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RESEARCH ARTICLE

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Wood species identification from Atlantic forest by near infrared spectroscopy

José HC Pace*[1]; João VF Latorraca[1]; Paulo RG Hein[2]; Jonnys P Castro[1]; Alexandre M Carvalho[1]; Carlos ES Silva[1]
(Pace, JHC; Latorraca, JVF; Hein, PRG; Castro, JP; Carvalho, AM; Silva, CES)
[1]Federal Rural University of Rio de Janeiro, Forest Institute, Department of Wood Technology, 23890-000, Seropédica, Brazil. [2]Federal University of Lavras, Department of Forest Science, 37200-000, Lavras, Brazil.

Abstract

Aim of study: Fast and reliable wood identification solutions are needed to combat the illegal trade in native woods. In this study, multivariate analysis was applied in near-infrared (NIR) spectra to identify wood of the Atlantic Forest species.

Area of study: Planted forests located in the Vale Natural Reserve in the county of Sooretama (19 ° 01'09 "S 40 ° 05'51" W), Espírito Santo, Brazil.

Material and methods: Three trees of 12 native species from homogeneous plantations. The principal component analysis (PCA) and partial least squares regression by discriminant function (PLS-DA) were performed on the woods spectral signatures.

Main results: The PCA scores allowed to agroup some wood species from their spectra. The percentage of correct classifications generated by the PLS-DA model was 93.2%. In the independent validation, the PLS-DA model correctly classified 91.3% of the samples.

Research highlights: The PLS-DA models were adequate to classify and identify the twelve native wood species based on the respective NIR spectra, showing good ability to classify independent native wood samples.

Additional keywords: native woods; NIR spectra; principal components; partial least squares regression.

Authors´ contributions: Original ideia: JHP, JVL and PRH. Material collection: JHP, JVL, AMC, JPC and CES. Study design: JHP, JVL and PRH. Data analysis: JHP and PRH. Manuscript preparation and revisions: JHP, JVL, PRH, AMC, JPC and CES. All authors read and approved the final manuscript.

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Correspondence should be addressed to José-Henrique Camargo-Pace: josehcpace@gmail.com

Introduction

The use of Atlantic Forest reforestation woods as a source of income and raw material aims to supply the domestic market of native wood, protect the few biome remnants and stimulate the forestry of timber species (Brancalion *et al.*, 2012). Forest certification encourages economic landscapes restoration and helps combat the illegality existing in the native timber trade, generating pressures on forest concessions holders and timber traders to know the origin of their material (Silva *et al.*, 2018). In general, illegal trade stems from the lack of proper wood identification (Bisschop, 2012), often because of limitations on the domain of the wood anatomical, physical and visual aspects (Ramalho *et al.*, 2018).

The traditional process to wood identification, depending on the species and location, involves costs and a long period of time, generating doubts in the wood commercialization and inspection in pile deposits and sawmills (Soares *et al.*, 2017). Therefore, it is necessary

to identify these timber found in the sawmill's yards quickly and efficiently, in order to assist and provide practicality to the inspection agencies, since timber can present different quantitative characteristics within the same species, whereas they are influenced by the climatic, soil conditions, silvicultural practices and forest density (Silva *et al.*, 2018).

Near-infrared spectroscopy (NIR) has been a promising technique for identifying forest species in a fast and practical way (Abasolo *et al.*, 2013; Meder *et al.*, 2014; Soares *et al.*, 2017; Ramalho *et al.*, 2018). The NIR-based technique can increase response speed and reduce operating costs, since it does not require the tree felling or the destruction of a piece of wood (Rosso *et al.*, 2013; Lazzarotto *et al.*, 2016). Therefore, NIR technology has been identified as a solution to help control the illegal timber trade (Ramalho *et al.*, 2017; Soares *et al.*, 2017; Ramalho *et al.*, 2018).

By using the NIR technique it is possible to make a large database on species, which will lead to an easy and quick identification, avoiding fraudulent transactions and, in addition to being able to make other types of estimates, such as the place of origin, the moisture wood content, estimate the density and degradation levels that it can present (Watanabe *et al.*, 2006; Tsuchikawa & Kobori, 2015; Lazarescu *et al.*, 2016; Silva *et al.*, 2018). NIR spectroscopy is based on the interaction of the electromagnetic radiation with the C-H, S-H, N-H and O-H bonds present in the material (Pasquini, 2003, Hein, 2012).

To extract information from the spectra, multivariate statistical analyzes are used. Chemometrics methods are used to correlate the NIR spectra with the woods quantitative or qualitative characteristics in order to recognize, develop classification models, plan and optimize experiments and calibrate multivariate regressions based on the materials spectral signature (Brereton & Lloyd, 2014; Hein *et al.*, 2017; Nascimento *et al.,* 2017; Ramalho *et al*., 2017; Soares *et al.*, 2017).

Thus, the objective of this study was to develop wood classification and identification models based on the spectral signature through principal component analysis and partial least squares discriminant analysis. This research aims to expand the spectral information of Brazilian Atlantic Forest species and to create fast solutions for the identification of unknown wood.

Material and methods

Wood collection

The study area is part of one of the largest collections of forest remnants of the Atlantic Forest, Vale Natural Reserve in Linhares, Espírito Santo, Brazil. The climate is hot and humid, with rainy summers and dry winters, being classified as Awi according to the Köppen system. Meteorological data from a 24-year historical series (1986-2010) show that the annual average temperature is approximately 24 °C and the average annual rainfall is 1,212 mm. In the reserve, research was developed with the species native from the reserve in homogeneous plantation of more than 30 years, originating from seeds of the reserve's own matrix. The plantations had spacing 3 x 2 meters and were fertilized in 400g NPK (5:14:3) (Mendonça *et al.*, 2017).

For the wood study of these homogeneous plantations, three trees per species were felled (Table 1). For the initial material recognition, the apparent density (15% of moisture) and the basic density were verified according to the NBR 7190 standards, with 10 specimens of each tree per species.

Wood samples from each tree, for all the species, were recorded in the library of Foresty Institute of the Rural University of Rio de Janeiro, documented with codes 7,730 to 7,765. With the help of a circular saw the samples produced with 3 x 3 x 10 cm dimensions (tangential, radial and longitudinal to the fiber direction) were used for spectroscopy. Heartwood and sapwood samples and near the bark and marrow were collected for all the collected trees, resulting in an average of 60 samples per species, totaling 696 spectra. All the samples were air-conditioned with equilibrium moisture at 12%.

Near Infrared Spectroscopy - NIR

The spectra were recorded in diffuse reflectance mode using a Fourier transform NIR spectrometer (MPA, Bruker Optik GmbH, Ettlingen, Germany). This Fourier transform spectrometer is designed for solids reflectance analysis, holding an integrating sphere that measures diffuse reflected infrared energy from a point of 150 mm². The spectral analysis was performed within the range from 12,000 to 3,900 cm^{-1} at the resolution of 8 cm^{-1} (each spectrum represents an average of 32 readings), according to the procedure described in (Ramalho *et al.*, 2017, 2018). The collected spectrum data are stored on the computer through the OPUS program, version 7.5. The readings were performed on both samples transverse surfaces, avoiding regions with cracks and other defects, creating a spectral average for each sample. For a better perception and extinction of noises contained in the spectra, a comparison of the data without pretreatment and with pre-treatments was done, being the first and second derivative (polinomial of second order

Table 1. List of species used and average values of wood density (g/cm³).

Code	Common name	Scientific name	ρ15	ρ	Family
A	Angico Preto	*Senegalia polyphylla* (DC.) Britton	1.02	0.80	Fabaceae
AD	Aderne	*Astronium graveolens* Jacq.	0.84	0.72	Anacardiaceae
C	Cerejeira	*Amburana cearensis* (Allemão) A.C. Sm.	0.60	0.44	Fabaceae
FS	Farinha seca	*Basiloxylon brasiliensis* (Allemão) K. Schum.	0.74	0.55	Malvaceae
G	Gonçalo-alves	*Astronium concinnum* Schott ex Spreng.	0.83	0.63	Anacardiaceae
JB	Jacarandá da Bahia	*Dalbergia nigra* (vell.) Allemão	0.78	0.63	Fabaceae
L	Louro	*Cordia trichotoma* (Vell.)	0.59	0.48	Boraginaceae
PA	Paineira	*Pachira endecaphylla* (Vell) Carv.-Sorb.	0.40	0.29	Malvaceae
PB	Pau Brasil	*Paubrasilia echinata* (Lam.) Gagnon, H.C. Lima & G.P. Lewis	0.97	0.79	Fabaceae
PS	Pequiá-sobre	*Aspidosperma pyricollum* Müll. Arg.	0.94	0.76	Apocynaceae
PSA	Pau sangue	*Pterocarpus rohrii* Vahl	0.47	0.39	Fabaceae
S	Sucupira	*Bowdichia virgilioides* Kunth	0.88	0.71	Fabaceae

ρ_{15} = Bulk density (15% of moisture); ρ = Basic Density.

and 15 points of each side) and SNV (Normal Standard Variate). (Lazzaroto *et al.*, 2016, Ramalho *et al.*, 2018).

Multivariate statistical analyzes

For the multivariate exploratory and the models calibration statistics, the statistical program Chemoface 1.61 was used (Nunes *et al.*, 2012). The species identification and separation was supported by chemometrics (translation of chemical spectra by mathematical models). After the database elaboration and the respective pre-treatments of the same, the multivariate analyzes were used.

Principal Component Analysis (PCA)

First, the analysis was used to identify which pretreatment of the data presented a better explanatory power. After this identification, an exploratory analysis was performed by the PCA using two-thirds of the total samples, considering the remaining third as independent samples of the statistical models creation, adopted by some authors (Nunes *et al.*, 2012; Lazarescu *et al.* 2016, Lazzaroto *et al.*, 2016, Soares *et al.*, 2017, Ramalho *et al.*, 2017, 2018, Costa *et al.*, 2018). The PCA was performed using 10 main components, in order to translate the groups and trends in the calibration database, extracting and identifying latent variables, thus reducing the database dimensional space.

Discriminant analysis by least squares regression (PLS-DA)

From the PLS-DA approach, the species were considered as a categorical variable presenting discrete values. In this study, the samples were grouped into different classes, as category A is represented by *Senegalia polyphylla* wood and so on (see Table 1). Then, the values 0 or 1 were assigned to all the samples in each category, and when the sample belonged to that category, the value 1 was assigned and when the sample did not belong to the category, the value 0 was assigned. Preliminary PLS-R models were performed to estimate each of twelve categories (A, AD, C... and S). Thus, a continuous value was estimated for each specimen from the twelve predictive models. In this approach the PLS-R model whose estimate was the highest continuous value indicated the category to which the sample belonged. The preliminary PLS-R models were evaluated by the coefficient of cross-validations determination (R^2_{cv}) or test set validation (R^2_p), root mean standard error ($RMSE_{cv}$ and $RMSE_p$), while the PLS-DA models were evaluated by success rate and by means of the graphic representation. The percentage of hits of unknown samples also reflects the robustness of the PLS-DA model. No outliers were detected in this database. This approach is described in detail in Costa *et al.* (2018).

Results

Material Recognition

For the data analysis, a total of 696 spectra were collected, adding robustness to the database for the model calibration and validation. Fig. 1 illustrates the difference in the visual appearance among the woods in terms of coloration, which possibly denotes chemical differentiations among the species.

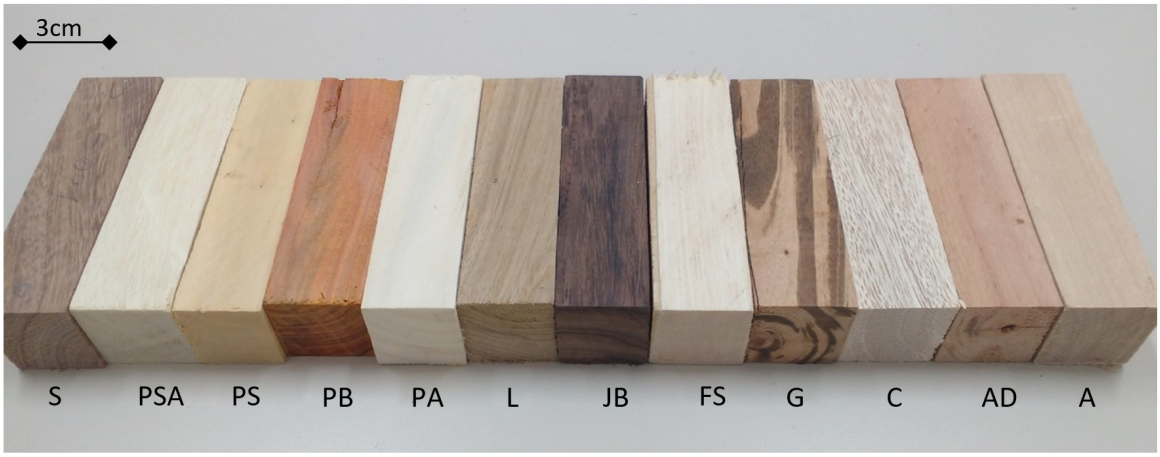

Figure 1. Specimens of each of the studied species.

NIR spectroscopy

The results obtained by means of the NIR spectra for each species can be observed in Fig. 2. The analyzed spectral variation was between 9,000 and 3,999 cm^{-1}. Observing the NIR absorbance graph, it is possible to notice that the upper and lower extremities of the spectra mean are given by the Angico spectrum and the Paineira spectrum, respectively, considering that both species also have the highest and the lowest density according to Table 2. The greatest distance or chemical difference between the spectra is comprised in the wavelength ranges from 7,000 to 5,300 cm^{-1} and also in another small range from 5,000 to 4,500 cm^{-1}. Amazonian species woods showed that the spectra average by species, also presented the same tendency according to the density (Nascimento *et al.*, 2017; Soares *et al.*, 2017).

Principal Component Analysis - PCA

The spectra complex behavior requires an analysis with a high power of interpretation, for trends or latent variables (main components). Through the PCA it was possible to identify the best way to work with the database, reducing the noise contained in the spectra. Therefore, it was possible to observe that the database without pre-treatment showed that the main

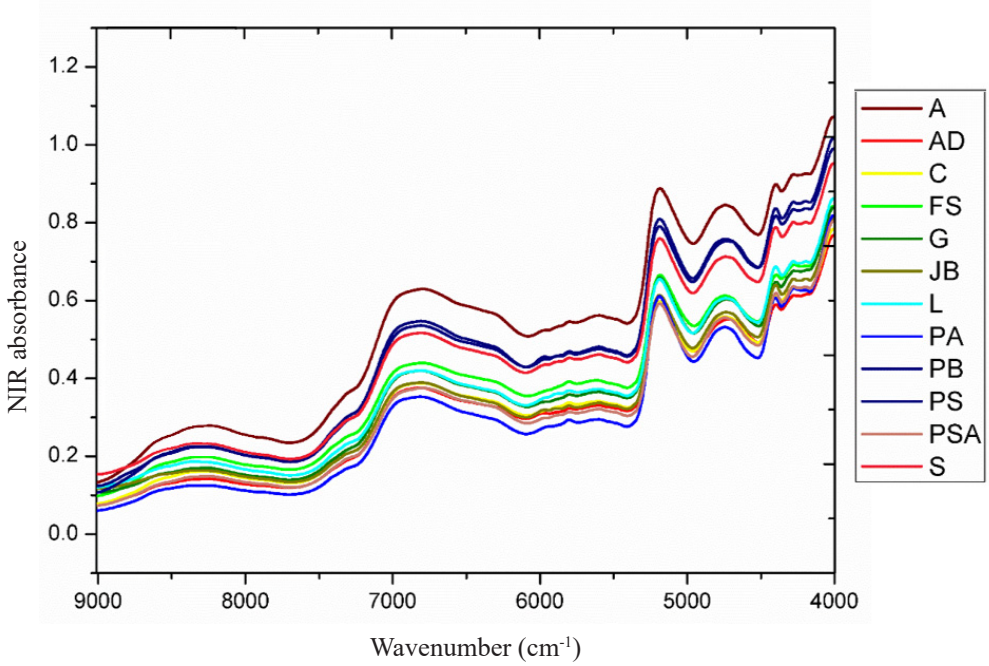

Figure 2. Average profiles of the NIR spectra for the 12 species.

Table 2. Explanation of the X variation (in%) through the values of the main components, applying treatments in the database for the spectra of the woods obtained by the NIR.

	Untreated	1 der	2 der	SNV
PC 1	99.84	99.10	98.24	98.63
PC 2	99.97	99.55	98.92	98.91
PC 3	99.99	99.71	99.24	99.16
PC 4	99.99	99.92	99.67	99.39

(1 der) (2 der) first and second derivative, (SNV) Standard Normal Variate.

components presented a better explanatory power of the total of the variance present in the analysis space (Table 2). It is observed that the database pre-treatment with the 1st derivative, was possible to obtain the closest values of the components without treatment, serving as a good option for evaluation, with good explanatory power. However only the first (CP1) explained more than 99% of the variance in the original (untreated) spectra database.

Using only the first and second main components, it was possible to generate score graphs with formation of large four groups, which are possibly associated to the wood density variation. (Fig. 3). This exploratory analysis of spectra behavior was very significant, using only the first two components due to the variance explanation percentage. Note that the first group is represented only by the scores related to Angico wood (bottom of the graph); the second group represented by wood scores of Pau Brasil, Sucupira, Pequiá-Sobre and Farinha Seca; the third group containing the wood scores of Louro, Gonçalo Alves, Jacarandá, Cerejeira, Aderne and Pau Sangue; and the fourth group containing only scores related to Paineira (upper).

Calibration and prediction of the model (PLS-R and PLS-DA)

Pre-modeling of each species through PLS-R gave some parameters described in Table 3. The PLS-R model calibration took 2/3 of the sample amount into account and the remaining 1/3 was reserved for testing the capacity of the PLS-DA model prediction, considering them as independent, unknown wood samples.

The species discrimination in PLS-R had its calibration fixed with 20 latent variables. In Table 3 it can be observed the number of latent variables to classify each species, quantity which was determined in a way that there was constancy in the quadratic error values of the cross validation. It can be noticed that the model calibration using the PLS-R provided a very significant modeling, due to the high values for the coefficients of determination (R^2_c) for the species, so that the robustness of the database allowed to obtain values between 0.74 to 0.94, corroborated by the small values of the cross-validation error ($RMSE_{cv}$), not exceeding 0.15. These results demonstrate that the model generated by PLS-DA presents a significant capacity to classify the native woods of different

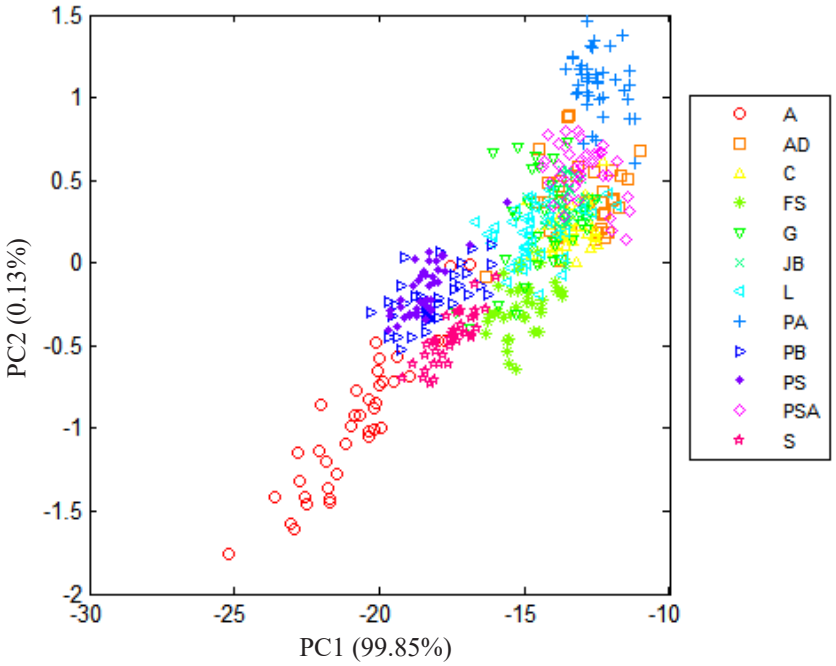

Figure 3. PCA scores of the 12 wood species indicating four groups of species.

Table 3. Statistics of PLS-R models used to classify PLS-DA, based on untreated spectra.

species	$RMSE_c$	R^2_c	$RMSE_{cv}$	R^2_{cv}	R^2_p	$RMSE_p$	VL
A	0.10	0.86	0.11	0.84	0.84	0.27	14
AD	0.12	0.78	0.13	0.74	0.75	0.25	17
C	0.12	0.84	0.12	0.81	0.80	0.18	12
FS	0.08	0.91	0.09	0.89	0.88	0.27	13
G	0.13	0.74	0.14	0.70	0.71	0.26	16
JB	0.12	0.81	0.13	0.79	0.78	0.28	15
L	0.12	0.82	0.13	0.80	0.80	0.27	17
PA	0.06	0.95	0.07	0.94	0.92	0.17	9
PB	0.11	0.83	0.12	0.81	0.80	0.26	17
PS	0.14	0.75	0.15	0.72	0.72	0.27	16
PSA	0.11	0.85	0.12	0.83	0.82	0.28	12
S	0.09	0.90	0.10	0.88	0.87	0.27	15

Calibration coefficient (R^2_c), cross-validation (R^2_{cv}) and prediction (R^2_p), calibration mean square error, cross validation and prediction ($RMSE_c$, $RMSE_{cv}$ and $RMSE_p$), latent variables (VL).

Atlantic forest families and species. In Table 4, it is possible to observe the classification power given by the PLS-DA cross-validation, in a way that four species (Farinha Seca, Jacarandá and Paineira) did not present an error in the classification of any sample, in this model generated by the PLS-DA, different from the Aderne and Pau-Brasil, which presented a percentage of classification error in cross-validation higher than 17 % and 22%, respectively. However, the average classification error for the generated model was less than 7%. This percentage exhibits close values obtained in the Amazon native wood species discrimination with species of Eucalyptus plantations (Ramalho *et al.*, 2018).

After the elaboration of the classification model by PLS-DA, it is necessary to test the predictive capacity of the same. The prediction was carried out using independent samples (1/3 of the total samples). The prediction showed excellent correct classification values, such that the percentage of accuracy exceeded 90%, for a total of 232 samples (Table 4). This value is very close to that of the calibration model. However, considering the classification errors, these were higher than those presented in the calibration model, guided by the same species (Aderne and Pau Brasil), however with larger values, close to 30%, raising the classification error percentage mean by PLS-DA to 9%. But even with this increase, the model still demonstrates an acceptance of its predictive ability of independent samples.

In the prediction of some species it is possible to observe that a remarkable classification was obtained, so that all samples of the dry flour, Jacarandá, Paineira and Pequiá-sobre, were correctly classified (Table 4), demonstrating the efficiency of the wood classification model by PLS-DA for these species of the Atlantic Forest.

Discussion

NIR Spectra

The spectra variations observed in the range from 7,000 to 5,300 cm^{-1} may help to explain some of the differences among woods due to high correlation with the main wood chemical constituents (Tsuchikawa & Korobi, 2015). In the range from 7,000 to 6,000 cm^{-1}, the overtones associated with OH and NH bonds are shown, promoting stretch-type vibrations associated with hydrogen bonds that interact with cellulose, hemicellulose and water (Soares *et al.* 2017). The crystalline and amorphous regions of cellulose are also related, at the wavelengths of 6,281 and 6,775 cm^{-1}, respectively (Watanabe *et al.*, 2006). The beginning of the spectra separation can be perceived within the range from 6,900 to 6,850 cm^{-1}, because in this range it is possible to perceive the readings of aromatic, phenolic and OH groups associated to lignin and extractives (Watanabe *et al.*, 2006; Schawnniger *et al.*, 2011). This is a point where the spectra differ the most, since the difference in the species coloration, especially in the core regions (when it is distinct), is notorious for the large extractives deposition occurring in this part of the material. Since that the extractives are also estimated by NIR spectroscopy, showing good correlations

Table 4. Samples classification by cross-validation and prediction of independent samples by the model generated in PLS-DA, with the database without pre-treatment.

	NIR (classification of spectra by species)												Correct classification		Total samples
	species	A	AD	C	FS	G	JB	L	PA	PB	PS	PSA	S	Nº	%	
Cross-validation	A	36	2								2			36	90.0	40
	AD		28			4	2							28	82.5	34
	C			36								5		36	87.8	41
	FS				39									39	100	39
	G			1		33						1		33	94.2	35
	JB						41							41	100	41
	L			1				39						39	97.5	40
	PA								40					40	100	40
	PB									28	8			28	77.7	36
	PS	1									38			38	97.4	39
	PSA			2			1					38		38	92.6	41
	S	1											37	37	97.4	38
	Independent samples													433	93.2	464
Test set validation	A	18										1		18	94.7	19
	AD	1	12			4								12	70.5	17
	C			20								1		21	95.2	21
	FS				20									20	100	20
	G		1			15						1		14	88.2	17
	JB						21							18	100	21
	L	1					1	17						17	90.5	19
	PA								20					20	100	20
	PB	1					2			12	4			12	63.1	19
	PS										19			18	100	19
	PSA											20	1	20	95.2	21
	S						1						18	19	94.7	19
total														209	91.0	232

(Schawnninger *et al.*, 2011; Tsuchikawa & Korobi, 2015), they are suitable to support the determination of chemical solutions for pulp production (Hein *et al.*, 2017).

Another point of great difference among the obtained spectra was the wavelength of 5,974 and 5,850 cm^{-1}, which are attributed to the aromatic lignin rings (Schawnninger *et al.*, 2011) and vibration of C-H bonds (Li *et al.*, 2015), respectively. After the wavelength of 5,300 cm^{-1}, the differences in the spectra presented an attenuation, so that this attenuation is associated with the OH bonds vibration with greater stretching and their deformation, presenting a connection with the water molecules structures (Pasquini, 2003, Baldin *et al.*, 2018), this can be proven by the homogenization and humidity control that the test specimens passed before the NIR readings inside the heated room.

Principal Component Analysis (PCA)

Although scores generated by PCA illustrate totally separate clusters, as it can be seen with some authors, differentiating species and/or families mainly when working in the wood and charcoal differentiation (Nigoski *et al.*, 2015, Ramalho *et al.*, 2017), some trends can also be observed, due to the existence of overlapping of some points (Meder *et al.*, 2014; Ramalho *et al.*, 2018), even the existence of a linearity in the scores graph (Abasolo *et al.*, 2013), also seen in Fig. 3. This linearity can be interpreted and divided into four large groups.

The PCA analysis translates the spectra chemical information, and with the scores graph (Fig. 3), it was possible to observe some groups. This separation among groups may be related to the density variation among the species (Table 1). The density is directly involved

with the wood anatomical and chemical characteristics (Nascimento *et al.*, 2017). In the chemical part it correlates with the proportion of the wood main chemical constituents (cellulose, hemicellulose, lignin and extractives) (Tsuchikawa & Korobi, 2015), since the NIR readings are based on the chemical changes. Some authors attest the elaboration of models with high capacity to classify and estimate basic density when using the near infrared spectra due to the wood chemical character that is associated with the density (Schwanninger 2011; Rosso *et al.*, 2013; Li *et al.*, 2015; Lazzaroto *et al.*, 2016; Hein *et al.*, 2017).

Therefore, it can be observed that the first group presents the species with the highest density, in the case of Angico (ρ_{15} = 1.08g / cm³), with the formation of the next group with less dense wood than in the first group, such as Sucupira, Pau Brasil and Pequiá-sobre. The third group was also formed by woods that present smaller densities than the previous group, with the participation of Cerejeira, Gonçalo-Alves, Pau sangue and Jacarandá. Finally, the fourth group is formed by the species that have the least dense wood of all, in the case of Paineira (ρ_{15} = 0.40g / cm³). In group three, the presence of Aderne and Gonçalo is observed, however, both species present a higher density than that found in this group, demonstrating a differentiation of the *Astronium* genus compared to the other species, suggesting more studies in relation to the genus.

Calibration and validation of the PLS-DA model

Results obtained in this study agreed with those of the literature, assisting in the studies for the Atlantic Forest conservation, since that chemometric technique for the wood and NIR recognition has already been used in the Amazonian biome. When tested predictive models to identify wood species, the accuracy percentage in PLS-DA classification reached values ranging from 0.90 to 0.99 (Soares *et al.*, 2017). Robust differentiation models of planted and native wood resulted in a cross-validation coefficient between 0.86 and 0.94 (Ramalho *et al.*, 2018), even with the identification of the place of origin of the *Swietenia macrophylla* wood. they obtained by PLS-R, coefficient of determination values greater than 0.90 (Silva *et al.*, 2018). Of the 464 samples used for PLS-R calibration, which were used to base the classification by the PLS-DA model, only 6.7% of the samples were classified incorrectly, showing reliability in the classification by the model, affirming the good capacity that the technique has in determining to which group a sample can probably be classified (Brereton & Lloyd, 2014). Remembering that the models can always be improved, the more information and the more robust the database, the better. However, there is some chemical characteristic of the sample that differs from the others within the same species, due to the great wood inherent heterogeneity, because of the presence of heartwood, scar marks and/or marks of old branches, proving that the technique is not perfect.

The model of classification generated by PLS-DA, translated the great capacity that the infrared spectroscopy presents to be used in the identification of different types of wood of the Atlantic Forest, corroborating with the results of some authors (Nigoski *et al.*, 2015; Silva *et al.*, 2018; Ramalho *et al.*, 2018). The PLS-R models reported in this study present relatively good values for the cross-validation coefficient (R^2_{cv}). Similar studies have presented high values for the determination coefficient. Lazarescu *et al.*, (2016) reported R^2 = 0.87 for predicting *Tsuga* sp. or *Albies* sp wood specimens. Soares *et al.* (2017) showed promising models for separating Amazonian timber while Ramalho *et al.* (2018) reported good classifications for differenting wood specimens from natural or planted forests.

These results strengthen the concept of the NIR technique use associated with multivariate statistics, for the classification and identification using the PLS-DA model, at the level of families, species, genera and even in hybrids (Abasolo *et al.*, 2013; Meder *et al.*, 2014; Nigoski *et al.*, 2015; Soares *et al.*, 2017; Baldin *et al.*, 2018; Ramalho *et al.*, 2018). These results can help the entities responsible for the timber trade control to be aware of this technological option due to the ease, speed and accuracy of the answers, since these are the main obstacles to combat the illegal timber trade (Bisschop, 2012).

Conclusion

The non-destructive near-infrared spectroscopy technique can also be used to identify Atlantic Forest woods. The use of chemometrics aided in the spectra translation making it possible to evidence the trends and behaviors of the studied forest species. The model created for some species showed great efficiency in the classification, both in calibration and validation, but for some species a greater wood variability to improve their calibration models. NIR spectroscopy in conjunction with PLS-DA can be considered a promising tool for control in the timber trade and in the species conservation.

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