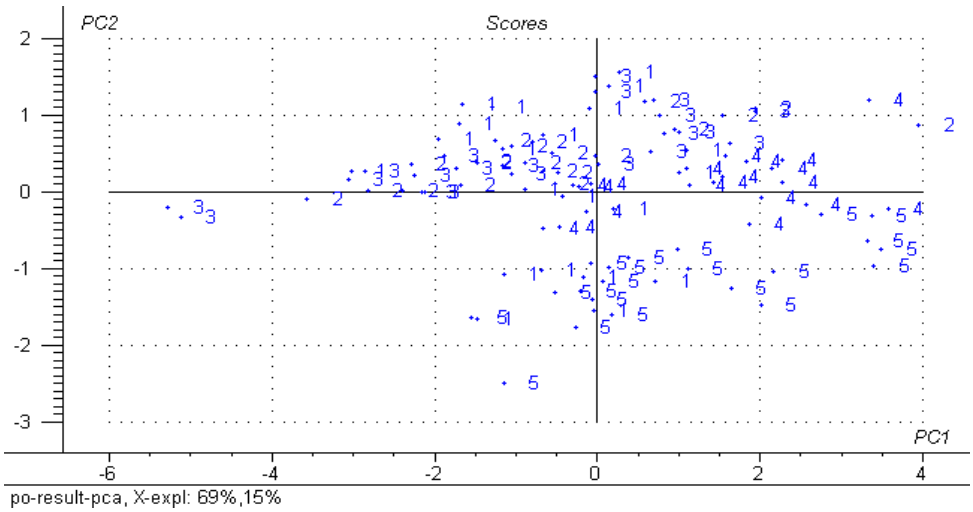

Fig. 7. PCA analysis of *Pometia* species

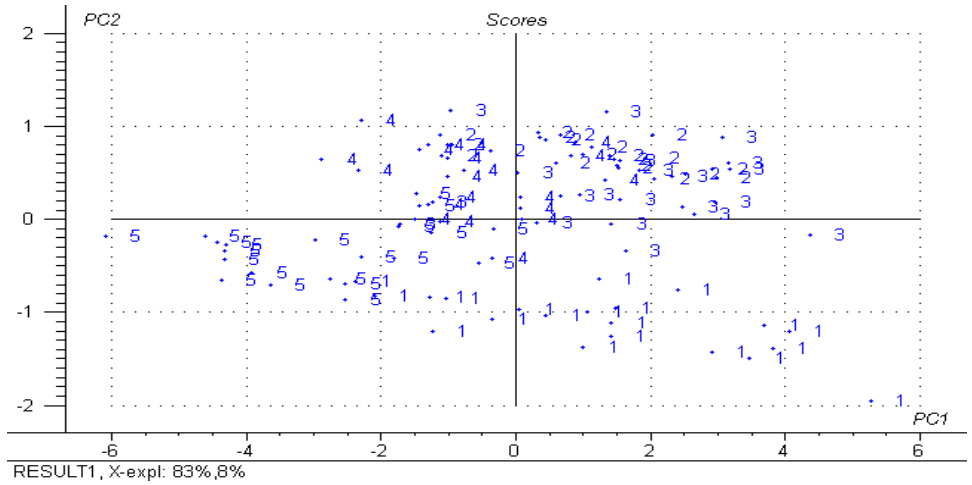

Fig. 8. PCA analysis of *Instia* species

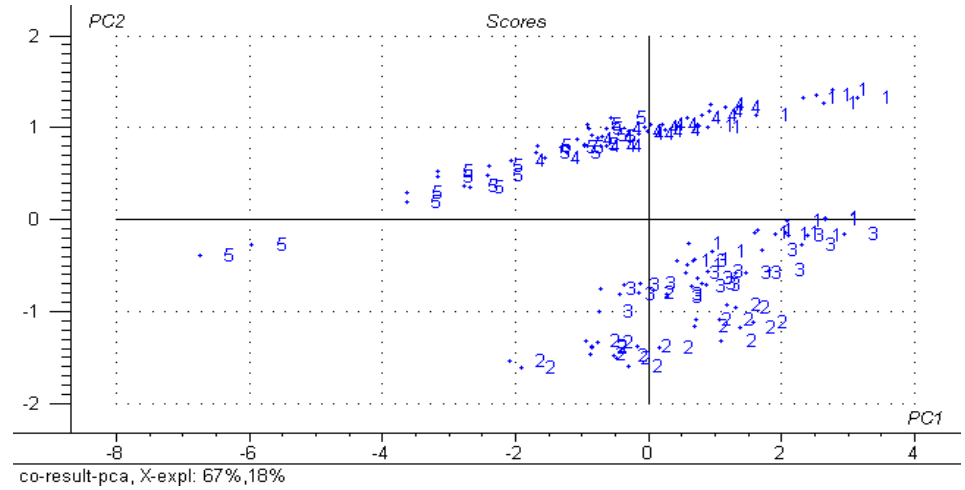

Fig. 9. PCA analysis of *Couratari* species

Table 3. Calibration and Validation Results of NIR Spectra (400 to 2500 nm) for Three Wood Species with Five Wood Blocks from Different Locations

Sample sets	Locat-ions	*Pometia*			*Instia*			*Couratari*		
		R^2	SEC /SEV	Correct samples	R^2	SEC /SEV	Correct samples	R^2	SEC /SEV	Correct samples
Calibration (n=70)	L 1	0.77	0.19	14	0.85	0.16	14	0.88	0.14	14
	L 2	0.28	0.34	2	0.77	0.19	14	0.88	0.14	13
	L 3	0.28	0.34	3	0.72	0.21	11	0.90	0.12	14
	L 4	0.76	0.20	14	0.81	0.18	14	0.94	0.09	14
	L 5	0.83	0.17	14	0.74	0.2	13	0.92	0.12	14
Total accuracy		67%			94%			99%		
Validation (n=70)	L 1	0.425	0.21	14	0.61	0.28	14	0.85	0.16	14
	L 2	0.19	0.37	1	0.69	0.22	14	0.85	0.16	13
	L 3	0.18	0.37	2	0.55	0.29	11	0.88	0.14	14
	L 4	0.72	0.21	14	0.74	0.21	14	0.92	0.11	14
	L 5	0.79	0.19	14	0.30	0.43	13	0.88	0.13	14
Total accuracy		64%			94%			99%		

In model one, which is based on the *Pometia* samples, the accuracy of the model calibration and validation were 67% and 64%, respectively. Forty-seven calibration samples and 45 validation samples were classified into the correct groups. The samples from the second and third tree were completely confused with each other. This was also revealed in the previous PCA analysis. Accuracy was low, 0%, and the coefficients of determination also were low, 0.18 to 0.19, and SEC/SEV was high, 0.34 to 0.37. It is possible that these two trees may have come from adjacent locations. The samples from the remaining wood blocks were all classified into the correct groups with an accuracy of 100%. In model two, which is based on the *Instia* samples, the total accuracy of the model calibration and validation were 94% and 94%, respectively. Except for three samples in the third wood block and one sample in the fifth wood block that were wrongly classified, all samples in other wood block were correctly classified. In model three, based on the *Couratari* samples, 69 samples in the model calibration and validation sets were classified into the correct groups, with a high accuracy of 99%. This result also corresponded to the previous PCA analysis of *Couratari* samples from five different locations.

Table 4 summarizes the prediction results for the three NIR models. In the prediction set of *Pometia* samples, 21 samples were identified correctly, with an accuracy of 60%.

Table 4. Identification Results of Unknown Samples from Different Locations using the Three PLS-DA Models

Samples	Locations	L 1	L 2	L 3	L 4	L 5
Pometia (n=35)	Correct samples	6	0	2	7	6
	Accuracy	(21/35) 60%				
Instia (n=35)	Correct samples	6	5	6	7	5
	Accuracy	(29/35) 83%				
Couratari (n=35)	Correct samples	7	7	7	7	7
	Accuracy	(35/35) 100%				

In the prediction set of *Instia* samples, the prediction accuracy was 83%. Twenty-nine samples were identified correctly, and six samples were placed into the wrong groups. Samples in the *Couratari* prediction set were entirely placed into the correct groups, with an accuracy of 100%.

CONCLUSIONS

The ability of near-infrared spectroscopy (NIR) to identify wood samples from different species and wood block samples from different locations was investigated. The conclusions are as follows:

1. In case I, NIR models based on the spectra from the three sections were tested. The total correctness of the model based on the spectra from the cross-sections was 100%. The identification results demonstrated that NIR can identify different wood species correctly.
2. In case II, three identification models were established based on trees from different locations. The calibration performances of *Pometia*, *Instia*, and *Couratari* were 67%, 94%, and 99%, and the accuracies of the prediction results of *Pometia*, *Instia*, and *Couratari* were 60%, 83%, and 100%, respectively. From the above results, it can be concluded that NIR has the potential to identify wood block samples from different locations. However, futher investigations are needed to achieve better identification accuracy.

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