Alternative identification of wood from natural fallen trees of the Lecythidaceae family in the Central Amazonian using FT-NIR spectroscopy

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HIGHLIGHTS

- FT-NIR spectroscopy was capable of discriminating wood from natural fallen trees from the Lecythidaceae family.
- Degraded samples carry 50% of the identification bands at the genus level.
- The spectral signature is the key to identifying wood types.
- The mathematical treatment (2nd derivate, Norris, and Savitzky-Golay smoothing) increased the identification accuracy.
- FT-NIR is a powerful tool for taxonomic purposes in accurate and non-destructive identification and classification of wood.

SUMMARY

The scientific identification of natural fallen trees in tropical forests is complex due to the lack of fertile material in field collection. The study evaluated the use of near-infrared spectroscopy with Fourier-transform (FT-NIR) in the discrimination of wood from fallen trees of the Lecythidaceae family. Seven trees were collected in the Central Amazonian region (Brazil), from which 63 specimens were prepared from the wood, and NIR spectra were obtained on different wood surfaces (total 756 spectra). Chemometric models were developed with a spectral data set, and the Mahalanobis algorithm was applied. The discriminant model with 2nd derivative spectra improved the identification capacity, resulting in errors < 5% in the identification of genus *Couratari* (3 ssp.), *Eschweilera* (2 ssp.), *Holopyxidium* (1 sp.) and *Lecythis* (1 sp.). The comparison of the spectral signatures of samples of fallen trees and wood library revealed that even when wood was exposed to environmental weathering, around 50% of the original bands were preserved, favouring discrimination at the genus level. The accuracy of the chemometric models developed indicates the applicability of FT-NIR spectroscopy integrative in identifying fallen trees from the Lecythidaceae family in the tropical forests.

Keywords: fallen wood, alternative taxonomy, Amazon woods, discriminant analysis, non-destructive methodology

Identificação alternativa de madeira de árvores caídas naturalmente da família Lecythidaceae na Amazônia Central utilizando espectroscopia FT-NIR

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A identificação científica de árvores caídas naturalmente em florestas tropicais é complexa devido à falta de material fértil na coleta de campo. O estudo avaliou o uso da espectroscopia no infravermelho próximo com transformada de Fourier (FT-NIR) na discriminação de madeira de árvores caídas da família Lecythidaceae. Sete árvores foram coletadas na região da Amazônia Central (Brasil), sendo que 63 corpos-de-prova foram preparados a partir da madeira, e espectros NIR foram obtidos em diferentes superfícies de madeira (total de 756 espectros). Modelos quimiométricos foram desenvolvidos com um conjunto de dados espectrais, e o algoritmo Mahalanobis foi aplicado. O modelo discriminante com espectros na 2ª derivada melhorou a capacidade de identificação, resultando em erros < 5% na identificação dos gêneros *Couratari* (3 ssp.), *Eschweilera* (2 ssp.), *Holopyxidium* (1 sp.) e *Lecythis* (1 sp.). A comparação das assinaturas espectrais de amostras de árvores caídas e da biblioteca de madeira revelou que mesmo quando a madeira foi exposta ao intemperismo físico e biológico, cerca de 50% das bandas NIR originais foram preservadas, favorecendo a discriminação em nível de gênero. A precisão dos modelos quimiométricos desenvolvidos indica a aplicabilidade integrativa da espectroscopia FT-NIR na identificação de árvores caídas da família Lecythidaceae em florestas tropicais.

Identification alternative du bois provenant d'arbres tombés naturellement de la famille des Lecythidaceae en Amazonie Centrale par spectroscopie FT-NIR

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L'identification scientifique des arbres tombés naturellement dans les forêts tropicales est complexe en raison du manque de matériel fertile lors des récoltes sur le terrain. L'étude a évalué l'utilisation de la spectroscopie proche infrarouge avec transformée de Fourier (FT-NIR) pour la discrimination du bois des arbres tombés de la famille des Lecythidaceae. Sept arbres ont été collectés dans la région de l'Amazonie centrale (Brésil), à partir desquels 63 spécimens ont été préparés à partir du bois, et des spectres NIR ont été obtenus sur différentes surfaces de bois (total 756 spectres). Des modèles chimiométriques ont été développés avec un ensemble de données spectrales et l'algorithme de Mahalanobis a été appliqué. Le modèle discriminant avec les spectres de 2[e] dérivée amélioré la capacité d'identification, entraînant des erreurs < 5% dans la classification des genres *Couratari* (3 ssp.), *Eschweilera* (2 ssp.), *Holopyxidium* (1 sp.) et *Lecythis* (1 sp.). La comparaison des signatures spectrales d'échantillons d'arbres tombés et de la xylothèque a révélé que même lorsque le bois était exposé aux intempéries environnementales, environ 50% des bandes originales étaient préservées, favorisant la discrimination au niveau des genres. La précision des modèles chimiométriques développés indique l'applicabilité de la spectroscopie FT-NIR intégrative pour identifier les arbres tombés de la famille des Lecythidaceae, provenant des forêts tropicales.

Identificación alternativa de madera de árboles caídos naturales de la familia Lecythidaceae en la Amazonía Central mediante espectroscopia FT-NIR

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La identificación científica de árboles caídos naturalmente en los bosques tropicales es compleja debido a la falta de material fértil durante las cosechas en el campo. El estudio evaluó el uso de espectroscopia de infrarrojo cercano por transformada de Fourier (FT-NIR) para discriminar madera de árboles caídos de la familia Lecythidaceae. Se recolectaron siete árboles en la región amazónica central (Brasil), de los cuales se prepararon 63 especímenes a partir de la madera y se obtuvieron espectros NIR en diferentes superficies de madera (total 756 espectros). Se desarrollaron modelos quimiométricos con un conjunto de datos espectrales y se aplicó el algoritmo de Mahalanobis. El modelo discriminante con los espectros 2a derivados mejoró la capacidad de identificación, resultando en < 5% de errores en la clasificación de los géneros *Couratari* (3 ssp.), *Eschweilera* (2 ssp.), *Holopyxidium* (1 sp.) y *Lecythis* (1 sp.). La comparación de las firmas espectrales de muestras de árboles caídos y de la biblioteca de madera reveló que incluso cuando la madera estuvo expuesta a la intemperie ambiental, aproximadamente el 50% de las bandas originales se conservaron, favoreciendo la discriminación a nivel de género. La precisión de los modelos quimiométricos desarrollados indica la aplicabilidad de la espectroscopia FT-NIR integradora para identificar árboles caídos de la familia Lecythidaceae, originarios de bosques tropicales.

INTRODUCTION

The Amazon Rainforest is home to one of the greatest forest diversities on the planet. One of the most recent taxonomic survey studies in the region recorded a total of 14,003 species belonging to 1,788 genera and 188 families of plant species (Cardoso *et al*. 2017). However, it is important to note that conservation, climatology and biotechnology studies in many areas of the Brazilian Amazonian face significant challenges in relation to the botanical taxonomy of this vast biota. With this in mind, it is not surprising that Brazil has the largest collection and species identification gaps in the Amazonian region (Schulman *et al.* 2007, Nascimento *et al.* 2022).

In a floristic inventory carried out in the Alto Solimões region, in Central Amazonian in Brazil, the most abundant botanical families were identified, including Fabaceae, Lecythidaceae, Burseraceae, Moraceae, Myristicaceae and Euphorbiaceae (Resex Rio Jutaí 2011). The Lecythidaceae family, which is part of the Ericales order, has a pantropical distribution, comprising 25 genera and approximately 340 species (Mori *et al.* 2015). According to the Brazilian Flora Checklist, the state of Amazonas is home to the greatest diversity of Lecythidaceae in the country, with 79 species distributed across seven genera (Smith *et al*. 2015, Cruz *et al*. 2021).

The Lecythidaceae are known internationally as the "chestnut family" due to the global trade in *Bertholletia excelsa* (Brazil nut) seeds, as well as the logging of species such as *Couratari* (tauari), *Lecythis* (jarana), and *Eschweilera* (matá-matá) (Procópio *et al.* 2010, Freitas and Vasconcellos 2019). The presence of specimens from this family serves as an indication of preserved or little disturbed floodplain forests (Prance and Mori 1979). Furthermore, it is notable that some tree species of this taxon are considered among the oldest, as evidenced by samples of silicified wood dating back to the Late Cretaceous found in both the Amazon Forest and the Atlantic Forest, which were identified as belonging to the genus *Lecythis* (Fernandes 1998, BFG 2015, BFG 2018).

In the Amazon rainforest, the identification of Lecythidaceae is often based on a combination of distinct vegetative characteristics. These traits include the predominantly arboreal habit, the release of a characteristic odour when the bark is cut, the presence of simple leaves arranged alternately, and the existence of cortical bundles in the bark that produce fibers, known as "envira". These vegetative traits provide a solid basis for species identification and are easy to observe. However, accurate identification of this taxon, both in terms of their external and internal morphology, requires a significant level of specialized knowledge on the part of botanists. Unfortunately, experts in this field are scarce throughout the world (Hopkins and Mori 1999).

The difficulty in identifying plant species is often associated with the availability of collected material. In many cases, it is necessary to analyse the reproductive organs of plants, but these organs are not always available. Sterile material can be evaluated by parabotanists in the field, but even then, identification errors can occur, often requiring specialist consultation (Fidalgo and Bononi 1984). For the identification of woody tissue, xylotheques (wood collections) and experts in wood anatomy play a key role. However, specialists in wood anatomy are a scarce professional category in Brazil. The identification and classification of wood depend mainly on microscopic characteristics, as more visible characteristics, such as colour, odour, and texture, can vary considerably but are still useful (INPA/CPPF 1991, Wheeler and Baas 1998, Freitas and Vasconcellos 2019). The correct description of anatomical traits of xylem tissue at the microscopic level, is one of the guarantees of scientific identification, with wood cells such as fibers, parenchyma, vessels, and rays being specific identities of this plant tissue (Santini Junior *et al.* 2021). Furthermore, other advanced plant identification techniques are being applied, such as cytology, genetics, molecular biology, biochemistry, carbon isotope analysis, and X-ray spectrometry. However, these techniques are onerous, time-consuming, and expensive (Vázquez *et al.* 2002, Fasciotti *et al.* 2015).

The circumscription of the chestnut family is still an issue that has not been completely resolved, with a lack of consensus on both inter- and intrafamily relationships within the group (Mori *et al.* 2015). Another situation that draws attention to the confusion in the identification of Lecythidaceae in the Brazilian Amazonian is the traditional recognition of common names for individuals of different genera and species (Bernal *et al.* 2011, Mori *et al.* 2015, Cysneiros *et al.* 2018). For example, Procópio and Secco (2008) identified eight different species of Lecythidaceae grouped under the name "tauari" in the northern region of Brazil. Therefore, wood identification in the field has proven challenging. Macroscopic characteristics, such as the external morphology of the shell or the presence of growth rings, are often insufficient for accurate identification at the species level. According to Rosa da Silva *et al.* (2022), distinguishing tropical wood species using only microscopic images presents a significant challenge owing to the diverse composition of xylem tissue and the variability among botanical species. They advocate for further research into image classification techniques utilizing machine learning specifically tailored to xylem microscopy.

One of the first records of identification of Lecythidaceae wood was reported by Diehl (1935), who indicated the presence of a homogeneous group characterized by bands of axial parenchyma, exclusively simple perforation plates, fibers with simple to indistinctly delimited punctuations, alternating intervascular punctuations and two types of punctuations on the rays of the vessels. Years later, Metcalfe and Chalk (1950) described the wood of this taxon and concluded that there was no clear distinction of the axial parenchyma. Therefore, this characteristic could not be used as a key to identify the wood of Lecythidaceae.

In general, the correct wood identification process must follow standards from the moment samples are collected, together with the respective herbarium receipts, as recommended by Barker (2008). Unfortunately, this approach is not always possible in regard to wood from trees that have fallen natural in the forest, as their fall is often associated with wind, lightning, old, sick individuals, or those infested by xylophagous organisms. In these situations, sterile material or quality vegetative material is often not found for identification purposes.

Non-destructive methodologies based on spectral signatures are becoming an effective and complementary alternative in plant identification, allowing taxonomic discrimination at different levels, from families, genera, species, and even morphotypes of various parts of plants, such as leaves, fruits, seeds and xylematic tissue. This approach has been shown to be fast and reliable compared to traditional taxonomy (Horikawa *et al.* 2015, Paiva *et al.* 2021, Nguyen *et al.* 2022).

Near-infrared spectroscopy (NIR) is an analytical technique that is based on vibrational spectroscopy and measures the interaction of electromagnetic radiation with the chemical components present in the sample. The NIR spectrum covers the wavenumber range of 12,000–4,000 cm^{-1} and is considered a "spectral signature" or "fingerprint" of the sample. This spectrum contains important chemical information about the type and number of functional groups, as well as the C–H, N–H, and O–H chemical bonds present in the sample (Durgante *et al.* 2013, Tang *et al.* 2018, Pasquini 2018).

Some botanical studies have validated the effectiveness of NIR spectroscopy. Castilho *et al.* (2008) and Severo (2010) demonstrated the usefulness of leaf fingerprinting in taxonomic classification. Lang *et al.* (2015, 2017) obtained high success rates in identifying seedlings and branches at the genus and family levels of Amazonian species using NIR. Hadlich *et al.* (2018) applied visible and NIR spectroscopy to recognize tree species from the bark tissue of tropical trees. In Brazil, few studies use NIR for botanical identification based on xylem tissue (wood), such as Braga *et al.* (2011), Nisgoski *et al.* (2018), Ramalho *et al.* (2018) and Pace *et al.* (2019). However, to date, no records of studies using NIR to discriminate wood from natural fallen trees in tropical forests have been found. In this sense, this study aimed to evaluate the use of near-infrared spectroscopy with Fourier-transform (FT-NIR) in the discrimination of wood from natural fallen trees of the Lecythidaceae family from the Central Amazonian.

MATERIALS AND METHODS

Study area and sample collection

The study was conducted in a tropical forest area in the Alto Solimões region, which covers the municipalities of Atalaia do Norte (Pau Mari and São Rafael communities), Benjamim Constant (Faustino Community) and Jutaí (Novo Apostolado, Porto Belo and São Raimundo communities), all located in the state of Amazonas, Brazil (Figure 1).

The region has a humid and superhumid tropical climate, with an average annual precipitation of 2,800 mm and an average temperature of 29 ± 2 °C. The average altitude in the region is approximately 65 m above sea level. From a geographical point of view, semi-flat terrains with yellow latosol soils predominate, being predominantly clayey, characterized by low permeability and fertility rates (Maia and Marmos 2010, Saldanha *et al.* 2018).

In the forest inventory carried out in the region, trees that were lying on the forest floor were selected. Before proceeding with the collection, visual inspections were carried out along the trunk (phytosanitary), recording the occurrence of fungi, termites, coleoptera, hollows, cracks, and wood with a high degree of degradation (mass loss > 50%). Dendrological parameters were measured, such as total height, commercial height, diameter at breast height (DBH), total volume, and the azimuth of each individual (Table 1). Most of the trees had damaged crowns and did not have fertile material for taxonomic identification purposes. In each case, roots were exposed, but the trunk appeared to be intact. The survey of fallen trees revealed a large occurrence of individuals from the botanical families Fabaceae, Lecythidaceae, Moraceae, Myristicaceae, and Euphorbiaceae, among others.

Seven matá-matá (*Eschweilera odora*) and tauari (*Couratari stellata*) trees from the Lecythidaceae (chestnut) family recognized by field experts (parataxobotanists FQ Reis and GA Mota) were selected for the study. Wooden discs with a thickness of 10 cm were cut at a height of 1.3 m on the tree (diameter at breast height, DBH) were removed using a chainsaw. Each disc was numbered and transported to the Wood Engineering and Artifacts Laboratory (INPA, Amazonas/Brazil). For anatomical identification purposes, a wedge corresponding to a quarter of the disc was removed using a band saw (Videira model), and this material was sent to the Wood Identification and Anatomy Laboratory (INPA, Amazonas/Brazil) for identification at the genus and species level using the comparison technique (Freitas and Vasconcellos 2019), with samples from the Botanical Collection Xylotheque (PCAC-INPA, Amazonas/Brazil). The remainder of each disc was transformed into specimens (20 × 20 × 30 mm), totalling nine replications per tree.

Obtaining NIR spectra

Initially, the samples were acclimated for a period of seven days (20 ± 2 °C and relative humidity of 65 ± 5%) to reduce the possible effects of instrumental deviations during the digitization of the spectral signature. The spectra were obtained

FIGURE 1 *Geographical location of the cities of Atalaia do Norte, Benjamin Constant and Jutaí (Amazonas/Brazil) where natural fallen trees were collected*

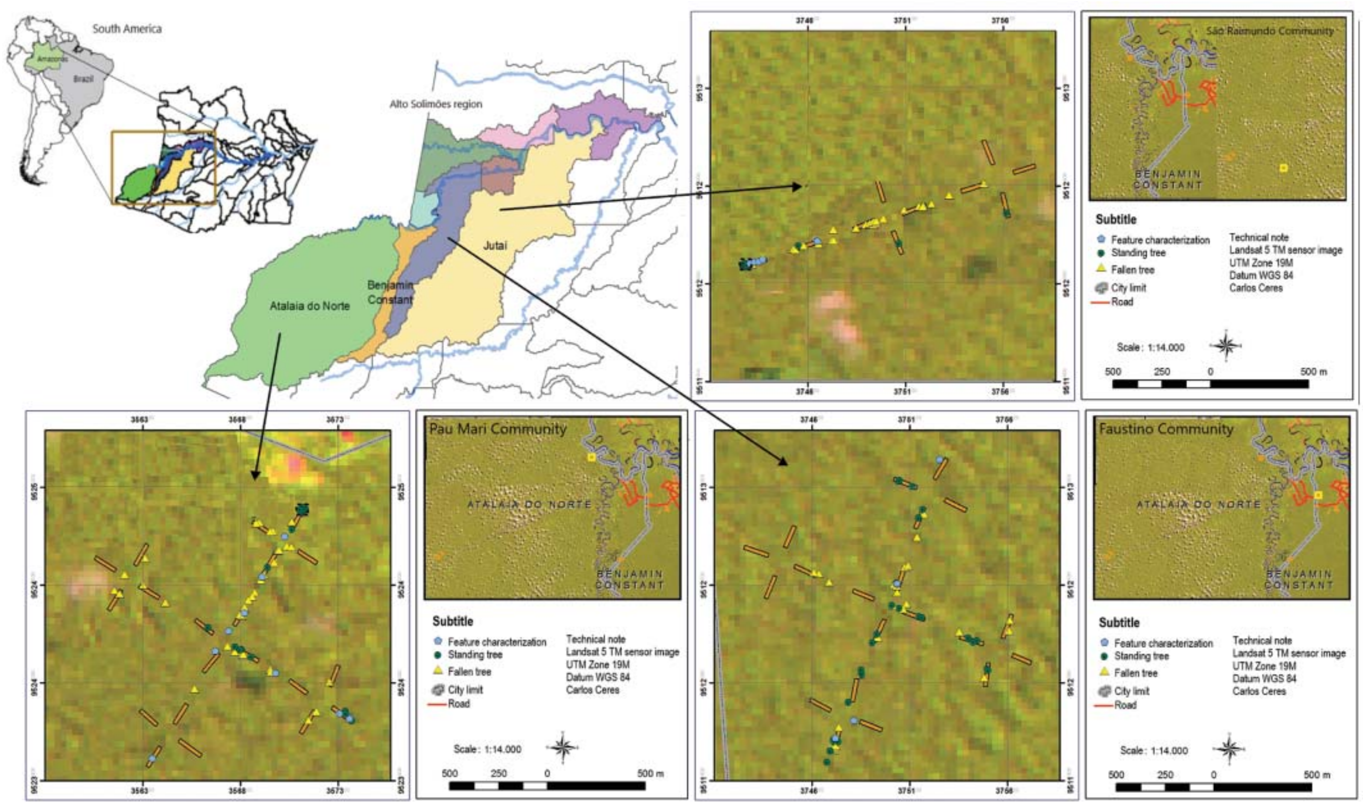


TABLE 1 *Natural fallen trees collected in the Alto Solimões region (Amazonas/Brazil)*

Identification		General characteristics of wood	Collection ocation	Az (°)	Alt (m)	HT (m)	HC (m)	DAP (cm)	VT (m^3)
Field	Xylotheque								
N° 18: Tauari *Couratari* sp.	*Couratari* sp.	Wood of medium density, straight grain, medium texture, apotracheal parenchyma and solitary vessels.	BC (Faustino): 3°06′ 39.6″S, 67°07′13.3″W	178	82	32.0	15.0	52.0	2.84
N° 286 Tauari *Couratari* sp.	*Couratari guianensis* Aubl.	High density wood, straight grain, medium texture, reticulated parenchyma, solitary vessels and multiples of two.	JU (Porto Belo): 3°17′ 19″S, 67°08′42.2″W	200	69	37.5	10.5	100.3	8.62
N° 362 Tauari *Couratari* sp.	*Lecythis usitata* Miers.	High density wood, slightly reversed cross grain, medium texture, reticulated parenchyma, solitary vessels and multiples of two with tylose obstruction.	JU (S. Raimundo): 3° 10′24″S, 67°13′22.3″W	160	56	22.0	11.5	18.5	0.30
N° 83 Matá-matá *Couratari* sp.	*Couratari stellata* A.C. Smith	Wood of medium-high density, straight grain, medium texture, reticulated parenchyma, solitary and multiple vessels of two and three with tylose obstruction.	BC (Faustino): 3°11′ 08.9″S, 67°08′59.4″W	229	89	18.6	12.5	20.5	0.35
N° 87 Matá-matá *Eschweilera* sp.	*Eschweilera odora* (Poepp. ex O.Berg)	High density wood, irregular grain, and medium to coarse texture, reticulated parenchyma, solitary vessels with tylose obstruction.	AN (Pau Mari): 3°11′ 06,5″S, 67°09′11″W	229	72	14.0	6.3	18.5	0.16
N° 163 Matá-matá *Eschweilera* sp.	*Eschweilera corea cea (*DC.) S.A.Mori.	High density wood, straight grain and medium texture. Reticulated apotracheal to paratracheal parenchyma, solitary vessels and multiples of two with tylose obstruction.	AN (S. Rafael): 3°27′ 0.9″S, 67°33′15″W	185	84	20.8	7.6	22.0	0.28
N° 312 Matá-matá *Eschweilera* sp.	*Holopyxidium* sp.	High density wood, straight grain and medium texture, reticulated and scalariform parenchyma, solitary vessels with tylose obstruction.	JU (N. Apóstolo): 3° 46′08″S, 67°26′32″W	180	68	26.0	14.5	26.0	0.66

AN: Atalaia do Norte; BC: Benjamin Constant; JU: Jutaí; Az: azimuth; Alt: Altitude; HT: total height; HC: commercial height; DBH: diameter at breast height; VT: total volume.

from the specimens using a near-infrared spectrometer with Fourier-transform – FT-NIR (Thermo Fisher Scientific, model Antaris II). The system uses RESULT™ software that operates at wavelengths from 10,000 to 4,000 cm^{-1}, with a resolution of 8 cm^{-1} and 96 scans – spectrum/sample of 16 scans (Torralvo *et al*. 2020*,* Nascimento *et al.* 2022). In each sample, four spectra were obtained in each plane (radial, tangential and transversal planes). Sample 'n' of the experiment (calibration and validation) was composed of 756 spectra (7 trees x 9 samples x 3 planes x 4 readings) that were used for multivariate analysis. From wood samples deposited in the Xylotheque/INPA/Brazil collection, 252 spectra were obtained and used in the evaluation of fallen wood models and spectral study (bands/reference).

Data processing and multivariate analysis

TQ Analyst™ software was used for multivariate analysis, and OMNIC™ was used for band evaluation. Prior to this procedure, to reduce the influence of various sources unrelated to the physical or chemical information carried by the raw spectra, the preprocessing technique, multivariate scatter correction (MSC), was applied.

When setting up the discriminant analysis, the dependent variables are categorical (genus/species), and the function's independent variables are the absorbance and wavelength of the NIR spectrum. The classification model developed consisted of a discriminant analysis that used the Mahalanobis algorithm (Mahalanobis distance – MD) to indicate grouping at two levels of botanical classification (genus and species) for wood from fallen trees of the Lecythidaceae family. MD works as a metric that determines the distance between a vector and the distribution. In the case of the NIR spectrum, the expression is based on the chemical bands that are possibly attributed to the class that is closest to the base in the MD.

All calibration and validation were developed on spectral data sets centred on the mean of each sample, where the sampling universe was composed of 75% samples for calibration and 25% for validation (Table 2). Random selection was performed to define the samples selected for each model.

The performance of the identification models was evaluated using the following parameters: Identification Index $_{(calibration/validation)}$ =N1/N2 x 100, where N1 = Number of samples correctly identified in the model; N2 = Total number of samples, and Maximum Classification Error =(∑E)/CA x 100, where ∑E = Sum of errors (calibration+ validation); CA = Total sample set.

RESULTS AND DISCUSSION

Discrimination of wood from fallen trees

The central aim of this study was to evaluate whether near-infrared spectroscopy is capable of distinguishing wood from natural fallen trees at the genus and species levels of the Lecythidaceae family. To our knowledge, no attempt has been made to discriminate this type of plant material using non-destructive techniques such as NIR spectroscopy. Traditional destructive wood identification methods are complex, time-consuming, and laborious and require specialization due to their dependence on physical, anatomical and visual characteristics of the xylem tissue.

The NIR spectral signature of the wood from fallen trees was used as input data for the discriminant analysis. The results showed a high identification rate for the calibration set (≥ 61%) and the validation set (≥ 86%), both at the genus and species level (Tables 3 and 4), highlighting the efficiency of the chemometric models. developed. Discriminant models n°. 5 (genus) and 4 (species) proved to be robust in classifying the xylem tissue of fallen trees. Furthermore, treatment of the spectra with the second derivative, Savitzky-Golay, and Norris smoothing improved the discrimination capacity, resulting in low error rates (< 5%). These results indicate that the mathematical treatment can enhance the quality of the NIR spectral signal, indicating correct identification of the wood; that is, when validating the model with samples of fallen trees (genus) that were not included in the calibrated set, the correct classification was 100%. Samples of Amazonian wood from the botanical collection (from the cities Presidente Figueiredo, Itacoatiara and São Gabriel da Cachoeira/ Amazonas/Brazil) were tested in the chemometric models and presented satisfactory results (77% correct identification) at the genus level; however, for species, the results showed incorrect classification.

NIR spectroscopy combined with multivariate analysis has proven to be a robust tool and can be adopted as an alternative method for the identification/classification of species from tropical or temperate regions for taxonomic purposes. This is because the results obtained are fast and highly reliable, according to literature reports (Durgante *et al*. 2013, Horikawa *et al*. 2015, Pace *et al*. 2019, Karlinasari *et al.* 2021). However, it is important to highlight that to date, no records of specific spectral models have been found for the taxonomic identification of natural fallen trees.

The variable used in the discriminant analysis was the Mahalanobis distance algorithm, MD (Figure 2 and 3), allowing the observation of four groupings (similarity), *Couratari, Eschweilera, Holopyxidium* and *Lecythis*, based on spectral

TABLE 2 *Summary of chemometric parameters used in FT-NIR modelling*

Chemometric method	Spectral region λ (cm^{-1})	Mathematical treatment	Smoothing	Data set
Discriminant analysis	9,882–4,119	No treatment 1st derivative; 2nd derivative	Savitzky-Golay; Norris	Calibration = 564 spectra Validation = 188 spectra Test = 252 spectra

TABLE 3 *Evaluation parameters of chemometric models for genus discrimination*

Chemometric models	Spectral treatment	Identification Index		Maximum Classification Error	Test*
		Calibration	Validation		
1	Raw spectra, Savitzky-Golay filter	83% (470 spectra)	93% (176 spectra)	14.55%	3% (8 spectra)
2	1st derivative Spectra, Savitzky-Golay filter	83% (470 spectra)	93% (176 spectra)	14.55%	19% (48 spectra)
3	1st derivative Spectra, Norris filter	61% (346 spectra)	86% (162 spectra)	32.80%	13% (33 spectra)
4	2nd derivative Spectra, Savitzky-Golay filter	83% (470 spectra)	100% (189 spectra)	14.55%	68% (171 spectra)
5	2nd derivative Spectra, Norris filter	98% (556 spectra)	100% (189 spectra)	1.46%	77% (194 spectra)

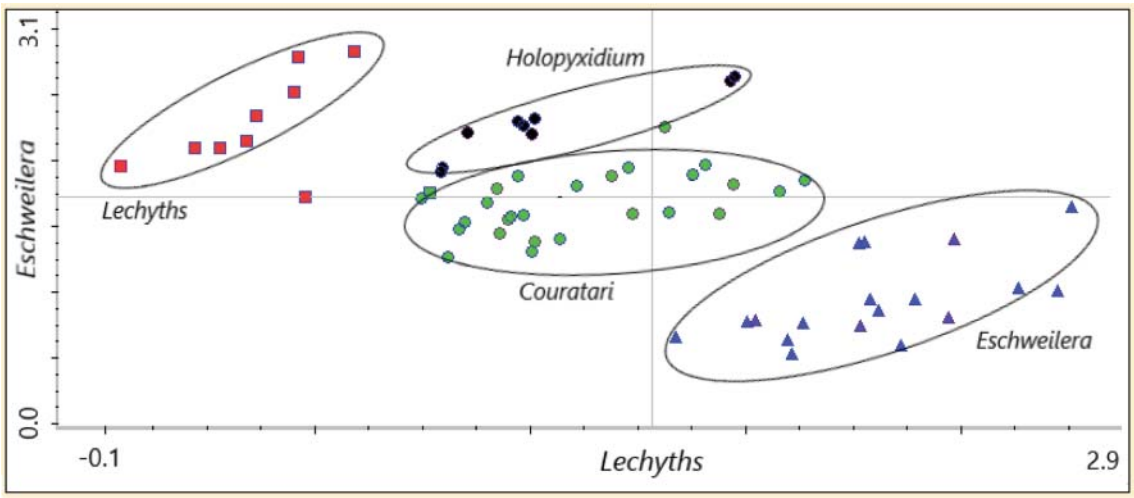
* Comparison with the Xylotheque sample; a more robust model is highlighted in bold

TABLE 4 *Evaluation parameters of chemometric models for species discrimination*

Chemometric models	Spectral treatment	Identification Index		Maximum Classification Error	Test*
		Calibration	Validation		
1	Raw spectra, Savitzky-Golay filter	86% (488 spectra)	88% (166 spectra)	13.49%	0%
2	1st derivative Spectra, Savitzky-Golay filter	86% (488 spectra)	88% (166 spectra)	13.49%	0%
3	1st derivative Spectra, Norris filter	91% (516 spectra)	88% (166 spectra)	9.79%	0%
4	2nd derivative Spectra, Savitzky-Golay filter	98% (556 spectra)	89% (168 spectra)	4.23%	9% (24 spectra)
5	2nd derivative Spectra, Norris filter	93% (527 spectra)	88% (166 spectra)	8.33%	0%

* Comparison with the Xylotheque sample; a more robust model is highlighted in bold

FIGURE 2 *Distribution of the "genus" calibration set of fallen wood of Lecythidaceae from the Mahalanobis distance algorithm*

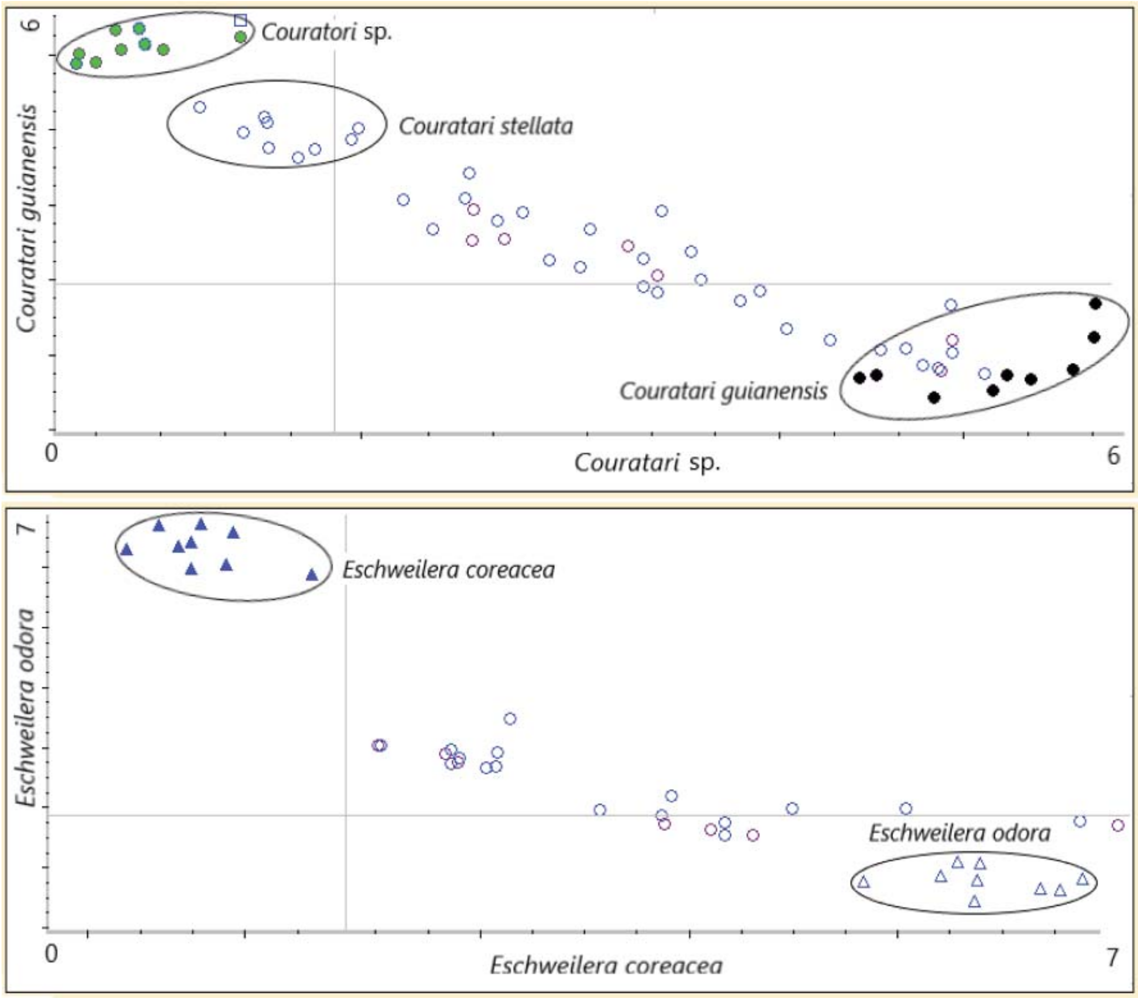


characteristics. In Figure 2, the MD is approximately 3, with significantly lower values for the genera *Holopyxidium* and *Lecythis*, which can be attributed to the similarity in the spectral bands of these genera. On the other hand, for the species *Couratari* (Figure 3A) and *Eschweilera* (Figure 3B), the MD was higher, approximately 6, suggesting that this behaviour may be related to botanical chemotaxonomic markers (Barbosa *et al.* 2006, Fasciotti *et al.* 2015, Nascimento *et al.* 2019).

Multivariate analysis plays a fundamental role in chemometric modelling, as it allows complex relationships between several variables to be explored. In the context of the NIR spectral signature, this technique combines absorbance with wavelength, incorporating a variety of information about the analyte of interest. This makes it possible to identify patterns, trends and potential clusters. Studies developed by Morozova *et al.* (2013) with NIR spectroscopy and MD sets validated the efficiency of this distance-based pattern recognition method and concluded that the MD algorithm presents reliable relationships when considering the qualitative characteristics of the samples. A study conducted by Wang *et al.* (2016) exemplifies the power of non-destructive methodology in combination with MD to evaluate defects in wood. The results of this study highlighted the robustness of the models developed and their superiority in comparison to other mathematical treatments.

Another relevant example is the study carried out by Davrieux *et al.* (2010), who used NIR spectroscopy in conjunction with the MD algorithm to discriminate charcoal from the native woods *Tabebuia serratifolia* and *Eucalyptus grandis*. In this case, the MD values obtained were 40 and 80, respectively, allowing validation of discrimination with a 100% accuracy rate. According to Morozova *et al.* (2013), shorter distances indicate spectral similarity with a class, and higher numbers indicate spectral dissimilarity. It is worth mentioning that NIR spectroscopy is based on the measurement of wavelength *x* absorbance, which is a variable closely associated with chemical concentration (Budinova *et al.* 2008, Prades *et al.* 2012). In this sense, the present studies can demonstrate the effectiveness of multivariate analysis in conjunction with NIR spectroscopy and the MD algorithm in identifying and classifying fallen wood in a precise and non-destructive way, enhancing its alternative use in alternative taxonomy.

Figure 3 *Distribution of the "species" calibration set of fallen wood in Lecythidaceae from the Mahalanobis distance algorithm: A – tauari (*Couratari *sp.,* Couratari guianensis *and* Couratari stellata*); B – matá-matá (*Eschweilera coreacea *and* Eschweilera odora*)*



Different chemometric models have been employed in studies that use NIR spectroscopy to analyse heat-treated wood, charcoal, and ancient and archaeological wood. These studies observed the anatomical, chemical and physical-mechanical degradation of the xylem matrix, according to Davrieux *et al*. (2010), Hwang *et al.* (2016), Tong and Zhang (2016), and Lengowski *et al*. (2018). *Exempli gratia*, Xie *et al*. (2015) compared the properties of archaeological and modern wood from *Phoebe zhennan* (Lauraceae) using Fourier-transform infrared analysis. The results revealed significant differences in the chemical components of the two categories of wood. The extractives and hemicellulose were degraded in the old wood, and the lignin concentration was higher. Spectral analysis of the bands with the highest absorbance indicated that the biologically younger material (tree recently cut down and non-biodegraded) presented higher peaks related to the concentration of chemical components in the wood.

In another study, Hwang *et al.* (2016) investigated archaeological pine wood in Korea using NIR spectroscopy (8,000–4,000 cm^{-1}) in conjunction with multivariate analysis. A correct prediction rate of 100% was obtained for the identification of wood from *Pinus densiflora* forma *erecta* Uyeki, *P. densiflora* Sieb. et Zucc., and *P. sylvestris* L. from Russia and Germany. Similar to the studies mentioned previously, the present research highlighted the ability of infrared spectroscopy to discriminate wood from natural fallen trees, even when they showed some degree of biological, chemical and physical degradation. These studies confirm the versatility and effectiveness of NIR spectroscopy in the analysis of a wide variety of wood types, including those with different degrees of degradation, thus contributing to significant advances in the characterization and identification of woody materials in diverse contexts.

NIR spectral signatures

Figures 4 and 5 show the spectral signatures of *Couratari stellata* and *Eschweilera odora* wood in the near-infrared region (10,000–4,000 cm^{-1}). In this range, the absorption bands correspond to the characteristic functional groups of the chemical components of wood (Schwanninger *et al.* 2011, Fahey *et al.* 2018).

FIGURE 4 *Spectral signature of* Couratari stellata*: A – Sample spectra of Xylotheque and fallen tree; B – spectrum of the Xylotheque sample with bands with higher NIR absorption; C – sample spectrum of natural fallen trees with bands with higher NIR absorption*

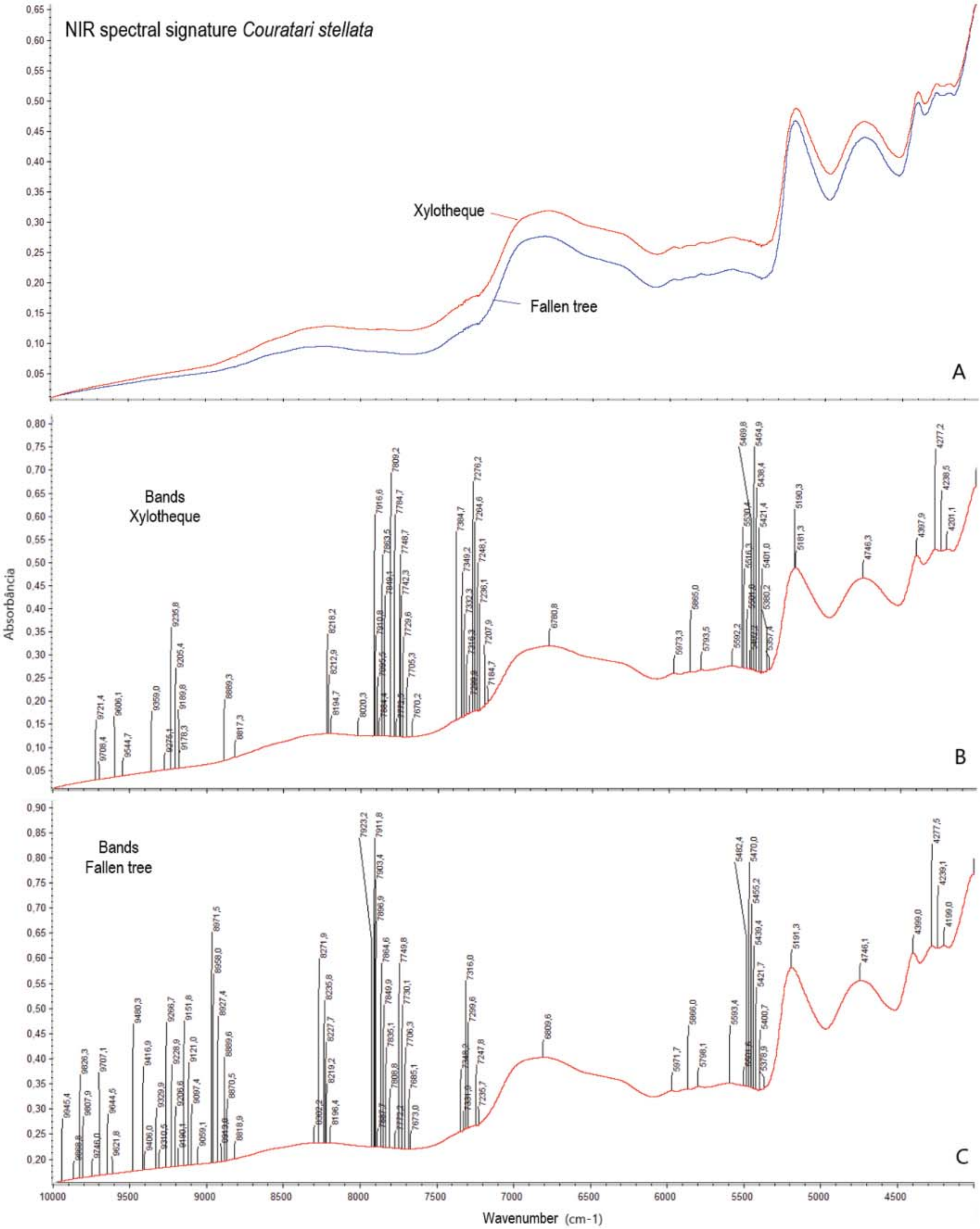
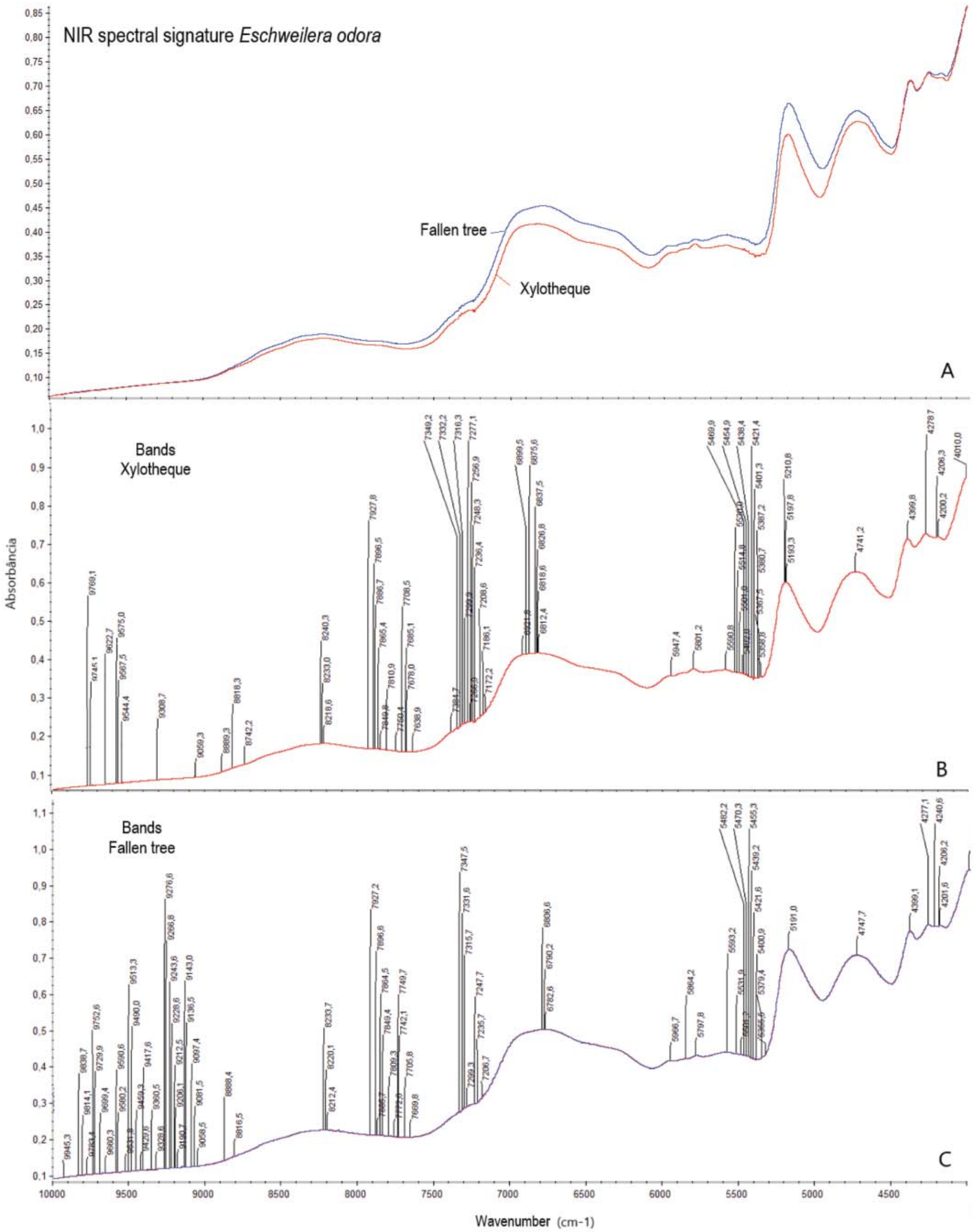


FIGURE 5 *Spectral signature of* Eschweilera odora*: A – Sample spectra of Xylotheque and fallen tree; B – spectrum of the Xylotheque sample with bands with higher NIR absorption; C – sample spectrum of natural fallen trees with bands with higher NIR absorption*



An initial observation of the spectra may suggest a possible similarity between the spectral signatures of fallen tree wood and samples from Xylotheque. However, a closer look reveals small differences. Spectral analysis by a chemometrics specialist reveals that this similarity does not exist, as certain NIR bands have been altered due to the physical, chemical, and biological weathering suffered by the samples when in direct contact with the soil. In Figure 4A, which presents the spectra of *C. stellata*, a discrepancy can be seen in the region from 6,800–5,300 cm^{-1}. In Figure 5A (*E. odora*), differences are identified in two ranges, 6,900–6,200 and 5,100–4,600 cm^{-1}. The characteristics of the bands with the highest absorption in relation to wavelength (cm^{-1}) can provide essential information for classification purposes. This explanation opens up the possibility of grouping based on genus and species, referring to the so-called "spectral signature" or "fingerprint" of the material (Ricci *et al.* 2015, Souza *et al.* 2017). Furthermore, Nascimento *et al.* (2023), when evaluating the biodegradation of lignocellulosic material by *Pleurotus* fungi, observed similar results in relation to the height of the bands in the near-infrared region, reaching the conclusion that the differences in absorbance are related to the concentration of chemical compounds, as well as degradation bands associated with the chemical bond characteristics of the samples.

In general, the appearance of the analysed spectra is quite similar. The spectral analysis was conducted using OMNIC® software, which highlighted the bands with the highest absorption in the spectra (Figure 4B, 4C, 5B and 5C). This information is important to facilitate the understanding of similarities or dissimilarities in the evaluated spectral universe.

Spectral evaluation of the botanical material covered in this study revealed significant differences that appear to be related to the chemical properties of the woody tissue. This may involve the quantity of primary metabolites, such as cellulose, hemicellulose and lignin, as well as the quantity and quality of extractives (secondary metabolites). According to Sandak *et al*. (2017), these groupings can be explained by the chemical and physical traits of the plant material. NIR spectra are represented by wavenumber versus absorbance, resulting from the amount of energy absorbed by the characteristic O–H, C–H, C–N and C=O bonds. The interpretation of spectra can be facilitated when there is a reference library containing peaks and digital signatures of compounds. Otherwise, interpretations of the bands depend on comparison with standard spectra (Schwanninger *et al*. 2011, Ricci *et al.* 2015).

Table 5 presents the bands observed in the spectral signature of *C. stellata* and *E. odora* wood, both from samples obtained from fallen trees and from the wood library. Band analysis indicates that the spectra of the fallen tree samples exhibit a band ratio higher than 50% compared to the Xylotheque samples, which initially served as a reference for the original bands, i.e., apparently undegraded samples. These results may be related to the effectiveness of classifying wood at the genus level, as shown in Table 3, where the results of the identification of samples from wood collections are included. However, this same assessment, when carried out at the species level with samples from the collection, resulted in low identification rates, as shown in Table 4.

The assignments of NIR bands for wood can be confirmed by other analytical methodologies, such as GC/MS, HPLC, and NMR (Tsuchikawa and Kobori 2015, Yeon *et al*. 2019, Park *et al*. 2021). In previous studies, the locations of the bands in relation to the wavenumber, the component that was likely absorbed at that location of the band and the vibration of the bond or structure associated with the chemical components of the wood were described (Kelley *et al.* 2004, Donald and Burns 2007, Schwanninger *et al.* 2011, Sandak *et al.* 2017).

Teye *et al.* (2013) indicated that in the region of 9,000–5,000 cm^{-1}, the carbonyl groups, ν(C–H) and the δ C–H, S–H, N–H, $-CH_2$ and $-CH_3$, correspond to the bonds of the polyphenolic, alkaloids, and terpenes structures (extractives). Souza *et al*. (2017) confirmed the effectiveness of cluster analysis using the NIR tool, making it possible to associate the separation of three plant species with characteristic bands of phenolic and flavonoid compounds in the region 8,663–3,757 cm^{-1}. In chemosystematics studies, the presence of a certain chemical class can explain the botanical groupings associated with environmental and evolutionary factors (Simões *et al.* 2017, Nascimento *et al.* 2019). Schwanninger *et al*. (2011) identified the main bands in the near-infrared region for wood, highlighting that the region of 6,717 and 6,060 cm^{-1} is related to the first overtone ν(O–H), while the peaks at 4,237 and 4,167 cm^{-1} correspond to δ(C–H), which may be related to the structure of cellulose. The bands at approximately 4,750, 5,780 and 7,812 cm^{-1} are mainly attributed to the first overtone δ(C–H) groups present in cellulose and hemicellulose. For aromatic compounds, the bands at 5,793 and 4,524 cm^{-1} are attributed to ν(C–H) of lignin. Most of these bands were confirmed in the spectra of the Xylotheque samples, as shown in Table 5.

Xie *et al*. (2015) investigated the infrared spectrum of old wood and associated bands ν(C=C) with the aromatic ring of lignin with greater intensity (concentration). In the present study, a similar behaviour was observed for the lignin bands for the signature of the fallen tree of *C. guianensis*, and for *E. odora*, ν(C–H) bands associated with cellulose and hemicellulose were observed in greater numbers for fallen wood.

The efficiency of Fourier-transform near-infrared spectroscopy (FT-NIR) has proven to be an effective tool in discriminating natural fallen wood from the Lecythidaceae family. This study revealed the ability to separate groups at the genus and species level using a multivariate statistical approach, taking advantage of characteristic absorption bands in the NIR region. This highlights that the observed clusters are influenced by the chemical and physical properties of the samples, with discriminant analysis acting as an effective tool for pattern recognition.

CONCLUSION

Fourier-transform near-infrared spectroscopy (FT-NIR) proved to be efficient in discriminating wood from fallen trees, both according to genus (*Couratari, Eschweilera, Holopyxidium* and *Lecythis*) and species (*Couratari* sp.*, C. guianensis, C. stellata, Eschweilera coriacea, E. odora, Holopyxidium* sp. and *Lecythis usitata*) belonging to the

TABLE 5 *Assignment of NIR absorption bands of wood of* Couratari stellata *and* Eschweilera odora.

Wood	**Vibration bands/ structure***	**Xylotheque wood**	**Fallen wood**
		λ (cm⁻¹)	
Couratari stellata	*v*(O–H); δ(O–H); *v*(C–H) = cellulose	4,238, 4,746, 5,190, 6,781, 7,772, 7,809, 7,785, 7,849, 7,863, 7,884, 7,895, 7,911, 7,917, 8,020, 8,195, 8,213, 8,218, 9,178, 9,190, 9,205, 9,236, 9,275, 9,359	4,746, 5,191, 7,772, 7,809, 7,835, 7,850, 7,865, 7,888, 7,896, 7,903, 7,912, 7,923, 8,196, 8,219, 9,179, 9,190, 9,207, 9,229, 9,310, 9,330, 9,406
	v(C–O–C); δ(C–H) = hemicellulose	4,398, 5,865, 7,670, 7,705, 7,730, 7,742, 7,749	4,399, 5,866, 7,673, 7,685, 7,706, 7,730, 7,750
	δ(C–H) = cellulose/ hemicellulose	5,357, 5,380, 5,401, 5,421, 5,438, 5,455, 5,470, 5,482, 5,501, 5,516, 5,530, 5,592, 7,276	5,379, 5,401, 5,422, 5,439, 5,455, 5,470, 5,482, 5,502, 5,593, 6,810
	v(C–H); *v*(C–H) + C–H_2; *v*(C–H) aromatic ring; *v*(C=C) aromatic ring = lignin	4,201, 4,277, 5,794, 5,973, 8,817, 8,889	4,199, 4,278, 5,798, 5,972, 8,228, 8,236, 8,272, 8,302, 8,819, 8,870, 8,890, 8,914, 8,927, 8,958, 8,971, 9,059, 9,097, 9,121, 9,152
	v(O–H) = lignin/extractives	7,185, 7,208, 7,236, 7,248, 7,265, 7,300, 7,316, 7,332, 7,349, 7,385	7,236, 7,248, 7,300, 7,316, 7,332, 7,348
	v(O–H) = water	5,181	-
	not assigned	9,545, 9,606, 9,701, 9,708	9,417, 9,480, 9,622, 9,645, 9,707, 9,746, 9,808, 9,826
			Spectral charge = 70,31%
Eschweilera odora	*v*(O–H); δ(O–H); *v*(C–H) = cellulose	4,741, 5,193, 6,812, 7,811, 7,850, 7,865, 7,887, 7,896, 7,927, 8,219, 9,309	4,748, 5,191, 6,783, 6,790, 6,807, 7,809, 7,849, 7,864, 7,886, 7,897, 7,927, 8,220, 9,191, 9,206, 9,212, 9,229, 9,244, 9,329, 9,360, 9,430
	v(C–O–C); δ(C–H) *v*(C–H) + δ(C–H); = hemicellulose	4,400, 7,257, 7,639, 7,678, 7,685, 7,705, 7,750	4,400, 7,670, 7,706, 7,750
	δ(C–H) = cellulose/ hemicellulose	5,359, 5,367, 5,381, 5,387, 5,401, 5,402, 5,421, 5,438, 5,455, 5,470, 5,501, 5,515, 5,530, 5,591, 6,818, 6,827, 6,837, 7,277	5,355, 5,379, 5,401, 5,421, 5,439, 5,455, 5,470, 5,482, 5,501, 5,532, 5,593, 5,864
	v(C–H); *v*(O–H); *v*(C–H) + C–H_2; *v*(C=C) aromatic ring = lignin	4,010, 4,200, 4,206, 4,279, 5,801, 6,875, 8,233, 8,240, 8,742, 8,818, 8,889, 9,059	4,201, 4,206, 4,277, 5,798, 8,224, 8,816, 8,888, 9,058, 9,081, 9,097, 9,136, 9,143
	v(O–H) =lignin/extractives	6,899, 6,922, 7,172, 7,186, 7,209, 7,236, 7,248, 7,300, 7,316, 7,332, 7,349, 7,385	7,207, 7,236, 7,248, 7,299, 7,316, 7,332, 7,347
	v(O–H) = water	5,198, 5,211	-
	not assigned	9,544, 9,567, 9,575, 9,623, 9,745, 9,769	9,267, 9,277, 9,417, 9,459, 9,490, 9,513, 9,532, 9,580, 9,591, 9,660, 9,699, 9,730, 9,753, 9,783, 9,814, 9,839, 994
			Spectral charge = 53,00%

* Literature: Kelley *et al*. (2004); Donald and Burns (2007); Workman and Weyer (2007); Zou *et al*. (2010); Schwanninger *et al*. (2011); Abe *et al*. (2013); Sandak *et al*. (2017); Varga, *et al*. (2017); Fahey *et al*. (2018).

Lecythidaceae family. The Mahalanobis distance algorithm, applied in discriminant analysis, accurately identified fallen wood based on the similarity and dissimilarity of NIR spectral signatures. This proved to be particularly valuable since, in field collection, identification was based only on popular denominations, such as matá-matá (*Eschweilera odora*) and tauari (*Couratari stellata*). The comparative analysis of the spectral signatures of samples, fallen trees and Xylotheque, revealed that even after exposure to the elements for some time, the wood from fallen trees still preserved approximately 50% of the original bands, which, in turn, favoured the discrimination of genus level. The accuracy of the NIR models indicates the applicability of this tool in an integrative way in taxonomy studies of woody materials from tropical forests, which are difficult to identify. This is due to the ability to analyse numerous samples quickly and effectively, eliminating the need to destroy samples, as occurs with traditional techniques.

DECLARATION OF INTEREST

The authors report no conflict of interest. The authors alone are responsible for the content and writing of this article.

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