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Prediction of wood and charcoal quality parameters of *Eucalyptus* and *Corymbia* clones using benchtop and portable NIR instruments

Caio Cesar Nemer Martins
Doctor Scientiae

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Thesis submitted to the Forest Science Graduate Program of the Universidade Federal de Viçosa in partial fulfillment of the requirements for the degree of *Doctor Scientiae*.

Adviser: Vinicius Resende de Castro

Co-advisers: Angelica de C. O. Carneiro
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“O maior presente Deus me deu, a vida me ensinou a lutar pelo o que é meu.”
(Charlie Brown Jr.)

ABSTRACT

MARTINS, Caio Cesar Nemer, D.Sc., Universidade Federal de Viçosa, December, 2025. **Prediction of wood and charcoal quality parameters of *Eucalyptus* and *Corymbia* clones using benchtop and portable NIR instruments**. Adviser: Vinicius Resende de Castro. Co-advisers: Angelica de Cassia Oliveira Carneiro and Paulo Ricardo Gherardi Hein.

Brazil ranks seventh among the world's largest producers of wood from planted forests. One of the main destinations of this raw material is the charcoal industry, with emphasis on the use of species from the genera *Eucalyptus* and *Corymbia*, due to characteristics such as rapid growth and high adaptability, which result in higher industrial yields. The growing demand of the industrial sector for high-quality wood and charcoal has driven the development and application of analytical techniques for their characterization. In this context, near-infrared (NIR) spectroscopy emerges as a promising tool, as it is a rapid, accurate, non-destructive, and cost-effective analytical technique when compared to conventional laboratory analyses. The appeal of this approach has been further strengthened by the emergence of portable NIR instruments, whose operational simplicity and portability allow analyses to be carried out directly in the field or in industrial environments, in addition to presenting lower acquisition costs compared to benchtop NIR instrument. This study aimed to predict quality parameters of wood and charcoal from *Eucalyptus* and *Corymbia* clones using benchtop and portable NIR instruments. To this end, the research was structured into four chapters. Chapter 1 presented a bibliometric analysis and a literature review on the use of benchtop and portable NIR instruments in the wood industry. Chapter 2 addressed the prediction of wood quality parameters of *Eucalyptus* and *Corymbia* clones using both types of NIR instruments. The portable NIR instrument showed a reduction in model performance parameters compared to the benchtop NIR; nevertheless, the results obtained were considered promising. Chapter 3 discussed the prediction of the energetic properties of charcoal from the same clones, also based on data obtained from both types of instruments. For *Eucalyptus* charcoal, the NIR instruments presented models with similar performance. However, for *Corymbia* charcoal, the portable NIR showed inferior model performance compared to the benchtop NIR. Chapter 4 explored the prediction of the apparent density of wood and charcoal based on spectral signatures obtained with benchtop (MPA) and portable (MicroNIR and Trinamix) NIR devices, as well as density values determined by X-ray densitometry. The models developed with the benchtop NIR instrument showed superior parameters compared to those obtained with portable NIR instruments for both wood and charcoal. Among the portable instruments, the parameters were similar for charcoal; however, in wood analysis, the MicroNIR exhibited superior performance compared to the Trinamix. The results of this thesis demonstrated that NIR spectroscopy, whether using benchtop or portable instruments, is an effective tool for characterizing qualitative parameters of wood and charcoal from *Eucalyptus* and *Corymbia* clones. Thus, the implementation of this non-destructive technology can contribute to process simplification and to the reduction of operational costs in the forestry sector.

Keywords: bioenergy; forest biomass; multivariate statistics; non-destructive techniques; x-ray densitometry

RESUMO

MARTINS, Caio Cesar Nemer, D.Sc., Universidade Federal de Viçosa, dezembro de 2025. **Predição de parâmetros de qualidade da madeira e do carvão vegetal de clones de *Eucalyptus* e *Corymbia* usando instrumentos NIR de bancada e portáteis**. Orientador: Vinicius Resende de Castro. Coorientadores: Angelica de Cassia Oliveira Carneiro e Paulo Ricardo Gherardi Hein.

O Brasil ocupa a sétima posição entre os maiores produtores mundiais de madeira proveniente de florestas plantadas. Um dos principais destinos dessa matéria-prima é a indústria de carvão vegetal, com ênfase no uso de espécies dos gêneros *Eucalyptus* e *Corymbia*, devido a características como rápido crescimento e alta adaptabilidade, que resultam em maior rendimento industrial. A crescente demanda do setor industrial por madeira e carvão vegetal de alta qualidade tem impulsionado o desenvolvimento e a aplicação de técnicas analíticas para sua caracterização. Nesse contexto, a espectroscopia no infravermelho próximo (NIR) surge como uma ferramenta promissora, por se tratar de uma técnica analítica rápida, precisa, não destrutiva e economicamente viável quando comparada às análises laboratoriais convencionais. O apelo dessa abordagem tem sido ainda mais reforçado pelo surgimento de instrumentos NIR portáteis, cuja simplicidade operacional e portabilidade permitem que as análises sejam realizadas diretamente em campo ou no ambiente industrial, além de apresentarem menor custo de aquisição em comparação com equipamentos NIR de bancada. Este estudo teve como objetivo prever parâmetros de qualidade da madeira e do carvão vegetal de clones de *Eucalyptus* e *Corymbia* utilizando instrumentos NIR de bancada e portáteis. Para isso, a pesquisa foi estruturada em quatro capítulos. O Capítulo 1 apresentou uma análise bibliométrica e uma revisão da literatura sobre o uso de instrumentos NIR de bancada e portáteis na indústria madeireira. O Capítulo 2 abordou a predição de parâmetros de qualidade da madeira de clones de *Eucalyptus* e *Corymbia* utilizando ambos os tipos de instrumentos NIR. O instrumento NIR portátil apresentou uma redução no desempenho dos parâmetros matemáticos dos modelos em comparação ao NIR de bancada. Ainda assim, os resultados obtidos foram considerados promissores. O Capítulo 3 discutiu a predição das propriedades energéticas do carvão vegetal dos mesmos clones, também com base nos dados obtidos pelos dois tipos de instrumentos. Para o carvão vegetal de *Eucalyptus*, os instrumentos NIR apresentaram modelos com desempenho semelhante. No entanto, para o carvão vegetal de *Corymbia*, o NIR portátil apresentou modelos com desempenho inferior aos obtidos com o NIR de bancada. O Capítulo 4 explorou a predição da densidade aparente da madeira e do carvão vegetal a partir de assinaturas espectrais obtidas com dispositivos NIR de bancada (MPA) e portáteis (MicroNIR e Trinamix) e de valores de densidade determinados via densitometria de raios X. Os modelos desenvolvidos com o instrumento NIR de bancada apresentaram parâmetros superiores aos obtidos com os instrumentos NIR portáteis, tanto para a madeira quanto para o carvão vegetal. Entre os instrumentos portáteis, os parâmetros foram similares para o carvão vegetal; contudo, na análise da madeira, o MicroNIR apresentou desempenho superior ao Trinamix. Os resultados da tese demonstraram que a espectroscopia NIR, seja com instrumentos de bancada ou portáteis, é uma ferramenta eficaz para caracterizar parâmetros qualitativos da madeira e do carvão vegetal de clones de *Eucalyptus* e *Corymbia*. Assim, a implementação dessa tecnologia não destrutiva pode contribuir para a simplificação de processos e para a redução de custos operacionais no setor florestal.

Palavras-chave: bioenergia; biomassa florestal; estatísticas multivariadas; técnicas não-destrutivas; densitometria de raios X

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CHAPTER 3: PREDICTION OF THE ENERGY PROPERTIES OF CHARCOAL OBTAINED FROM *Eucalyptus* AND *Corymbia* BIOMASS USING PORTABLE AND BENCHTOP NIR SPECTROMETERS

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LIST OF ABBREVIATIONS AND ACRONYMS

AC	Ash content
ARD	Apparent relative density
BD	Basic density
C	*Corymbia*
CCA	Canonical Correlation Analysis
CL	Clone
CRIST	Cellulose crystallinity
DS	Direct Standardization
E	*Eucalyptus*
EXT	Extractives
FC	Fines content
FIR	Far-infrared
FCC	Fixed carbon content
GY	Gravimetric yield
HOLO	Holocelluloses
IL	Insoluble lignin
LV	Latent variables
NIR	Near-infrared spectroscopy
MIR	Mid-infrared
PCA	Principal component analysis
PDS	Piecewise Direct Standardization
PLS-R	Partial least squares regression
PLS-DA	Partial least squares discriminant analysis
R^2	Coefficient of determination
R^2c	Coefficient of determination for calibration
R^2cv	Coefficient of determination for cross-validation
R^2p	Coefficient of determination for prediction
RPD	Ratio Performance to Deviation
RMSEc	Root mean square error for calibration
RMSEcv	Root mean square error for cross-validation
RMSEp	Root mean square error for prediction
S/G	Syringyl/Guaiacyl ratio

SL	Soluble lignin
SBC	Slope and Bias Correction
SNV	Standard normal variation
TL	Total lignin
VMC	Volatile matter content

SUMMARY

GENERAL INTRODUCTION

The planted forest sector has established itself as one of the main productive bases for various industrial chains, including the pulp and paper, wood panel, solid wood, sawmill, and charcoal production segments (XIONG *et al*., 2024; KISSANGA *et al*., 2024; N'TAMBWE NGHONDA *et al*., 2025; O'BRIEN *et al*., 2025). In addition to its economic benefits, this sector plays a relevant role in mitigating environmental impacts by contributing to the reduction of native forest deforestation, long-term carbon sequestration and storage, as well as the restoration of degraded areas through vegetation cover recovery (PAYN *et al*., 2015; SASMITO *et al*., 2023 BASKENT; KAŠPAR; BASKENT, 2025).

On the global stage, Brazil, China, and the United States of America stand out as the leading countries in forest productivity (FAO, 2022). Among these, Brazil is noteworthy not only for its production volume but also for its adoption of sustainable practices, advances in genetic improvement, silvicultural techniques, and favorable edaphoclimatic conditions for forest cultivation (SILVA LOPES *et al*., 2022; PUNHAGUI; JOHN, 2022). According to the 2025 report by the Brazilian Tree Industry (IBÁ), Brazil reached 10.5 million hectares of planted forests in 2024, with 8.1 million hectares cultivated with of *Eucalyptus* species, accounting for 77.1% of the national planted area.

Despite the dominance of *Eucalyptus* in Brazil's forest sector, species and hybrids of the *Corymbia* genus have been considered promising alternatives, especially for energy purposes. These species exhibit desirable attributes such as high basic density (above 600 kg/m³), resistance to adverse climatic conditions, and good adaptability to planting spacing, making them suitable for charcoal production (OLIVEIRA *et al*., 2023; MELO *et al*., 2024; MASSUQUE *et al*., 2024).

Brazil is also the world's largest producer and consumer of charcoal, with a production of 6.6 million tons in 2024, nearly all of which was destined for domestic consumption, particularly by the pig iron and steel industries (IBÁ, 2025). In these sectors, charcoal is valued as a cleaner reducing agent, with lower sulfur and ash content compared to mineral coal, in addition to having mechanical properties suitable for supporting iron ore loads in blast furnaces (COSTA *et al*., 2024).

In this context, the quality of wood and charcoal becomes a critical factor for industrial performance. Traditionally, the characterization of these materials is performed using destructive laboratory analyses, which are accurate but costly, time-consuming, and require specialized infrastructure. As an alternative, non-destructive techniques have been successfully employed in the characterization of lignocellulosic materials, notably near-infrared (NIR) spectroscopy, which is widely used to predict physical, chemical, and energy-related characteristics (SHRESTHA *et al*., 2023; TSUCHIKAWA; INAGAKI; MA, 2023), as well as X-ray densitometry, which enables accurate estimation of the apparent density of wood and its derivatives (MARTINS *et al*., 2025).

NIR spectroscopy is particularly effective in evaluating biologically derived materials such as wood and charcoal due to the presence of organic chemical bonds (C–C, C–H, O–H, N–H), whose interaction with infrared radiation generates informative spectral signatures. This technique can be coupled with multivariate statistical models to estimate complex characteristics such as cellulose crystallinity, syringyl/guaiacyl (S/G) ratio of lignin, extractives content, holocellulose content, lignin content, basic wood density, gravimetric yield, apparent relative density, fines content, and the chemical composition of charcoal (ABREU NETO *et al*., 2021; LIMA *et al*., 2022; LOUREIRO *et al*., 2022; MIRANDA *et al*., 2024).

Although most studies use benchtop NIR instruments, which offer high resolution and a wide spectral range, portable NIR devices are emerging as viable and promising alternatives. These devices offer lower cost, portability, and the ability to collect data directly in the field or industrial environments, enhancing real-time decision-making (SANDAK *et al*., 2021; MEDEIROS *et al*., 2025). However, the reduced spectral range of these devices (varies depending on the instrument) compared to benchtop instruments (12.500–3.500 cm^{-1}) raises concerns about the accuracy of predictive models derived from such spectra, especially when applied to materials such as charcoal and wood from the *Corymbia* genus, for which studies are scarce.

Density is widely recognized as one of the most important indicators in the assessment of wood quality, due to its relatively simple determination and strong correlation with various physical and functional properties, including dimensional stability (SARGENT, 2022), carbon sequestration capacity (EVANS *et al*., 2022; SERRA-MALUQUER *et al*., 2022). In this context, the use of more precise analytical techniques, such as X-ray densitometry, has intensified. This method offers significant advantages, as it is non-destructive, rapid, requires no reagents or solvents, and enables accurate determination of apparent density along the wood's radial profile (CASTRO *et al*., 2020; MORAES *et al*., 2023; BARBOSA *et al*., 2024).

Therefore, this study introduces an innovative methodological framework to address existing scientific gaps in the quality assessment of wood and charcoal from *Eucalyptus* and *Corymbia* using both benchtop and portable near-infrared (NIR) spectroscopy. The literature review evidences the limited number of investigations employing portable NIR devices for the characterization of these materials, as well as the absence of studies integrating non-destructive approaches, particularly the combination of X-ray densitometry and NIR spectroscopy for estimating apparent density. Considering these gaps, the research was organized into four chapters.

Chapter 1 provides a bibliometric and comprehensive literature review on the application of benchtop and portable NIR instruments in the forest-based industrial sector, emphasizing recent technological advancements and emerging research directions. It also contextualizes the relevance of the Brazilian forest sector, with particular attention to the cultivation of *Eucalyptus* and *Corymbia* clones. The chapter highlights the wide-ranging applications of NIR spectroscopy for evaluating wood and its derivatives, demonstrating the feasibility and operational advantages of portable instruments. Additionally, it examines calibration transfer strategies among NIR devices, underscoring their importance for harmonizing measurements and promoting the broader adoption of this technology in industrial environments.

Chapter 2 focuses on predicting wood quality attributes of *Eucalyptus* and *Corymbia* clones using benchtop and portable NIR spectrometers. Through the application of multivariate statistical methods, including Principal Component Analysis (PCA) and Partial Least Squares Regression (PLS-R), both instrument types demonstrated satisfactory predictive capacity. The findings confirm that NIR spectroscopy provides reliable estimates of quantitative wood properties from fast-growing plantations destined for bioenergy production, reinforcing its potential as a strategic tool for identifying superior genotypes in forest breeding programs.

Chapter 3 aimed to estimate the energy parameters of charcoal produced from *Eucalyptus* and *Corymbia* clones using benchtop and portable NIR instruments. Multivariate statistical analyses, including PCA and PLS-R, showed that the models developed for *Eucalyptus* charcoal exhibited similar performance with both instruments. This finding highlights the potential of portable NIR instruments as viable alternatives, especially considering their lower cost and operational convenience. However, the models developed for *Corymbia* charcoal exhibited inferior performance when using the portable device compared to the benchtop equipment.

Chapter 4 aimed to predict the apparent density of wood and charcoal based on spectral signatures obtained from benchtop and portable NIR instruments, associated with density values determined by X-ray densitometry. The application of multivariate statistical techniques (PCA and PLS-R) demonstrated a strong correlation between the two methods (NIR and X-ray densitometry) for estimating the apparent density of wood and charcoal. The global models developed for wood exhibited superior statistical parameters compared to those obtained for charcoal. Furthermore, the spectral signatures acquired using the benchtop NIR instrument resulted in models with higher statistical performance for predicting apparent density when compared to those generated from the spectral signatures of portable instruments.

In summary, this research advances the understanding of how near-infrared (NIR) spectroscopy, in both its benchtop and portable options, can be effectively applied to the qualitative and quantitative characterization of lignocellulosic materials. By integrating non-destructive analytical approaches, this study not only validates the potential of portable NIR instruments as reliable and cost-effective alternatives to laboratory analyses but also contributes to the development of more sustainable, faster, and lower-cost methodologies for assessing the quality of wood and charcoal. The findings provide a solid scientific foundation for future innovations in forest biomass characterization, supporting genetic improvement programs and processes related to industrial optimization.

OBJECTIVES

General objective

To predict the quality parameters of wood and charcoal from *Eucalyptus* and *Corymbia* clones for energy use using benchtop and portable NIR instruments.

Specific objectives

i. To carry out a bibliometric analysis and a literature review on the use of benchtop and portable near-infrared (NIR) instruments in the forest-based industrial sector.

ii. To predict the S/G ratio, cellulose crystallinity, structural chemical composition, and basic wood density of fast-growing plantation wood using benchtop and portable NIR instruments.

iii. To predict the gravimetric yield, apparent density, fines content, and proximate chemical composition of *Eucalyptus* and *Corymbia* charcoal using benchtop and portable NIR instruments.

iv. To predict the apparent density of wood and charcoal from *Eucalyptus* and *Corymbia* clones using NIR spectroscopy with benchtop and portable instruments, combined with X-ray densitometry.

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CHAPTER 1

OVERVIEW, STATE OF THE ART, AND PERSPECTIVES ON THE USE OF PORTABLE AND BENCHTOP NIR SPECTROMETERS IN OPTIMIZING THE CHARACTERIZATION OF WOOD PRODUCTS

OVERVIEW, STATE OF THE ART, AND PERSPECTIVES ON THE USE OF PORTABLE AND BENCHTOP NIR SPECTROMETERS IN OPTIMIZING THE CHARACTERIZATION OF WOOD PRODUCTS

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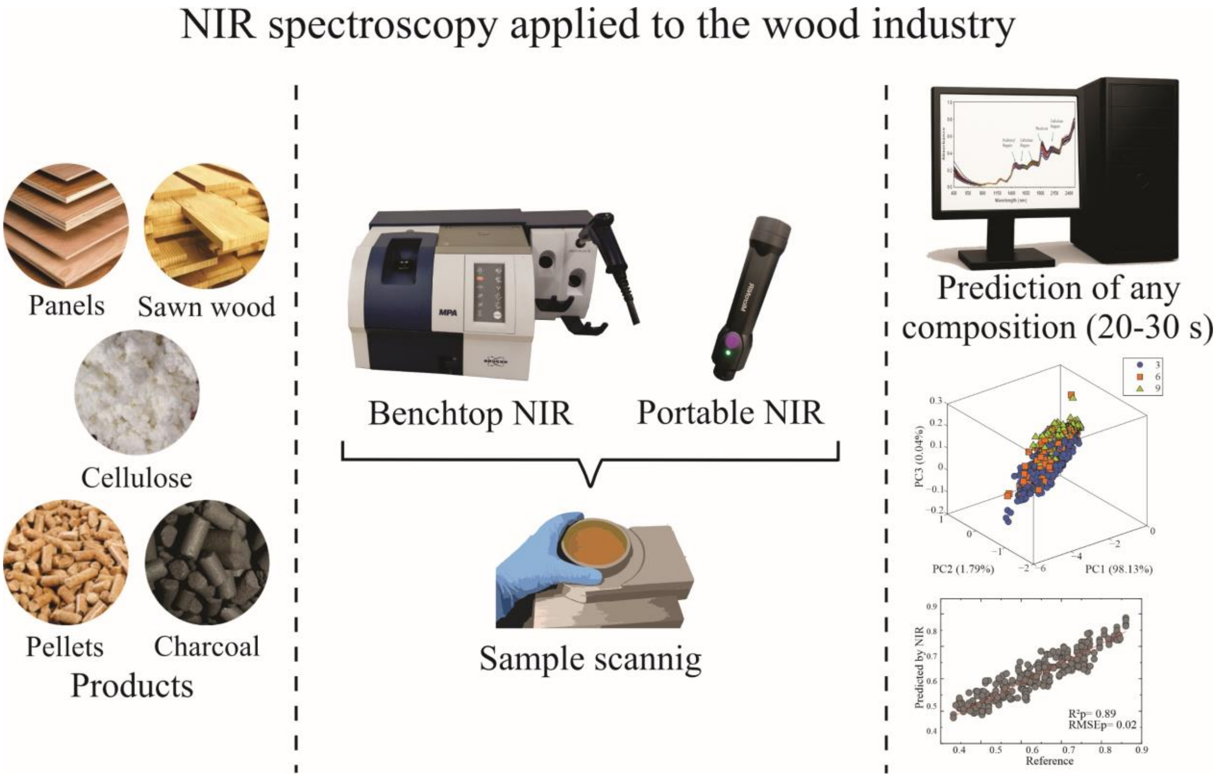
OVERVIEW, STATE OF THE ART, AND PERSPECTIVES ON THE USE OF PORTABLE AND BENCHTOP NIR SPECTROMETERS IN OPTIMIZING THE CHARACTERIZATION OF WOOD PRODUCTS

ABSTRACT

Non-destructive evaluations of the physicochemical properties of wood and its products represent promising alternatives to conventional laboratory analyses, as they offer fast, reliable information with minimal impact on the materials being assessed. In this context, near-infrared (NIR) spectroscopy has been successfully applied in the forest-based industrial sector. With technological advances, portable versions of NIR equipment allow real-time estimation of desired parameters directly in the field or industrial environment. This study aimed to carry out a bibliometric analysis and literature review on the use of both benchtop and portable NIR instruments in the forest-based industrial sector. This review aims to guide future research on the rapid and efficient characterization of forest wood products, in line with the United Nations Sustainable Development Goals (SDGs), particularly SDG 7 (Affordable and Clean Energy), SDG 12 (Responsible Consumption and Production), and SDG 13 (Climate Action). It also seeks to identify gaps in scientific knowledge to promote the development of new studies in this area. A total of 155 publications, released between 1997 and 2025, were retrieved from scientific databases and analyzed bibliometrically using VOSviewer software. The results indicate an average annual growth rate of ~7.5% in publications related to the topic. The literature shows that NIR spectroscopy has provided relevant information for the forest-based industrial sector, especially when combined with multivariate statistical methods. However, a lack of studies using portable NIR equipment was observed, highlighting a significant gap in the practical application of this technology. Therefore, it is recommended that further research explore the use of these devices in real-time conditions, aiming for greater representativeness of actual operational scenarios.

Keywords: Lignocellulosic materials. Quality control. Multivariate analysis. Wood property prediction. Non-destructive evaluation.

Graphical abstract



1. INTRODUCTION

The planted forest sector plays a vital role in the global economy, as its production is destined for the cellulose and paper industry (PENNELLS *et al*., 2020), charcoal (PROTÁSIO *et al*., 2021), sawn wood (SILVA-ALBUÊS *et al*., 2024; SENG HUA *et al*., 2022), wooden boards (BARBIRATE *et al*. 2020), among others. In addition to the industrial advantages, this sector also offers environmental benefits such as reducing deforestation (CHU; GRAFTON; NGUYEN, 2022), increasing long-term carbon sequestration and storage (WARING *et al*., 2020), and the rehabilitation of degraded areas with the vegetal cover occupation (ZHANG *et al*., 2021).

The countries that lead the global ranking of planted forest productivity are China, the United States of America, and Brazil (FAO, 2022). However, the Brazilian forestry market deserves to be highlighted due to the significant cellulose and charcoal production, influenced by factors inherent to forestry cultivation such as favorable climatic conditions, development of silvicultural techniques, advancement of genetic improvement programs in the selection of new genotypes and expansion of commercial plantations over the years (SILVA *et al*., 2022a; SILVA *et al*., 2022b). According to the Ibá (2025), Brazil reached 10.5 million hectares of planted forests for industrial crops in 2024. Of this total, approximately 8.1 million hectares are areas cultivated with the genus *Eucalyptus* due to its high adaptability and rapid growth (IBÁ, 2025).

Despite the predominance of the genus *Eucalyptus* in commercial plantations in Brazil, the genus *Corymbia* presents itself as a market option. Characteristics such as high density, with trees expressing wood basic density above 600 kg/m^3 at the age of seven (LOUREIRO *et al*., 2019), tolerance to adverse weather conditions (NAHRUNG *et al*., 2011) and resistance to planting density (MONTEIRO *et al*., 2020) accredit its use, mainly in charcoal producing industries due to the compatibility of desirable characteristics for this purpose.

Therefore, with the selection of new genetic materials, it is essential to know the wood's variability, composition, and characteristics to obtain maximum product yield (LIANG *et al*., 2020). Conventional laboratory analyses for wood characterization are expensive, use dangerous and restricted reagents and equipment, require extended periods, and are destructive. Thus, the specimens' physical, chemical, mechanical and anatomical properties are identified, but the capacity for final use is altered, resulting in the disposal of these materials after analysis (LI *et al*., 2020).

Non-destructive techniques are promising alternatives for quick and low-cost characterization without altering the material's original properties (PIMENTA *et al*., 2023). Among the available methods, near-infrared spectroscopy (NIR) stands out, being considered the main non-destructive one in research involving forest genetic improvement (BEĆ; GRABSKA; HUCK, 2020). The NIR technique has been successfully used in the qualitative and quantitative evaluation of wood and its products, as it meets the above-mentioned premises (RAMALHO *et al*., 2017; LI *et al*., 2022).

When correlated with the results of conventional laboratory analyses, the information obtained about the chemical constituents of the analyzed material through spectral signatures makes it possible to generate multivariate statistical models that explain valuable information about the required materials (AMARAL *et al*., 2020). It is essential to highlight that all aspects related to NIR spectroscopy are of technical-scientific interest since the simplification of the selection process of genetic materials contributes to optimizing industrial processes due to less time and cost of the analysis of interest.

These advances highlight the need for rapid and efficient characterization of forest-based wood products, in alignment with the United Nations Sustainable Development Goals (SDGs), particularly SDG 7 (Affordable and Clean Energy), SDG 12 (Responsible Consumption and Production), and SDG 13 (Climate Action). This approach helps reduce the use of chemical reagents and the generation of laboratory waste, while promoting the rational use of raw materials to minimize losses in both field and industrial operations. In this context, portable NIR has become an increasingly promising tool, enabling direct applications in the field and industrial processes.

In addition to all the advantages offered by the benchtop NIR instrument, the portable NIR allows spectral acquisitions to be carried out at the evaluation site itself, for example, in industries or forests that require the manager to make quick and assertive decisions (TOSCANO *et al*., 2022). Furthermore, the lower acquisition cost of the instrument compared to the benchtop one and the versatility and practicality of use provided by a single instrument are attractive characteristics for its use in the forest-based industrial sector. Zhu *et al*. (2022) report that these instruments' spectral range, wavelength range and resolution are reduced. However, multivariate statistical models can be built due to the presence of molecule bonds (N-H, S-H, O-H and C-H) within the given spectral region.

Therefore, advancing research using portable NIR instruments is well justified to enhance the efficiency and reliability of wood and wood-product characterization. Despite significant progress, the application of portable NIR sensors in this field still faces several underexplored challenges and limitations. These include the influence of sample conditions, sampling intensity, spectral acquisition methods, environmental factors, sensor variability, storage time, moisture variation, and product type, as reported by Medeiros *et al*. (2024), Medeiros *et al*. (2025), and Martins *et al*. (2026).

Given the above, the objective of this study was to carry out a bibliometric analysis and literature review on the use of benchtop and portable NIR instruments in the forest-based industrial sector. Furthermore, based on studies found in literature, gaps in scientific knowledge on the topic were identified, aiming to contribute to the development of future studies.

2. BIBLIOGRAPHIC REVIEW

2.1. Bibliometric and bibliographic review methodology

The data was collected in the Scopus and Web of Science Core Collection databases on September 29, 2025. The search was carried out based on the abstracts, keywords and titles of the works with the terms commonly used in the literature to describe the technique and the respective raw materials studied: ("Near Infrared Spectroscopy" OR "NIR" OR "NIRS" OR "Benchtop NIR instrument" OR "Portable NIR instrument" OR "Benchtop NIR Spectrometer" OR "Portable NIR Spectrometer") AND ("Partial least squares regression" OR "PLS regression" OR "PLS-R" OR "Principal component analysis" OR "PCA" OR "Partial least squares discriminant analysis" OR PLS-DA) AND ("*Eucalyptus" OR "Corymbia" OR "Eucalyptus* wood" OR "*Coymbia* wood" OR "*Eucalyptus* charcoal" OR "*Corymbia* charcoal"). The Boolean operators OR, AND, and the resources of quotation marks and parentheses were used to assemble the search equation to minimize the associated noise. A timeless search was established, and research and review articles were included in the pre-established theme. Theses, dissertations and abstract and other texts of event annals were not included in the search.

The selected works were exported in BibTeX format from all databases and compiled in RStudio (version 2022.12.0+353, RStudio, Inc., Boston, USA) using the Bibliometrix package for R (version 4.1.3, R Foundation for Statistical Computing, Vienna, Austria) to eliminate duplicates. The chosen articles were organized into a single file and exported in CSV and Excel. RStudio was used to analyze citations, the number of publications over time, and the thematic map. Furthermore, VOSviewer (version 1.6.19) was employed to evaluate the co-occurrence of plus keywords. At the same time, Microsoft Excel 2019 (Microsoft, Redmond, WA, USA) was used to analyze the volume of annual publications and the number of citations by country. The search returned 235 documents, 107 in Scopus and 128 in WOS. Seventy-five duplicate works were excluded, resulting in 160 compiled documents. The results of the descriptive data analysis are shown in Table 1.

Table 1 - Descriptive characteristics of the extracted raw data.

Description of documents	
Timespan	1997:2025
Sources (Journals, Books, etc)	72
Documents	160
Annual Growth Rate, %	7.47
Document Average Age (years)	9.81
Types of documents	
Research Articles	158
Review Articles	2
Description of authors and author collaborations	
Authors	488
Authors of single-authored docs	2
Single-authored docs	2
Co-authors per Doc	4.82
International co-authorships %	9.37
Citations and references	
Average citations per document	16.18
References	2171

Source: Results from the database obtained by the software.

2.2. Document screening from 1997 until September 2025

According to the search, the first article on the topic analyzed was published in 1997, showing an average growth rate of 7.47% per year. Only 10.6% (n=17) of articles were published between 1997 and 2007. This assumed that in the last 18 years (2008 to 2025) 89.4% (n=143) of research on the topic was published (Figure 1).

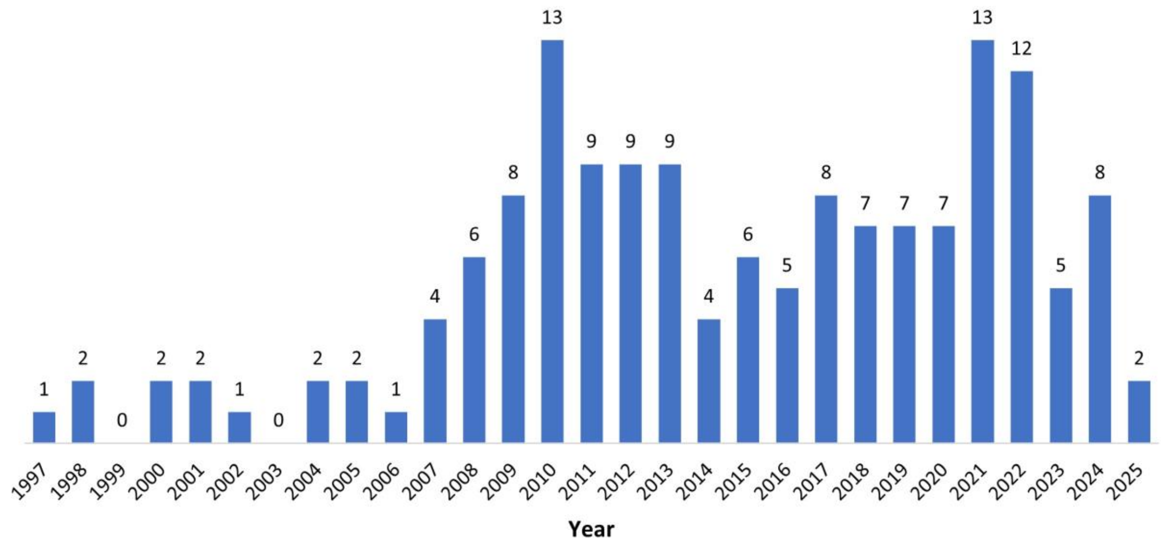


Figure 1- Number of articles (y axis) published from 1997 to September 29, 2025.

The progress observed in the last 18 years may be associated with factors such as the advancement of commercial plantations (IBÁ, 2025), selection of new clones via genetic improvement programs that meet industrial demands, the use of NIR spectroscopy to reduce time and cost in characterizing wood and its products, in addition to the simplification of NIR instruments through portable versions. Thus, recent studies have been carried out to contribute new information to academia and industry.

Although the number of research articles on this topic is on the rise, the bibliometric review identified only two review articles registered in the literature. Even so, the information included in this manuscript presented a divergent approach to what was carried out in our study. This fact demonstrates the need for more reviews on this topic to identify existing information and verify the gaps in scientific knowledge so that future studies can be conducted.

2.3. Scientific production and collaboration between countries

The country with the highest number of publications is Brazil (n=76), followed by Australia (n=38), China (n=33), France (n=27), United States (n=23), Portugal (n=23) and Chile (n=13). The other countries presented scientific production in the area equal to or less than 12 works published within the period analyzed. This figure (Figure 2a) also suggests that Brazil, Australia and China are the most productive and influential countries in using NIR spectroscopy in the forest-based industrial sector and present different patterns of collaboration with other countries.

Additionally, Figure 2a-b shows a positive correlation between the volume of publications and citations of countries. Thus, it was possible to observe that Brazil, Australia, China, and France together represent around 86.8% of publications and 70.42% of the citations, considering the 9 most cited countries. In addition to the number of publications, the number of citations is another parameter that reinforces the relevance of research in these countries, not only based on the number of works published but also on the depth and quality of the research carried out (SOUZA *et al*., 2024).

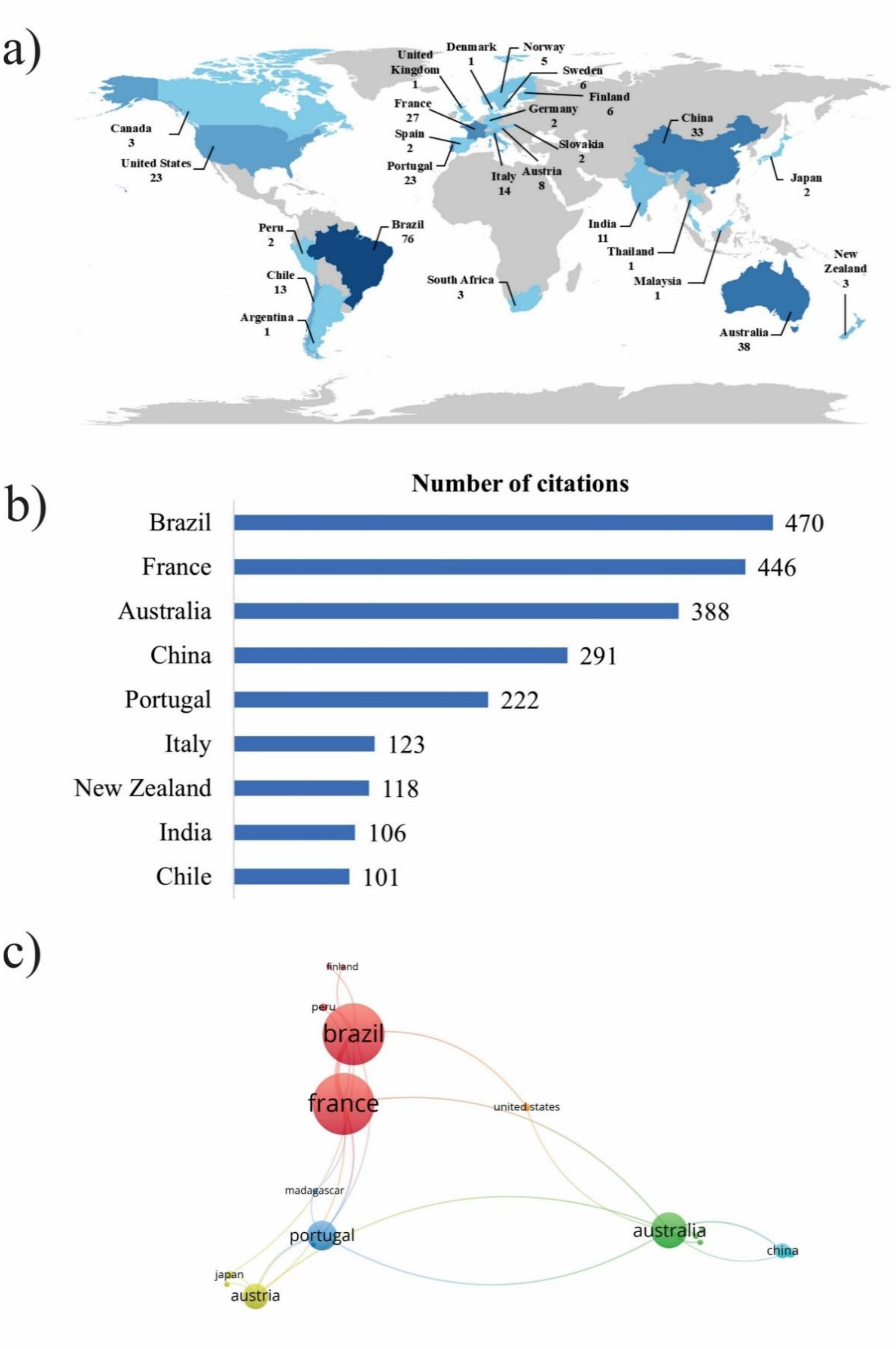


Figure 2- Bibliographic survey on the countries with the largest number of published documents (a), cited documents (b) and cooperation between countries (c).

In relation to Figure 2c, a network of collaboration between countries was observed in the production of research articles on the use of portable and benchtop NIR instruments in the industrial timber sector. Each node on the map corresponds to a country, and its size is proportional to the number of publications (SILVA *et al*., 2020). The connections between the nodes indicate the existing cooperation between these countries, and the density of the lines is proportional to the frequency and intensity of this cooperation (JIA *et al*., 2023). Regarding cooperating countries, Brazil, Australia, and France stand out. Thus, 6 nodes are linked to Brazil, 5 to Australia and 4 to France. It was possible to observe that China cooperates closely with Australia, which is ratified by the number of productions and citations from these countries.

Another aspect that deserves to be highlighted is the cooperation between Brazil and France. As seen in Figure 2a-b, these countries are among the leaders in the number of publications and citations, which justifies this proximity. Thus, it was concluded that countries such as Brazil, France, and Australia have greater representation of international collaboration than others involved in this topic.

2.4. Co-occurrence of keywords

The co-occurrence of keywords makes it possible to analyze the research field and the most covered topics. Furthermore, these results reveal publication patterns and can serve as tools for disseminating knowledge and helping to identify gaps related to the topic (SOUZA *et al*., 2024). Thus, 1006 plus keywords were found, 30 of which had several citations equal to or greater than 10 (Figure 3).

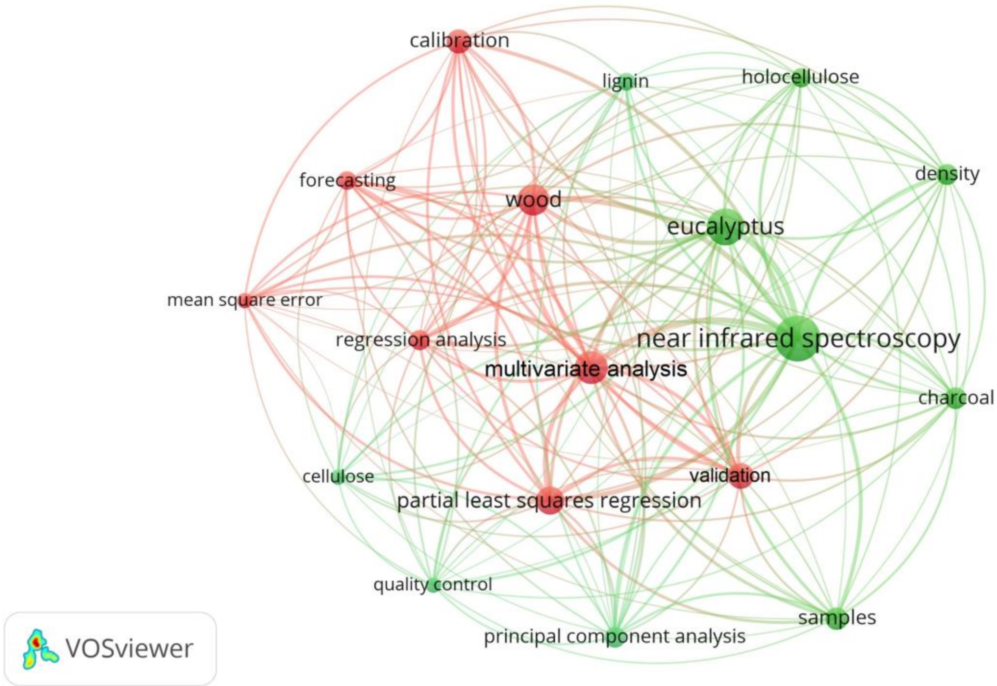


Figure 3 - Co-occurrence for all keywords, considering the bibliometric analysis between the years 1997 and 2025, in the Scopus Web of Science© database.

The size of each circle represents how often a term appears, while the distance between circles reflects the degree of connection among recurring keywords (PACHECO *et al*., 2024). The results depict keywords grouped into two clusters (green and red). The green cluster brings together terms associated with the chemical and physical characteristics of wood. The red cluster, on the other hand, encompasses keywords related to data processing using NIR spectroscopy, particularly in applications involving quality control of forest products.

The bibliometric analysis revealed a substantial volume of publications and scientific knowledge on the subject, especially regarding the keywords "near-infrared spectroscopy," "wood," and "eucalyptus." Although the terms "portable NIR spectrometer," "portable NIR instrument," and "*Corymbia* wood" were included in the database search, they did not appear in the co-occurrence network. This absence suggests that these themes, despite already showing promising potential in previous studies, remain underexplored and warrant further investigation.

Studies published over the last 28 years (1997–2025) demonstrate the participation of a broad range of authors and countries, as well as highlight the most frequently used keywords in this research area. Nevertheless, no publication was identified that simultaneously integrates and critically evaluates the use of both benchtop and portable NIR devices within the forest-based industrial sector. Therefore, considering the bibliometric findings and the extensive literature review, the present study gains relevance by addressing this gap and contributing to the ongoing development of wood-related technologies and industrial applications.

2.5. Scientific mapping

The thematic map is subdivided into four quadrants so that each represents the type of influence that each term presents within the theme, as reported by López Belmonte *et al*. (2020). The lower right quadrant refers to emerging themes that are relevant in the area, however, are still underdeveloped. The lower left quadrant presents the basic themes that are likely relevant but with intermediate development. The upper left quadrant, in turn, presents well-established niche themes in the area. Finally, the upper right quadrant shows the highly consolidated themes in the evaluated study area (Figure 4).

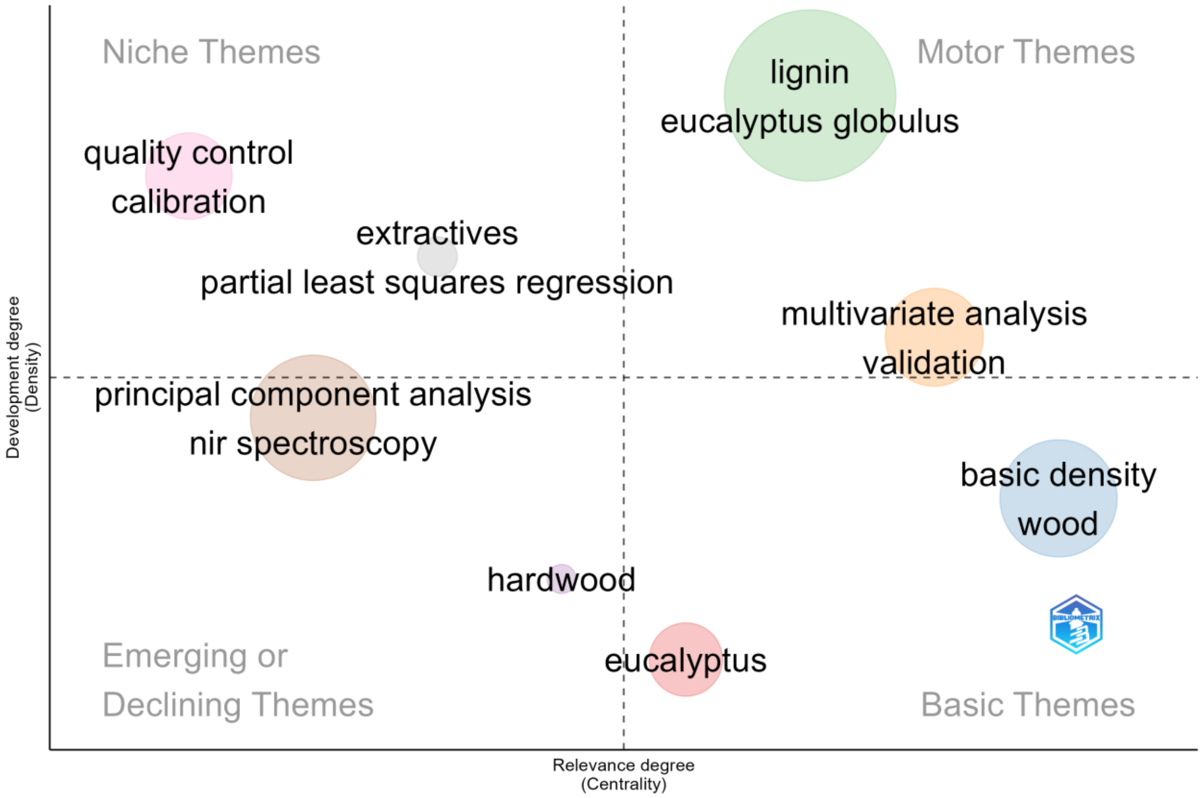


Figure 4 - Thematic map of the use of NIR spectroscopy in the forest-based industrial sector between 1997-2025.

The size of the circles for each term is directly proportional to the number of citations in articles in the area, and the position of each represents the density and relevance of these terms so that centrality is directly linked to the significance of each topic. In this way, it was possible to observe that terms related to wood quality, such as “quality control”, “extractives”, and “lignin”, were allocated in the upper left and right quadrants. The same trend occurred for terms linked to NIR spectroscopy, such as “calibration”, “partial least squares regression”, “multivariate analysis”, and “validation”.

This behavior may be associated with the increase in studies related to the characterization of wood's chemical and physical properties, influenced by the selection of new clones via genetic improvement. Thus, new studies were developed aiming to optimize the characterization of wood and its products since NIR spectroscopy, in addition to being a non-destructive technique (RAMALHO *et al*., 2017; AMARAL *et al*., 2020; LIMA *et al*., 2022a), is fast, simple and reliable for predicting the information of interest (LI *et al*., 2022).

Furthermore, it was observed that although the terms “principal component analysis” and “NIR spectroscopy” are in the lower left quadrant, the terms have the potential to consolidate in the future since the circle belonging to these words had considerable size concerning the others, indicating that they are highly cited in the literature. In this sense, the thematic map was essential to demonstrate the relevance and consolidation of using NIR spectroscopy in the forest-based industrial sector. Therefore, the bibliometric analysis highlights the evolution and consolidation of the use of NIR spectroscopy in the forest-based industrial sector, especially for wood characterization and process optimization.

3. BIBLIOGRAPHIC REVIEW

3.1. Forest production and exploitation for wood purposes

Forest exploration and production for wood purposes involves practices and steps that aim to extract, manage, and sustainably use forest resources. This activity can be carried out both in native forests and in commercial forest plantations, being governed by principles that seek to associate economic exploitation with environmental conservation (PRADO CAPANEMA *et al*., 2022; LIMA *et al*., 2024). To meet the requirements of sustainability and preservation of ecosystems, the exploitation of native forests requires compliance with legal and technical requirements that vary according to the legislation of each country (URRUTH; BASSI; CHEMELLO, 2022). Thus, the amount of wood exploited in native forests became insufficient to supply the industrial wood sector, so commercial forest plantations were presented as an alternative for providing wood.

Brazil stands out in the world concerning forestry cultivation due to the adoption of advanced technologies, genetic improvement of forest species and hybrids, and favorable climatic and soil conditions (FLORÊNCIO; MARTINS; FAGUNDES, 2022). These factors enable the rapid growth in height and diameter of species cultivated for different purposes (AFONSO; MILLER, 2021; MYNT *et al*., 2021). Ibá (2025) pointed out that the productivity of *Eucalyptus*, the main commercially planted genus in Brazil, was estimated at 35 m^3/ha/year (with bark). For comparison purposes, during the same period, the average productivity of eucalyptus internationally ranged from 10 m^3/ha/year to 25 m^3/ha/year, reinforcing the importance of the Brazilian forestry sector in the global context (PROTÁSIO *et al*., 2019).

Because it is a highly adaptable genus, species and hybrids of *Eucalyptus* are cultivated throughout all regions of Brazil, although most production remains concentrated in the Southeast and Central-West. Among the species most widely grown in the country, *Eucalyptus grandis*, *E. urophylla*, and *E. camaldulensis* stand out (IBÁ, 2025). In relation to hybrids, the most prominent combination is the cross between *E. urophylla* and *E. grandis*. As noted by Gonçalez *et al*. (2014), traits such as water-deficit tolerance from *E. urophylla* and the strong rooting capacity and vigorous field growth typical of *E. grandis* support the use of this cross to obtain higher-quality genetic material. By bringing together the complementary characteristics of both species, the resulting hybrid exhibits superior adaptive performance

The woods of the genus *Eucalyptus* and its hybrids are primarily intended for the paper and cellulose industry, as well as steel (using charcoal as a reducing agent), wood panels and sawn wood (PENÍN *et al*., 2020; SENG HUA *et al*., 2022). It is well known that, the selection of species and hybrids through genetic improvement for various industrial purposes directly influences product quality. Therefore, genetic materials with compatible and desirable characteristics are selected for each manufactured product.

In the cellulose and paper sector, clones are selected for characteristics such as high cellulose content, low lignin content, higher syringyl/guaiacyl ratio (S/G), and less extractives, in addition to rapid vegetative growth (GHANI; LEE, 2021; VIEIRA *et al*., 2021). For the steel sector, wood with high-density values, associated with higher lignin content, produces better quality charcoal with increased gravimetric yield, fixed carbon content and an apparent density (PROTÁSIO *et al*. 2019; SANTOS *et al*., 2020). To expand its use in products with higher added value (furniture, flooring, frames, among others), the wood of this type of eucalyptus must present desirable market characteristics, such as greater dimensional stability after drying, retention of the original color, adequate physical-mechanical properties and ease of machining (MIAO; PAN; XU, 2022).

The choice of genetic material to be planted must be based on soil and climate requirements, in addition to the final use of wood, which depends on its technological characteristics (TRUGILHO *et al*., 2015). In this context, studies related to the industrial viability of wood *Corymbia* reveal that species like *C. citriodora*, *C. maculata*, *C. torelliana* and some of their hybrids are recommended for the establishment of commercial forest plantations (LOUREIRO *et al*., 2021; COSTA *et al*., 2022). According to Loureiro *et al*. (2019), the hybrids of the genus *Corymbia* present desirable characteristics for the steel and coal industries, such as high basic density and high levels of total lignin in the wood. Such characteristics enable the production of charcoal with greater energy density, calorific value and lower degree of friability (PROTÁSIO *et al*. 2021).

Another possible application of *Corymbia* is for pulp and paper production. Costa *et al*. (2022) compared the industrial performance of biomass *Eucalyptus* and hybrids of *Corymbia* for cellulosic pulp production. Based on industrial parameters, the authors found promising results for the hybrid *C. citriodora* × *C. torelliana* (clone 4), such as with high basic density value, lower total lignin content, higher xylan content, higher purified yield and lower production cost per ton of air-dried cellulose. Therefore, the authors concluded that this hybrid *Corymbia* may be a possible alternative depending on the desirable industrial parameters.

Therefore, the industrial use of wood of this type, *Eucalyptus* and *Corymbia,* can be recommended for various applications. The genus *Eucalyptus* is most used in the Brazilian forestry market, and the genus *Corymbia* has potential for expansion but requires adjustments, especially regarding the development of genetic improvement programs for species and robust hybrids to obtain desirable characteristics that serve the forestry market.

3.2. Fundamentals of spectroscopy in the infrared region

Infrared (IR) is a region of the electromagnetic spectrum beyond the visible spectrum; that is, its wavelengths are longer than visible light (Figure 5). This spectrum range is concentrated between microwaves and visible light, with wavelengths ranging from 780 to 100.000 nm (Tsai; Hamblin, 2017). It can be divided into three subcategories: near-infrared (NIR), mid-infrared (MIR), and far-infrared (FIR).

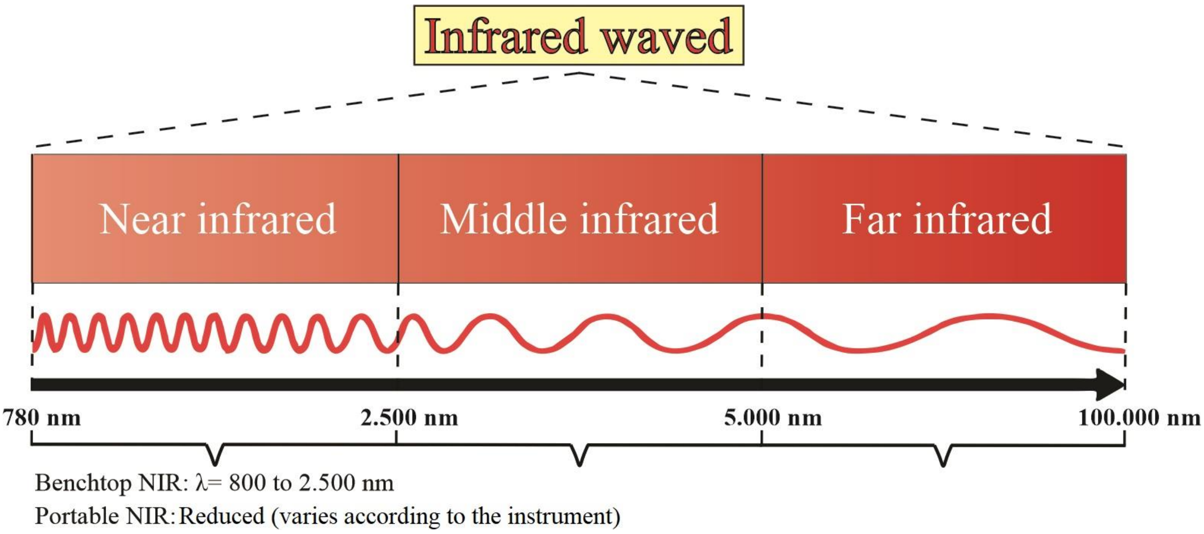


Figure 5 - Wavelengths and absorption bands corresponding to benchtop and portable NIR.

NIR spans the wavelength range from 780 to 2.500 nm and is used in applications such as remote sensing, materials analysis and communication technologies (PASQUINI, 2003). MIR is the infrared region with wavelengths 2.500 to 5.000 nm and is frequently used in spectroscopy to analyze chemical composition (SU; SUN, 2019). FIR, in turn, covers the wavelength range from 5.000 to 100.000 nm and can be applied to heat detection, communications and thermal imaging technologies (OZAKI, 2021). Therefore, the focus of this review was based on the NIR region, in which the principles of interaction, the advantages of its use and its applicability in the industrial wood sector were described.

The NIR technique is recognized as a non-destructive analytical method capable of efficiently determining molecular structures and quantitative variables in a wide range of organic materials (PASQUINI, 2018). Its operation relies on vibrational spectroscopy, which evaluates how NIR light interacts with the sample (NAES *et al*., 2002; PASQUINI, 2003). Because NIR radiation has longer wavelengths and therefore lower energy, its interaction induces only vibrational and rotational changes in the molecules being analyzed. This interaction occurs when the chemical bonds within the material resonate with the electromagnetic wave, meaning that the electric field generated by the bond's vibration aligns with the incoming radiation (OZAKI *et al*., 2021). During the process, the spectrometer directs near-infrared radiation onto the sample, while sensors detect the resulting variations in the vibrational behavior of its chemical components. These constituents absorb, reflect, and transmit the radiation in characteristic ways, as illustrated in Figure 6.

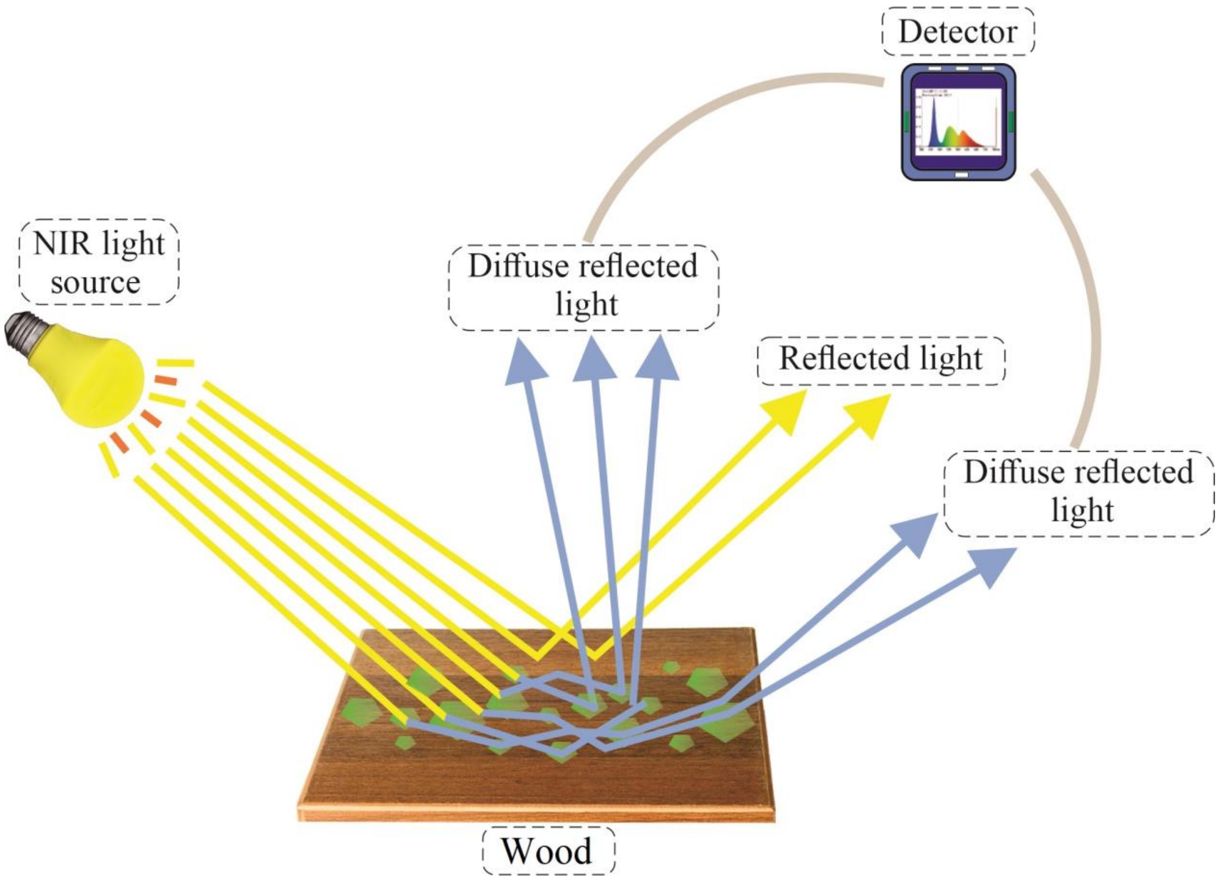


Figure 6 - Interaction of near-infrared light with the sample studied.

Within a wavelength range (780-2500 nm), some frequencies are absorbed or not absorbed (FERRARI; MOTTOLA; QUARESIMA, 2004). Therefore, the intensity of light absorption in contrast to the wavelength constitutes the absorption spectrum of a substance or sample, which causes the compression and stretching of the molecules, resulting in a wave movement of the atoms according to the elements and types of bonds (PASQUINI, 2003). Due to the absorption response, the NIR spectrum resembles a fingerprint, with each kind of material emitting a specific spectral signature.

In the forest-based industrial sector, the first records of studies that used NIR spectroscopy were reported at the end of the 1980s, emphasizing the work carried out by Birkett and Gambino (1989). Initially, NIR spectroscopy was treated as an alternative method for quickly analyzing the lignocellulosic components of wood, considering the predominance of conventional laboratory methods. As the technique became more widespread, work covering wood's physical and mechanical properties advanced significantly. In this context, Table 2 presents the main variables estimated using the NIR technique and their respective spectral ranges for different materials and products in the wood forest-based industrial sector.

Table 2 - Main chemical groups and corresponding NIR spectral ranges for lignocellulosic materials.

Material / Product	**Main chemical groups**	**Optimized spectral range (nm)**	**Main spectral assignment**	**Parameters estimated with higher accuracy**
Wood	Amorphous and crystalline cellulose, hemicelluloses, lignin, extractives	1140–1590	O–H and C–H vibrations (cellulose and hemicellulose); aromatic C–H (lignin)	Density, moisture content, cellulose content, holocellulose content, lignin content, extractives content, crystallinity, S/G ratio
Cellulose pulp	Cellulose, residual hemicelulose	1420–1560	O–H and C–H vibrations associated with cellulose	Moisture content, brightness degree, crystallinity
Wood-based panels	Lignin, synthetic adhesives, extractives	1200–1700	C–H and N–H (resins and lignin)	Resin content, moisture, apparent relative density
Charcoal	Condensed aromatic groups and graphitic structures	1110–1200	C–H and C=C bonds	ash content, gravimetric yield, apparent relative density, volatile matter

				content, fixed carbon content
Pellets	Cellulose, lignin, extractives	1150–1550	Combined C–H and O–H vibrations	Lignin content, ash content, calorific value

It is important to emphasize that the water content has a strong influence on the NIR spectral response, as it can mask or shift absorption bands associated with O–H and C–H bond vibrations, directly affecting the calibration and accuracy of predictive models (AMARAL *et al*., 2020; MEDEIROS *et al*., 2023). In the case of charcoal, the simplification of the chemical structure resulting from the carbonization process reduces the diversity of detectable functional groups, which may limit the precision of compositional estimations (COSTA *et al*., 2019; ABREU NETO *et al*., 2021; MARTINS *et al*., 2025).

After spectral acquisition, the application of multivariate statistical methods becomes essential for interpreting the data and predicting the variables of interest. In this context, principal component analysis (PCA), partial least squares discriminant analysis (PLS-DA) and partial least squares regression (PLS-R), are used in a complementary manner to extract qualitative and quantitative information from the spectra.

3.3. Multivariate statistical analysis applied in the forest-based industrial sector

3.3.1. Principal Component Analysis (PCA)

Multivariate statistics is a technique in which numerous variables are studied simultaneously. It can be classified as quantitative when the objective is to estimate sample variables or qualitative when the intention is to classify the data according to the desired characteristic (WANG *et al*., 2022). The choice of methods to be used depends on the objective of the research.

The PCA is the most used technique in qualitative spectral data analysis. This analysis aims to transform complex data into relevant information so that it becomes easier to visualize. PCA analysis helps the construction of two-dimensional graphs containing statistical information and the possibility of grouping between similar samples using the available variables (BURNS; CIURCZAK, 2008; RAMALHO *et al.*, 2017).

Principal components are defined according to the direction of maximum variance in the dataset. Each subsequent component captures the highest remaining variance, so that PC1 contains the greatest proportion of the data's variability, followed by PC2, PC3, and so forth (SCHWANNINGER *et al.*, 2011; DIESEL *et al.*, 2014). By transforming the original variables into this new set of principal components, most of the information (variance) can be retained while reducing the dimensionality of the dataset, with minimal loss of chemical information.

Several studies in the literature demonstrate how PCA has been applied to NIR spectroscopy within the forest-based industrial sector. Costa *et al*. (2018a) investigated how spectral acquisition procedures and wood anisotropy affect predictive modeling of wood density using a benchtop NIR instrument. They analyzed test specimens of *Eucalyptus urophylla* × *Eucalyptus grandis* (2.5 × 2.5 × 5.0 cm), collecting spectra from radial and tangential surfaces, as well as from cross sections machined with circular and band saws. PCA revealed that, for the radial, tangential, and transverse surfaces machined by either saw type and collected using an integrating sphere, the first two components accounted for 100% of data variability: 99% explained by PC1 and 1% by PC2. Radial and tangential spectra overlapped, indicating similar spectral characteristics, whereas transverse spectra formed distinct groups depending on the machining method, highlighting surface quality as a key factor in discriminating wood samples.

Using the same type of instrument, Santos *et al*. (2020) estimated moisture content in hybrid *E. urophylla* × *E. grandis* wood during ten stages of drying, from fiber saturation to the anhydrous state. Spectra were collected from radial, tangential, and cross-sectional surfaces machined with both saw types, as well as using an integrating sphere and an optical fiber probe. The first two components of the band-sawn transverse samples explained 99.90% of total variability (PC1 = 99.41%; PC2 = 0.50%). Moisture-related spectral variation was most evident in the transverse surface due to the greater exposure of anatomical features, which enhanced light–cell wall interaction. Among acquisition methods, the integrating sphere provided clearer separation among moisture classes, with fewer overlapping spectra compared to the optical fiber.

Lima *et al*. (2022b) evaluated the use of PCA to classify wood wastes from 12 Amazonian species for potential charcoal production. Samples consisted of 72 pieces per species (4.0 × 4.0 × 3.0 cm), with surfaces sanded to remove chainsaw marks. Spectra collected from radial and transverse sections showed very high explained variance: for radial surfaces, PC1 and PC2 accounted for 99.90% and 0.07% of variability, respectively (totaling 99.97%), while for transverse sections, PC1 explained 99.81% and PC2 0.13% (totaling 99.94%). The authors observed clustering tendencies for some species, particularly in transverse spectra, showing that NIR spectroscopy is a fast and effective tool for differentiating wood waste from various Amazonian species, especially when grouping materials intended for charcoal production.

Ramalho *et al*. (2017) investigated the differentiation of charcoal produced from native and planted wood, as well as the effect of final carbonization temperature, using a benchtop NIR system. They analyzed four Cerrado (Brazilian Savana) native species and two *Eucalyptus* clones, using samples of different dimensions for each group. Charcoal produced at 300, 500, and 700 °C showed temperature-dependent spectral patterns. PCA performed on data grouped by temperature produced three clusters corresponding to the carbonization temperature. When spectra were pre-processed with a first derivative, it became possible to distinguish between charcoal from native and planted forests, but only for the 300 °C carbonized samples. For higher temperatures, NIR scores overlapped, preventing clear separation. The study demonstrated that NIR spectroscopy can be applied to identify the origin of charcoal, especially at lower carbonization temperatures.

Vieira *et al*. (2021) examined the discrimination of both wood and charcoal from four Myrtaceae species native to southern Brazil using a benchtop NIR instrument. Three trees per species were sampled, with discs taken at breast height and subdivided into regions near the pith, intermediate zones, and near the bark. Two spectra per anatomical section (transverse, radial, and tangential) were obtained. PCA of untreated spectra showed limited separation, but applying a second derivative enhanced discrimination among species. For wood, all anatomical positions allowed species differentiation; for charcoal, greater dispersion occurred, but the radial and tangential sections, particularly near the bark, yielded the best separation results.

Thus, it was observed that PCA is a valuable tool in studies related to the industrial wood sector, demonstrating success in the qualification of lignocellulosic materials. As this analysis only requires information on spectral signatures, studies that presented greater sampling and spectrum collection variability, such as the use of different native woods and sample collection surfaces, presented the most promising results.

3.3.2. Partial least squares regression (PLS-R)

A PLS-R is a technique used to predict properties from spectral information. PLS maximizes the covariance between input and output data, with the model resulting from this technique being the relationship between the latent variables, which can be linear or not (HEIN; LIMA; CHAIX, 2010). The method begins with the calibration of the model, in which the data from the matrix (HEIN; PAKKANEN; SANTOS, 2017; RAMALHO; ANDRADE; HEIN, 2018).

The calibration equation makes it possible to predict the composition of unknown samples belonging to the population that originated in the calibration with good reliability. From the spectrum reading, the data is transformed into a numerical matrix that makes it possible to optimize the available information and correct the effects caused by differences in the particle size (density and orientation) of the samples to predict their composition. It is crucial that the samples under study represent all the variability existing in the population and that the reference measurements are carried out accurately (PASQUINI, 2003).

After calibrating the model for a given parameter (Figure 7), the accuracy of the calibration must be tested through model validation, which can be performed through cross-validation or external/independent validation (SCHWANNINGER *et al*., 2004). Cross-validation employs the same samples involved in the calibration test. The process involves segregating some samples and building a model with the rest. The prediction is based on the initially segregated samples, with the samples selected by the methods leaving one out in batches, systematically or randomly (LOUREIRO *et al*., 2022). Independent validation requires an external set of samples for measuring spectra and performing conventional analyses, increasing the reliability and validity of the validation process (MEDEIROS *et al*., 2023).

According to Pasquini (2003), external validation should preferably be used in the model construction, as this method presents more reliable, i.e., closer to reality results. Cross-validation should be used when few samples are available or due to the high cost of laboratory analyses.

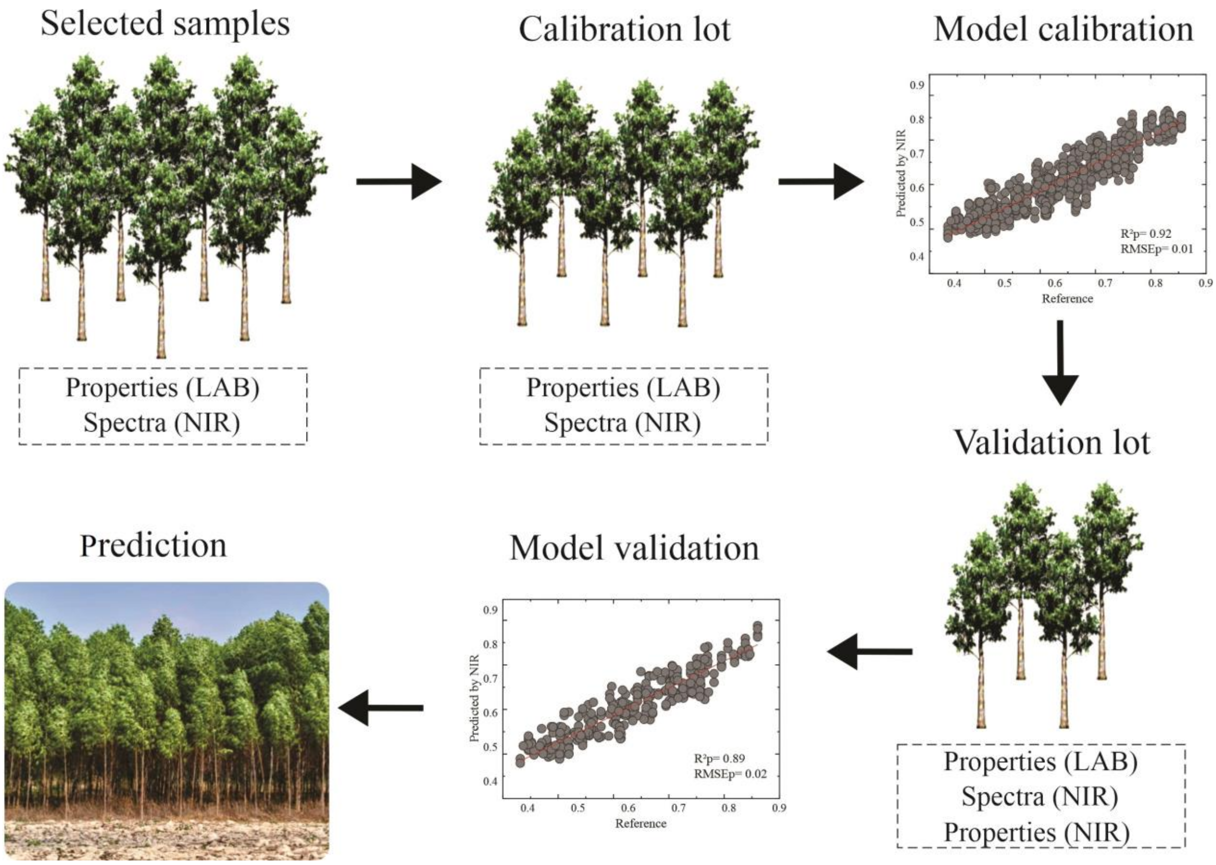


Figure 7 – Calibration and validation of multivariate statistical models.

The reliability of the models is represented by the calculation of the mean squared prediction error (RMSE) and coefficient of determination (R^2), where the RMSEcv is the prediction error generated in cross-validation. The R^2 demonstrates the relationship between the values obtained by laboratory analyses and those predicted in the same samples' models (SCHIMLECK *et al.*, 2022). RMSEp is the prediction error arising from independent validation, and RMSEc is the standard calibration error, the average deviation of the results of laboratory analyses and NIR spectra (NASCIMENTO *et al.*, 2017; MANLEY; BAETEN, 2018). Such parameters also provide basis for choosing the best models. In this sense, the reference values for each parameter to classify the reliability of the models indicate that the R^2 must be close to 1 and the RMSEc, RMSEcv and RMSEp close to the standard error of laboratory analyses (NUNES *et al.*, 2011; MUÑIZ *et al.*, 2012), as shown by Eq.1 and 2:

$$RMSE = \sqrt{\sum_{i}^{N} \frac{(y_i - y_1)^2}{N}} \quad (1)$$

$$R = \sum_{i=1}^{N} (\hat{y}_i - \bar{\hat{y}})(yi - \bar{y}) \,/\, \sqrt{\sum_{i=1}^{N} (y_i - \bar{y})^2} \sqrt{\sum_{i=1}^{N} (\hat{y}_i - \bar{\hat{y}})^2} \quad (2)$$

Where ŷ is the estimated value, ŷ with bar is the estimated average value, y represents the observed values and ȳ the observed average values. N is the number of samples belonging to each evaluated subset (test or training).

The ratio performance to deviation (RPD) is another parameter commonly used to check the model's efficiency regarding the samples' natural variation. The RPD is calculated for the calibration and validation models separately, being the relationship between the standard deviation of the reference data and the cross-validation standard error (RMSEcv) or independent validation standard error (RMSEp) (WILLIAMS; SOBERING, 1993). RPD reference values can be grouped into three classes: class "A" models with RPD > 2.0 are considered models of excellence, presenting R^2 values between 0.80 and 1.00; class "B" models with RPD between 1.4 and 2.0 are models considered adjusted, presenting R^2 varying between 0.5 and 0.8 and class "C" models with RPD < 0.5 are models considered unreliable, presenting $R^2 < 0.5$ (FERN, 2002).

Several studies in the forest-based industrial sector have employed PLS-R to predict wood properties and characteristics of derived products. Amaral *et al*. (2021) examined the calibration of basic density using NIR spectra collected on three anatomical surfaces (transverse, radial, and tangential) of *Eucalyptus urophylla* × *Eucalyptus grandis* wood. Among the evaluated treatments, spectra measured on the transverse face generated the most accurate model ($R^2cv = 0.85$; RMSEcv = 25.5 kg/m³). In contrast, the tangential surface yielded the weakest performance (R^2cv = 0.53; RMSEcv = 46.8 kg/m³). The authors also reported that mathematical preprocessing did not significantly improve the performance of models based on transverse spectra.

Miranda *et al*. (2023) investigated wood phenotyping in hybrid *Corymbia torelliana* (CT) × *Corymbia citriodora* (CC) and *Eucalyptus dunnii* (ED) using a benchtop NIR system. Sawdust samples were obtained from bark to bark at DBH. Two modeling strategies were tested: one with 25 CTO×CCT samples and another combining these with 36 EDU samples (61 total). For the first and second approaches, R^2cv values ranged from 0.60–0.73 for basic density, 0.37–0.65 for extractives, 0.56–0.53 for total lignin, 0.63–0.66 for the S/G ratio, and 0.52–0.77 for kraft pulp yield. Based on widely accepted statistical criteria, the authors considered all models suitable for classifying wood in genetic improvement programs.

Loureiro *et al*. (2022) used a benchtop NIR instrument to estimate chemical and physical properties of *Eucalyptus urophylla* wood (1–6 years old) from fast-growing plantations. Spectra were collected from groundwood (40–60 mesh) and from composite height samples. Independent validation produced encouraging results, with R^2p of 0.768 for density, 0.912 for extractives, 0.936 for ash, and 0.697 for carbon content. The authors emphasized that the sampling strategy using groundwood could be readily adapted to drilling-based methods used in tree breeding programs, potentially increasing efficiency in clone selection.

Liang *et al*. (2020) explored the prediction of holocellulose and lignin in raw material for pulp production using NIR spectroscopy combined with variable-selection techniques. Wood discs from eucalyptus, acacia, and poplar were ground and sieved (40–60 mesh). Various selection algorithms (ENIV-MC, ARCS, GA, and SPA) were compared. The ARCS method outperformed the others, providing more accurate predictions with fewer variables; AACS-PLS models produced R^2p values of 0.89–0.92 and RPD values of 2.84–3.69. As a result, the authors concluded that these models are suitable for predicting properties of mixed-species raw material.

Medeiros *et al*. (2023) evaluated water desorption behavior in different pulp types using NIR spectra. Four pulps (bleached eucalyptus, bleached and unbleached pine, and Chemithermomechanical pulp - CTMP pine) were tested at various moisture levels. Across conditions, R^2p values ranged from 0.89 to 0.98 and RMSEp from 5.1% to 18.3%. The study also assessed calibration transfer among pulp types, and the transferred models maintained satisfactory accuracy. Thus, the authors considered the approach promising for monitoring moisture variation in pulp and paper industries.

Costa *et al*. (2018b) built PLS-R models to estimate gravimetric carbonization yield (GCY), apparent relative density (ARD), and final carbonization temperature (FCT) of eucalyptus charcoal. Spectra were collected on radial and tangential surfaces. GCY and FCT were successfully predicted (R^2cv = 0.96 and 0.85), while ARD could not be accurately estimated. The study indicated that NIR models may be used to anticipate charcoal quality during industrial processing.

Abreu Neto *et al*. (2021) investigated the estimation of charcoal density and dynamic hardness using NIR spectroscopy. Nine species were analyzed, including six *Eucalyptus*, one *Corymbia citriodora*, and two hybrids. Specimens were carbonized at 300, 450, 600, and 750°C. PLS-R produced robust results, with R^2 of 0.89 for density (450°C) and 0.91 for dynamic hardness (750°C) when SNV preprocessing was applied. The study demonstrated the efficiency of coupling NIR with multivariate analysis for rapid assessment of charcoal properties.

Sandak *et al*. (2021) assessed the potential of a portable NIR device for quality control in the production of glued laminated timber. Spectra were collected at five random points along the edges of *Fagus sylvatica* boards. Although mechanical properties cannot be directly linked to specific vibrational modes, the indirect correlations derived from chemical and physical features allowed the prediction of several surface-related properties. The authors considered the results promising, especially given the exploratory nature of the study, and suggested that pre-gluing NIR assessments may enhance quality control in laminated-wood manufacturing.

Toscano *et al*. (2022) used a portable NIR instrument to estimate the moisture content of industrial wood chips composed of mixed species. Three models with different preprocessing techniques yielded R^2p values between 0.94 and 0.96 and RMSEp between 1.99% and 2.44%. These results confirm the feasibility of using portable NIR devices in operational environments, even with their narrower spectral range relative to benchtop systems.

Medeiros *et al*. (2024) evaluated the basic density of *Eucalyptus grandis* wood chips at varying moisture levels using both portable and benchtop NIR instruments. Spectra were collected from saturated and hygroscopic-equilibrium moisture content-samples. PLS-R models achieved R^2p values of 0.77–0.85, and performance was not affected by moisture variation. This indicates that basic density can be reliably estimated in freshly harvested or yard-dried material, improving decision-making in production chains.

Gomes *et al*. (2024) predicted energetic properties of Cerrado (Brazilian Savana) wood using a portable NIR instrument. Samples of *Handroanthus roseoalba*, *H. heptaphyllus*, and *Piptocarpha rotundifolia* were analyzed on radial and tangential surfaces, then carbonized for laboratory determination of charcoal characteristics. PLS-R models yielded R^2cv values of 0.49–0.87 for volatile matter, 0.48–0.88 for fixed carbon, and 0.49–0.85 for ash. Among the evaluated conditions, charcoal produced at

500 °C provided the most reliable predictions, and models based on spectra from the transverse surface showed superior accuracy.

Given the above, it was observed that NIR spectroscopy can predict the quality of wood and its products. The studies mainly evaluated presented models classified as class A (RPD > 2.0 and R^2 between 0.80 and 1.00) and B (RPD between 1.4 and 2.0 and R^2 between 0.5 and 0.8) for the different variables analyzed. However, knowledge about the predictive capacity of predictive models using portable NIR instruments is still scarce, presenting an opportunity for future studies to compare benchtop and portable instruments and verify their efficiency.

3.3.3. Partial least squares discriminant analysis (PLS-DA)

In NIR spectroscopy applications, PLS-DA is used to model the relationship between spectral predictor variables and categorical response variables. The method is an extension of the PLS regression approach and extracts latent variables that maximize the covariance between the spectral data and the class information (HÖSKULDSSON, 1988; CASTRO *et al*., 2023).

For classification purposes, the original class vector is transformed into a binary (dummy) matrix Y. This matrix contains n rows, each representing a sample, and G columns, corresponding to the number of classes. Each element of the matrix indicates whether sample i belongs to class g, using the values 1 for membership and 0 for non-membership. Through this transformation, the initial class vector becomes an $n \times G$ matrix suitable for model calibration (TIAN *et al*., 2021).

After calibration, the PLS algorithm generates predicted values for every combination of sample and class. These predictions do not necessarily correspond exactly to 1 or 0 but rather fall within this range. Values closer to 1 indicate a higher probability that the sample belongs to the corresponding class, while values near 0 suggest the opposite (ZHANG *et al*., 2023). The final classification of each sample is assigned according to the class with the highest predicted value (MARK; BRADLEY, 2016).

Research conducted in the forest-based industrial sector has applied PLS-DA to classify wood properties and derived products. For instance, Lima *et al*. (2022a) investigated the classification of Amazonian wood wastes intended for bioenergy. Using a benchtop NIR spectrometer, they analyzed residues from twelve native species, collecting spectra from radial and transverse surfaces and determining basic density and moisture on a wet basis. The most efficient classification model they obtained was developed from first-derivative spectra collected on radial surfaces, achieving 97.9% accuracy during validation with an independent set of samples. The authors noted that some low-density woods were misclassified, yet they emphasized that NIR spectroscopy remains a rapid and reliable approach for distinguishing branch wood from Amazonian species based on basic density, supporting more sustainable use of these resources for energy production.

Novaes *et al*. (2023) examined how the condition of the wood surface affects species identification among six Amazonian trees. Three trees per species were sampled, and 350 specimens were prepared using both chainsaw and circular saw cuts. Their PLS-DA models achieved 99.2% accuracy when spectra were collected from surfaces cut with a chainsaw and 95.2% accuracy for specimens cut with a circular saw. These findings indicate that species can be reliably pre-classified regardless of the tool used during sample preparation, which is particularly useful in field identification, inspection procedures and commercial activities involving Amazonian timber.

Another application of PLS-DA was explored by Costa *et al*. (2024), who evaluated the quality of cellulose nanofibrils produced from commercial bleached eucalyptus kraft pulp. They analyzed CNF suspensions at concentrations ranging from 0.05 to 6.00% using NIR spectra collected in either absorption or transmission mode, depending on sample translucency. Transmission was more appropriate for lower concentrations, while higher concentrations required absorption measurements. External validation with unknown samples resulted in 96.7% accuracy. Suspensions at 3.00% yielded higher correct classification rates than those at 6.00%. Although spectral pretreatments did not improve the predictive capacity of the models, removing non-fibrillated CNFs and samples treated with TEMPO reagents enhanced performance. The authors concluded that these spectral signatures could be integrated into routine laboratory analyses for continuous monitoring of CNF quality.

Costa *et al*. (2019) applied PLS-DA to differentiate commercial charcoal products. Using a benchtop NIR spectrometer, they acquired spectra on transverse and radial surfaces through both integrating sphere and optical fiber setups. Their results showed that charcoal brands and charcoal quality levels, represented by fixed carbon content, could be classified with over 95% accuracy. The study also demonstrated that spectra can be collected directly from unprepared charcoal surfaces, avoiding the need for sanding the material prior to measurement.

The potential of PLS-DA for screening purposes was reinforced by Mancini *et al*. (2018), who analyzed 106 ground samples of virgin wood and processing residues. Their models classified treated wood and virgin wood with complete accuracy, and distinguished virgin wood from glued laminated wood with a correct classification rate of 96.45. These results show the value of NIR spectroscopy combined with multivariate analysis for identifying different categories of wood waste and manufactured wood products.

Finally, Sandak *et al*. (2020) assessed the performance of low-cost portable NIR devices for detecting natural defects in wood, including knots, decay, resin pockets and reaction wood. Twenty-five discs of *Picea abies* were analyzed with three portable instruments covering the visible and near-infrared ranges. The MicroNIR device demonstrated superior performance in rapidly identifying defects, largely due to its compact integrated design, which reduces electrical noise and improves the signal-to-noise ratio. Despite these advantages, its higher cost compared to the other prototypes tested may limit its accessibility.

Thus, it was observed that PLS-DA presents promising results in discriminating qualitative data within the forest-based industrial sector. Studies have demonstrated that classification models are robust, primarily when significant differences exist between the samples evaluated. We can mention the different species of wood, surface, and spectrum collection plan for the assessed samples. As an opportunity, studies collecting spectra in the field using portable NIR instruments could be instrumental in classifying wood and charcoal from native forests, contributing to reducing illegal deforestation through inspection by responsible environmental agencies. In the industrial environment, developing PLS-DA models to classify the quality of wood products in real-time presents a promising aspect since optimizing processes is of commercial interest.

3.3.4. Improvement of multivariate statistical models

Strategies such as mathematical spectra treatments, removal of outliers, and spectral range selection are used to obtain statistical models with superior results. Mathematical treatments of spectra are used before building models and seek to minimize problems related to spectral noise interference or even maximize the extraction of spectral information that has a low correlation with the evaluated property (OZAKI, 2012).

According to Agelet and Hurburgh (2010), the main mathematical treatments used are first derivative, second derivative, normalization, and SNV (Standard Normal Variate). During the model construction routine, each pre-treatment is applied to the spectra, and, posteriorly, multivariate statistical models are obtained by the software-specific applications such as Chemoface, Unscrambler, OPUS, MATLAB, and RStudio. Therefore, the choice of the model that best meets the evaluated parameter/characteristic is based on the ranking defined by the mathematical parameters described previously.

Outliers are samples that exhibit different behaviors about the rest of the data and are considered irrelevant for building models (CHEN *et al*., 2005). As a way to detect the presence of possible outliers, the construction of the graph leverage × waste student presents itself as an alternative. Leverage is a measure of sample dispersion in relation to the data's center or average, indicating each sample's performance in calibrating the model. The leverage value close to zero demonstrates that the sample in question is insignificant when calibrating the models. However, when differences are observed between the experimental measurements of a sample in relation to the others in the calibration set, this sample influences the model, which may be negative (ZHENG-FENG *et al*., 2016). Another method to identify outliers is the graph scores, where the axes are the main components. In this way, the analyzed samples are chemically like each other. If the behavior of a sample is discrepant in relation to the others, it can be considered an outlier.

Finally, the spectral range selection method presents another alternative to optimize multivariate statistical models. According to Pasquini (2003), spectra present variables that provide diverse information. However, some of these variables present information that results in noise, low correlation, or even redundancy. Therefore, selecting appropriate spectral regions is necessary to eliminate information that could negatively interfere with the accuracy of the models. This step consists of choosing the spectral regions that best interact with the analyzed variable since specific wavelength ranges capable of providing more information are known in the literature, emphasizing the chemical components of wood (TSUCHIKAWA; KOBORI, 2015). As a result of this selection, the models present improvements in mathematical parameters and stability in relation to collinearity, in addition to simplifying the interpretation of model relationships (XIAOBO *et al*., 2010).

3.4. Comparison between benchtop and portable NIR instruments

Studies in the forest-based industrial sector were primarily based on bench instruments, aimed mainly at the cellulose and paper sector and as a phenotyping tool for genetic improvement programs. However, portable versions of the NIR instrument were introduced on the market in 2010, therefore, to date, few studies have been found for wood, and no studies have been found for charcoal using spectra of the material itself, which highlights the importance of new studies in the forest-based industrial sector.

The main differences between benchtop and portable NIR instruments are related to analytical performance, practical application, and the infrastructure required for operation. Benchtop equipment is traditionally used in laboratory environments and stands out for offering greater spectral stability, higher resolution, and a broader spectral range, typically between 800 and 2.500 nm (AMARAL *et al*., 2021; LIMA *et al*., 2022). These features allow for more precise and detailed analyses, making them ideal for the development of robust calibration models and the chemical highly reliable characterization of samples. In addition, these instruments operate under controlled conditions of temperature, humidity, and lighting, which favors the reproducibility of results (COSTA *et al*., 2018b).

On the other hand, portable NIR instruments have been developed to meet the growing demand for fast and real-time analyses directly in industrial or field situations. These instruments are compact, lightweight, durable, and less expensive compared to benchtop models. Their spectral range is more limited (varies between instruments), which may restrict the identification of certain important spectral bands (MEDEIROS *et al*., 2024; GOMES *et al*., 2024).

Nevertheless, portable instruments offer operational flexibility, require less training for use, and do not depend on complex laboratory infrastructure, making them ideal for continuous process monitoring, routine inspections, and decentralized quality control (LIANG *et al*., 2020; SANDAK *et al*., 2021). Table 3 presents the main characteristics that differentiate benchtop and portable NIR.

Table 3 - Key differences between benchtop and portable NIR instruments.

Characteristic	Benchtop NIR	Portable NIR	References
Size and weight	Large and heavy	Compact and lightweight	Medeiros *et al*. (2024)
Portability	Stationary, requires a laboratory	High, can be used in the field	Martins *et al*. (2025); Martins *et al*. (2026)
Precision and accuracy	High, with greater spectral resolution	Lower than benchtop, but sufficient for quick use	Toscano *et al*. (2022)
Spectral range	Broader and more detailed	Limited, depending on the model	Medeiros *et al*. (2025)
Ease of use	Requires technical knowledge	Generally simpler, user-friendly interface	Brito *et al*. (2017)
Cost	High cost	Relatively lower cost	Sandak *et al*. (2021)
Maintenance	Complex	Simple, but with limitations	Zhang *et al*. (2022)
Common applications	Research and quality control laboratories	Precision agriculture, food, pharma, field use	Hein *et al*. (2017)
Power requirement	Stable power source needed	Battery-powered or external portable power	Kappacher *et al*. (2022)
Calibration and validation	More robust and frequent	Limited, may require occasional technical support	Panchuk *et al*. (2017)
Examples of analysis in the forest-based industrial sector	- Estimation of moisture content - Classification of wood species - Analysis of lignin, cellulose and hemicellulose - Quality control of pellets and briquettes - Estimation of apparent density	- Rapid field moisture measurement - Wood species screening - Control at the reception of raw materials - Biomass analysis for energy - Wood drying assessment - All analyses performed with benchtop NIR	Costa *et al*. (2018b); Costa *et al*. (2024); Liang *et al*. (2020); Ramalho *et al*. (2018); Miranda *et al*. (2024); Feng *et al*. (2018); Abreu Neto *et al*. (2021)

In terms of cost-effectiveness, portable NIR presents itself as a promising alternative for operational analyses, as it reduces response time, minimizes the need for sample collection and transportation, and allows forest managers to make immediate decisions in industrial processes (MEDEIROS *et al*., 2025). However, for applications that require greater analytical precision and method validation, benchtop instruments are the preferred option due to the higher accuracy of multivariate statistical models.

Based on this information, table 4 includes both benchtop and portable NIR instruments, with distinct spectral ranges, representing the diversity of equipment currently available for spectroscopic analyses. This instrumental variety enables the comparison of the applicability of different devices in the characterization of wood sector products, covering conditions ranging from controlled laboratory environments to field measurements.

Table 4 - Configuration and operating mode of the main NIR instruments.

Category	Brand	Model	Spectral range (nm)	Typical material
Benchtop	Bruker	MPA II	800–2.500	Liquids, solids, powders
Benchtop	Bruker	MPA III	780–2.530	Liquids, solids, powders
Benchtop	Bruker	TANGO II	800–2.500	Liquids, solids, powders
Benchtop	SFTec	IR1000 / IR1600 Series	900–2.500	Solids, liquids, gases
Portable	VIAVI	MicroNIR OnSite	908 – 1.676	Solids, powders
Portable	Trinamix	PAL Two	1.300–2.350	Solids, recycled materials, plastics
Portable	Bayspec	Breeze™ Handheld (VIS-NIR-SWIR)	400–2.500 (e.g., 400–1.700 for VIS-NIR-SWIR	Solids, industrial materials
Portable	ZEISS	AURA® handheld NIR	950–1.650	Solids (diffuse reflection)
Portable	SFTec	IR2200 handheld NIR	900–1.700 / 900–2.500 (configurable)	Solids, powders
Portable	IRIS Technology	Visum Palm™	900–1.700	Solids, furniture, textile
Portable	BUCHI	ProxiScout™	1.350–2.550	Solids, production analysis

Therefore, the choice between a benchtop and a portable NIR instrument should consider not only the technical requirements of the analysis but also the logistical, economic, and operational aspects associated with the production process (SANDAK *et al*.; 2021; GOMES *et al*.; 2025). In this context, criteria such as operating spectral range, optical resolution, mechanical robustness, thermal stability, ease of calibration, spectral acquisition speed, and compatibility with different sample types (solid, granular, or fragmented) become decisive. Furthermore, factors such as field usability, level of automation, maintenance cost, and availability of technical support should also be evaluated.

The strategic combination of benchtop and portable instruments represents a complementary and effective approach, enabling the integration of high-precision laboratory analyses with real-time monitoring in industrial environments. This integration enhances quality control and traceability of wood products while optimizing decision-making in harvesting, processing, and technological characterization stages of the wood production chain.

3.5. Applications and implications of using portable NIR instruments in industrial environments

With the advancement of sensor miniaturization and the development of embedded chemometric algorithms, portable NIR instruments have assumed an increasingly strategic role in industrial process control (SANDAK *et al*., 2020; TOSCANO *et al*., 2022). The adoption of this technology in production environments represents a significant shift in how quality is monitored and managed throughout production chains.

The use of portable NIR enables real-time analysis directly on the production line, allowing for the early detection of quality deviations and the immediate implementation of corrective actions (MEDEIROS *et al*., 2025). This agile response capability is particularly valuable in forestry-based industries with high demands for uniformity and traceability, such as pulp and paper producers, charcoal manufacturing, and wood panel industries. The ability to obtain immediate data on critical process parameters eliminates the need for lengthy delays associated with conventional laboratory analysis, thereby reducing cycle times and enhancing operational efficiency (GOMES *et al*., 2024; PAN; YU; YANG, 2024).

Furthermore, the use of this technology considerably reduces reliance on conventional analytical laboratories (TSUCHIKAWA; KOBORI, 2015). By enabling direct analysis of raw materials, intermediates, and final products, portable NIR instruments lower logistical and operational costs associated with sample transportation and preparation, as well as the use of chemical reagents (LEBLON; ADEDIPE; HANS, 2013). This supports a more sustainable approach by minimizing the disposal of chemical substances and the consumption of laboratory resources.

However, the effective implementation of portable NIR instruments requires careful consideration of organizational and human factors. Despite the simplified interface of modern equipment, reliable use of the technique depends on adequate training of personnel. Operators must be capable of handling the instruments correctly, understanding basic operating principles, following calibration protocols, and interpreting results as needed. The development and maintenance of robust multivariate statistical models, suited to the inherent variability of industrial processes, require specialized technical support, particularly during the initial stages of implementation (SANDAK; SANDAK; MEDER, 2016; DEEPA; SHUKLA; KELKAR, 2024). Continuous monitoring of these models throughout their operational application is essential to ensure that predefined parameters are consistently met.

From an economic perspective, investment in portable NIR instruments presents a highly promising tendency. Although the initial acquisition cost may be considered significant, these instruments are generally less expensive than benchtop NIR instruments, making them a more accessible alternative for decentralized implementation in industrial settings (SANDAK *et al*., 2021). Additionally, the benefits of analytical automation and real-time monitoring tend to outweigh the costs over time (MEDEIROS *et al*., 2024). Reduced losses, improved process stability, and more efficient use of inputs result in direct gains in productivity and quality. Moreover, companies that incorporate advanced analytical technologies into their operations strengthen their competitive position and demonstrate alignment with increasing demands for innovation, traceability, and operational efficiency.

Thus, the adoption of portable NIR instruments in industrial contexts represents a shift toward a smarter, more economical, and sustainable production model. By integrating real-time analysis, operational autonomy, and process intelligence, this technology not only enhances quality control capabilities but also redefines the dynamics of modern industrial operations. However, factors such as local conditions (temperature, relative humidity and sample moisture), the properties to be determined, the spectra collection surface of the samples, as well as the material used (degree of purity, granulometry and sample heterogeneity) present challenges that can directly influence the estimates and precision of the models (COSTA *et al*., 2018a; RAMALHO *et al*., 2019). Therefore, new studies must investigate the extent to which the information obtained in the laboratory environment may differ from the field and/or industrial environment due to the control of factors external to the process.

3.6. Calibration transfer between benchtop and portable NIR instruments

Calibration transfer between benchtop and portable NIR instruments has become a consolidated strategy for enabling rapid and accurate analyses in industrial environments, while maintaining the traceability and robustness of analytical models originally developed under laboratory conditions (FOLCH-FORTUNY *et al*., 2017; WORKMAN, 2018).

Although benchtop spectrometers provide advantages such as greater spectral stability, higher resolution and improved environmental control, portable NIR devices are designed to prioritize operational versatility, making them suitable for real-time and in-field measurements (TOSCANO *et al*., 2022). These contrasting characteristics create obstacles when attempting to directly transfer calibration models from one type of instrument to another. To address this issue, several mathematical and statistical strategies are commonly adopted, including Direct Standardization (DS), Slope and Bias Correction (SBC), Piecewise Direct Standardization (PDS) and Canonical Correlation Analysis (CCA) (ZHANG *et al*., 2022). Such techniques help harmonize the spectral matrices generated by different sensors, which in turn allows models to be validated using data collected on distinct instruments.

Because portable devices inherently operate with constraints related to spectral coverage, light source intensity and detector performance, transferring calibrations built on benchtop equipment can be particularly challenging (MISHRA; PASSOS, 2021; MEDEIROS *et al*., 2025). For this reason, assembling a representative set of standard samples that reflects the expected variability of the application environment becomes essential for achieving effective cross-calibration (YANG *et al*., 2019). In industrial contexts, where uniformity of results is crucial for maintaining product quality and supporting operational decisions, establishing trustworthy calibration transfer procedures is therefore a fundamental aspect of analytical workflow.

From an operational standpoint, the development of hybrid or adaptive models capable of dynamically adjusting based on measurements obtained in field and industrial environments represents a promising trend. These models, when combined with continuous learning techniques, allow algorithms to be updated in response to new process conditions or raw material variability, thereby enhancing analytical resilience.

Research on calibration transfer of NIR spectra in the forest-based industrial sector is still limited, with only two studies published so far. The first, conducted by Zhang *et al*. (2022), investigated the transfer of calibration models among portable NIR instruments to estimate lignin content in wood samples used for pulp production. The study included five species (*Pinus massoniana*, *Cunninghamia lanceolata*, *Acacia*, *Eucalyptus* and *Populus*) and applied several statistical strategies to transfer models from a master to a target instrument. The authors tested direct standardization (DS), slope and bias correction (SBC), piecewise direct standardization (PDS) and canonical correlation analysis (CCA). The best results were obtained using the DS and PDS methods, which produced R^2 values above 0.79 and demonstrated high predictive performance after calibration transfer.

A second study, carried out by Medeiros *et al*. (2025), examined the feasibility of transferring calibrations between benchtop and portable NIR instruments for predicting the basic density of *Eucalyptus grandis* wood at different moisture levels (140%, 30% and 12%). Ninety-five cubic wood samples measuring 3.0 × 3.0 × 3.0 cm were prepared, and spectra were acquired directly on the transverse surface using both types of instruments. The authors evaluated three approaches: matrix correction, variable selection and external validation. The models developed from each spectral matrix showed coefficients of determination ranging from 0.74 to 0.92, indicating strong predictive potential using raw or harmonized spectral data. During the calibration transfer stage, the predictive coefficient of determination reached 0.93. The best results were obtained for samples with moisture content close to 30%. The study also showed that calibrations developed with the benchtop instrument were more robust and presented greater transferability to other devices.

Although calibration transfer between benchtop and portable NIR instruments involves technical challenges, it represents an important opportunity to expand the use of NIR spectroscopy in decentralized industrial environments. The implementation of standardized procedures, the development of robust statistical models and ongoing validation efforts are essential to bridge the precision achieved in laboratory conditions with the operational flexibility required in field applications.

3.7 Scientific gaps and suggestions for future research

The use of NIR, especially in relation to portable instruments, is characterized as a promising tool for non-destructive analysis of forest products. However, there are significant limitations, such as the scarcity of studies under real operating conditions, in-depth studies on sensor variability in estimates, the effects of environmental factors, and the influence of moisture content and storage time on spectral acquisitions.

This, in turn, may be related to the low level of collaboration among researchers around the world. Given that the equipment can be costly, sharing databases and/or equipment can contribute significantly to resolving doubts about the accuracy of estimates. Thus, it is suggested that future work explore the use of portable NIR spectrometers in industrial and forest environments under different climatic and operational conditions, in addition to investigating robust calibration methods that consider the variability of materials and equipment. Comparative studies of portable and benchtop spectrometers can also contribute to validating the reliability of mobile devices, expanding their practical applicability in the forest-based industrial sector.

4. FINAL CONSIDERATIONS

This review used the visual representation of bibliometric coupling and keyword co-occurrence from 1997-2025 to illustrate the evolution of themes and central research focus areas. It was found that the studies that applied NIR spectroscopy in the industrial wood sector mainly used the benchtop NIR instrument. As it is a recent technology, studies using portable NIR instruments are scarce for characterizing wood and its products. To fill this gap in scientific development, new studies using such instruments are necessary so that their precision and robustness can be evaluated. The literature reports that studies that used portable NIR instruments in the forest-based industrial sector reported promising results, reinforcing the possible advantages of using these instruments for benchtop NIR, such as lower acquisition cost instruments, little and/or no sample preparation due to greater instrument mobility, the possibility of use at the study site, among others. From future perspectives, studies are expected to evaluate not only wood but also its products. Furthermore, studies conducted in the field or the industries are alternatives that would make it possible to assess the characteristics of interest in real-time, resulting in characterization processes that are closer to reality.

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CHAPTER 2

COMPARISON OF BENCHTOP AND HANDHELD NEAR-INFRARED SPECTROSCOPY FOR PREDICTING WOOD PROPERTIES IN FAST-GROWING PLANTATIONS FOR BIOENERGY APPLICATIONS

COMPARISON OF BENCHTOP AND HANDHELD NEAR-INFRARED SPECTROSCOPY FOR PREDICTING WOOD PROPERTIES IN FAST-GROWING PLANTATIONS FOR BIOENERGY APPLICATIONS

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COMPARISON OF BENCHTOP AND HANDHELD NEAR-INFRARED SPECTROSCOPY FOR PREDICTING WOOD PROPERTIES IN FAST-GROWING PLANTATIONS FOR BIOENERGY APPLICATIONS

ABSTRACT

The forestry sector requires fast, accurate and low-cost techniques to control the quality of wood used in bioenergy generation. Near-infrared spectroscopy (NIR) is a promising technique that meets these requirements. This study aimed to predict the S/G ratio, cellulose crystallinity, structural chemical composition and wood basic density from fast-growing plantations using benchtop and portable NIR instruments. Two trees of 15 clones (11 *Eucalyptus* and 4 *Corymbia* clones) aged 84 months were evaluated. Wood discs with 10 cm thickness taken longitudinally (0, DBH, 25, 50, 75 and 100%) from each stem were ground to obtain composite samples. In each composite sample, 20 spectra were collected, resulting in a matrix of 600 spectra for each instrument (benchtop and portable). Principal component analysis (PCA) was employed to verify the distribution and similarity of spectral data, and partial least squares regression (PLS-R) was used to develop predictive models. PCA showed accumulated variance >99.0% of the spectral data for both instruments. The PLS-R models using the benchtop NIR instrument showed prediction coefficients (R^2p) ranging from 0.69 to 0.93 for *Eucalyptus* clones and from 0.82 to 0.96 for *Corymbia* clones. The portable NIR instrument fitted models with R^2p ranging from 0.58 to 0.80 and 0.69 to 0.81 for *Eucalyptus* and *Corymbia* clones, respectively. In general, benchtop and portable NIR instruments showed promising results. They can predict the quantitative indices of wood from fast-growing plantations used in bioenergy generation, presenting themselves as valuable tools for selecting superior clones via genetic improvement programs.

Keywords: Quality control. Wood phenotyping. Multivariate statistics. Syringyl/guaiacyl ratio. Non-destructive techniques.

1. INTRODUCTION

Wood from planted forests instead of petroleum-based products has been gaining prominence in Brazil and worldwide due to its renewable nature, reduction of CO_2 emissions, and temporary carbon storage capacity of wood during use (PENA-VERGARA *et al*., 2022). The versatility of using wood from planted forests allows it to be used for various energy purposes, such as producing charcoal and firewood by direct combustion (ASARE *et al*., 2022; LIMA *et al*., 2022). Thus, fast-growing species that can adapt to different soil and climate regions are desirable in planted forests, so species and hybrids of the *Eucalyptus* and *Corymbia* genera have been used in the forestry market.

The *Eucalyptus* genus is the most widespread in planted forests in Brazil. According to the Ibá report (2025), the forest planted with this genus corresponds to 8.1 million hectares, resulting in 77.1% of the planted area in the country. Regarding its average productivity, in 2024, *Eucalyptus* reached an average annual increase of 33.7 m^3/ha/year (with bark) in Brazil, which can be associated with advances in the sustainable management of forest plantations, pest and disease control, soil fertilization, combined with favorable edaphoclimatic conditions for cultivation (IBÁ, 2025; DESTA; TEKLEMARIAM; MULUGETA, 2023).

The advancement of genetic improvement programs allowed the genus *Corymbia*, established in Brazil between the 1970s and 1980s, to become competitive with the genus *Eucalyptus*, mainly for energy use. At ages close to 6 years, studies conducted by Melo *et al*. (2024) and indicate high productivity for *Corymbia* (40 m^3/ha/year) and *Eucalyptus* (65 m^3/ha/year). In addition, other studies have obtained results indicating that wood from both genera, at 7 years of age, had basic density values above 600 kg/m^3, low gum exudation, resistance to adverse conditions (water deficit, frost, and wind), and planting density (LOURENÇON *et al*., 2013; LOUREIRO *et al*., 2019; MIRANDA *et al*., 2024).

Forestry industries constantly select new clones with desirable characteristics through genetic improvement programs. To optimize the selection process and reduce the costs of laboratory analyses, it is necessary to have techniques capable of predicting wood quality parameters in a simple, fast and reliable way. Among the non-destructive techniques, NIR spectroscopy stands out. Because it is of biological origin, wood has organic chemical bonds in its composition, which allows its quality to be assessed based on the spectral signatures generated by NIR.

A significant part of the studies in the literature addressing the use of NIR spectroscopy in the forestry sector used benchtop instruments to collect data. However, portable instruments offer the advantages of reduced cost, portability of the instrument and the possibility of assessing the material at the study site itself (WANG *et al*., 2015; TOSCANO *et al*., 2022). The main disadvantage is that the spectral range of the portable NIR instrument (11000-6000 cm^{-1}) is reduced compared to most benchtop instruments (12500-3500 cm^{-1}) (SANTOS *et al*., 2013; ZHU *et al*., 2022). However, most studies evaluating wood spectra use the 9000 to 4000 cm^{-1} range due to static noise and the lack of relevant information (LIMA *et al*., 2022a; LIMA *et al*. 2022b). In this sense, both equipment collect data in the presented range, allowing their use. However, it is necessary to evaluate whether reducing the spectral range of the portable NIR results in a loss of quality and reliability of multivariate statistical models to estimate wood quality.

Studies using portable NIR instruments have already been reported in forestry (SANDAK *et al*., 2020; HAO; WANG; ZHANG, 2021; SANDAK *et al*., 2021; MEDEIROS *et al*., 2024). However, there is still a lack of information on the efficiency of the portable NIR instrument in estimating the chemical and physical properties of wood from *Eucalyptus* and *Corymbia* clones. Considering the scarcity of information on the efficiency of portable NIR instruments in estimating wood quality, particularly for clones of the genera *Corymbia* and *Eucalyptus*, which have high potential for energy applications, this study stands out for its originality by employing such instruments to predict wood quality for energy purposes. Furthermore, few studies on models estimate essential characteristics for the energy sector, such as cellulose crystallinity and wood lignin's syringyl/guaiacyl (S/G) ratio.

Based on these gaps in scientific knowledge and considering the hypothesis of comparable accuracy between benchtop and portable NIR instruments, this study aimed to predict the S/G ratio, cellulose crystallinity, structural chemical composition and basic density of wood from fast-growing plantations with benchtop and portable NIR instruments. Once the potential of NIR instruments to predict these properties is proven, their use can be recommended for forestry companies as phenotyping tools for genetic improvement programs.

2. MATERIAL AND METHODS

2.1. Obtaining the material

The clonal test was established in commercial plantations located in Itamarandiba, Minas Gerais, Brazil (latitude 17º 44’ 45” S; longitude 42º 45’ 11” W; altitude 1000 m). The predominant soils are Oxisols, particularly the Typical Dystrophic Red Oxisol and the Typical Dystrophic Red-Yellow Oxisol, with clayey to very clayey texture and good structure. The region has a tropical climate with a dry season, characterized by humid summers and dry winters, an average annual temperature of approximately 21°C, and an average annual rainfall of 1166 mm.

Fifteen commercial clones of the genera *Eucalyptus* spp. and *Corymbia*, 84 months old and planted at a spacing of 3 × 3 m, were evaluated. For each clone, two trees of average diameter were selected, and discs 10 cm thick were removed longitudinally from the stems at six different positions (0, DBH, 25, 50, 75, and 100%) for analysis of the wood’s chemical and physical properties.

2.2. Laboratory physical-chemical analysis

A sample of each tree along all longitudinal positions was used to determine the chemical structural composition of the genetic materials. The samples submitted to the analyses were the fractions retained between the 40 and 60 mesh sieves (ASTM, 1982). The absolutely dry mass of the wood was determined according to the TAPPI 264 om-88 standard (TAPPI, 1996a). The total extractive content was determined according to TAPPI 204 om-88 (TAPPI, 1996b) in duplicate, replacing ethanol/benzene with ethanol/toluene. Soluble and insoluble lignins were determined following TAPPI UM250 (TAPPI, 1991) and TAPPI T 222 om-02 (TAPPI, 2002). The sum of the insoluble and soluble lignin contents determined the total linin. The holocellulose content was obtained by difference, subtracting the total lignin, extractives and ash content from 100.

Using liquid chromatography, the syringyl/guaiacyl (S/G) ratio of lignin was determined with 200 mg of absolutely dry sawdust free of extractives, with a sample composed of each tree along all longitudinal positions. The alkaline oxidation analysis with nitrobenzene was performed in duplicate, following the procedure described by Lin and Dence (2012).

Samples composed of all longitudinal positions of the tree were used, and the fraction of sawdust retained on the 270 mesh sieve was collected to analyze cellulose crystallinity. The analyzed material was fixed on quartz slides in 0.1 g using PVA glue, forming a thin, compact, homogeneous layer. The crystallinity index was calculated using X-ray diffraction (XRD). XRD patterns were obtained at room temperature using a D8-Discover X-ray diffractometer (Bruker), with a θ-2θ scan from 10 to 40° and a step of 0.05°/s.

The Segal crystallinity index (SEGAL *et al*., 1959) was calculated in duplicate for each treatment. Crystallinity was investigated based on the peak intensity of only two points: the flat peak (200) around 2θ = 22.7° and at 2θ = 18.5° representing the amorphous halo. Therefore, the index compares the crystalline portion of the main peak (200) concerning its overall intensity, as shown by Eq. 1:

$$IC = \frac{(I_T - I_A)}{I_T} \, x \, 100 \qquad Eq.(1)$$

Where, CI is the Segal crystallinity index, I_T is the total intensity of the (200) peak and I_A is the intensity of the amorphous halo.

The wood basic density was determined by collecting samples 1.30 m above the ground. To do this, the average obtained from the basic density of two opposite wedges passing through the core of the disc with a thickness of 2.5 cm was calculated according to the ABNT NBR 11941 standard (ABNT, 2003). The results of the mentioned physical-chemical characteristics can be seen in Table 1.

Table 1 – Chemical and physical properties of wood from *Eucalyptus* and *Corymbia* clones.

CL	**S/G**	**CRIST (%)**	**HOLO (%)**	**IL (%)**	**SL (%)**	**TL (%)**	**EXT (%)**	**BD (kg/m^3)**
C1	2.98 ± 0.01	66.09 ± 1.19	65.41 ± 1.07	24.75 ± 0.38	2.31 ± 0.22	27.05 ± 0.25	7.54 ± 0.93	600.0 ± 0.0
C2	2.42 ± 0.01	69.19 ± 1.00	61.51 ± 0.34	26.74 ± 0.23	2.96 ± 0.12	29.70 ± 0.35	8.79 ± 0.46	631.0 ± 10.0
C3	3.56 ± 0.01	69.85 ± 0.50	66.26 ± 1.16	24.21 ± 0.38	2.42 ± 0.20	26.62 ± 0.58	7.11 ± 0.65	586.0 ±0.0
C4	2.65 ± 0.01	66.22 ± 0.21	66.48 ± 0.67	23.27 ± 0.47	2.48 ± 0.24	25.74 ± 0.45	7.77 ± 0.23	635.0 ± 0.0
E1	3.05 ± 0.00	65.89 ± 1.58	66.85 ± 0.95	25.51 ± 0.87	3.03 ± 0.10	28.53 ± 0.82	4.61 ± 0.13	519.0 ± 10.0

E2	2.55 ± 0.01	88.11 ± 7.07	65.08 ± 0.39	26.61 ± 0.34	2.86 ± 0.09	29.46 ± 0.34	5.45 ± 0.08	546.0 ± 20.0
E3	2.94 ± 0.00	79.03 ± 2.29	69.04 ± 0.26	25.75 ± 0.08	2.69 ± 0.18	28.44 ± 0.18	2.85 ± 0.10	472.0 ± 0.0
E4	2.60 ± 0.02	75.13 ± 4.69	65.69 ± 0.14	26.34 ± 0.21	3.20 ± 0.31	29.54 ± 0.10	4.77 ± 0.31	517.0 ± 40.0
E5	2.37 ± 0.01	69.98 ± 0.54	66.60 ± 0.68	26.28 ± 0.19	2.63 ± 0.20	28.91 ± 0.33	4.99 ± 0.52	551.0 ± 20.0
E6	2.69 ± 0.00	70.47 ± 2.02	65.04 ± 0.57	26.40 ± 0.19	3.29 ± 0.14	29.68 ± 0.10	5.27 ± 0.67	522.0 ± 0.0
E7	2.52 ± 0.02	71.93 ± 2.18	62.88 ± 1.10	29.00 ± 0.21	3.14 ± 0.15	32.15 ± 0.32	5.73 ± 0.24	438.0 ± 0.0
E8	2.66 ± 0.00	73.40 ± 0.07	67.66 ± 0.85	26.94 ± 0.59	3.30 ± 0.08	29.90 ± 0.77	3.43 ± 0.71	483.0 ± 0.0
E9	2.63 ± 0.01	70.57 ± 1.20	64.64 ± 0.86	27.91 ± 0.35	3.31 ± 0.08	30.89 ± 0.58	4.79 ± 0.56	486.0 ± 60.0
E10	2.81 ± 0.00	72.44 ± 0.72	64.69 ± 0.63	27.76 ± 0.20	3.26 ± 0.12	30.96 ± 0.32	4.29 ± 0.34	534.0 ± 10.0
E11	2.38 ± 0.00	76.23 ± 0.14	64.14 ± 0.87	29.57 ± 0.18	2.08 ± 0.12	30.73 ± 0.42	5.55 ± 0.15	492.0 ± 10.0

*CL = Clone; C = *Corymbia*; E = *Eucalyptus*; S/G = Syringyl/Guaiacyl ratio; HOLO = Holocelluloses; CRIST = Cellulose crystallinity; SL = Soluble lignin; IL = Insoluble lignin; TL = Total lignin; EXT = Extractives. BD = Basic density.

2.3. Preparation of samples for analysis using the NIR technique

Wood discs (thickness 10 cm) were taken longitudinally from the tree at positions 0, DHB, 25, 50, 75, and 100% and kept under laboratory conditions until they reached equilibrium humidity with the environment. Soon after, the discs were ground, and composite samples were prepared for each tree/clone. The samples were sieved using 40 and 60-mesh sieves, with the material retained on the 60-mesh sieve being used.

2.4. Spectra acquisition

The ground wood samples were kept in a climate-controlled room at approximately 20°C and relative humidity of approximately 65% until they reached an equilibrium moisture of around 10-12% (dry basis). Immediately after, NIR spectra were acquired using a benchtop and portable device.

The benchtop instrument used was a Fourier transform (FT) MPA NIR spectrometer manufactured by Bruker Optik GmbH (Ettlingen, Germany), operating with OPUS software version 7.0. Spectra were obtained by diffuse reflection of the integrating sphere (12500-3500 cm^{-1}) with a resolution of 8 cm^{-1}. Sixteen scans were performed for each collected spectrum. Subsequently, the averages of these scans were calculated and compared with the standard to obtain the absorption spectrum of the specimen. Background compensation was performed every 10 min during spectral acquisition, and the light emission from the MPA window was shielded. However, the spectral range used for the calculations comprised the 9000-4000 cm^{-1} interval since the band selection method was applied to eliminate possible noise.

The portable instrument used was the MicroNIR On-site from Viavi Solutions Inc. (CA, United States), which was connected to a computer for storage of spectral data using the Spectral Solutions software from Viavi Solutions Inc. The spectra acquisition covered the 11000-6000 cm^{-1} range, with a resolution of 5.6 nm and 125 spectral variables. Each spectrum resulted from 16 scans in diffuse reflectance mode. Twenty readings were performed per sample on each instrument (benchtop and portable), with the samples being homogenized between each reading, totaling 600 spectra for each instrument.

2.5. Multivariate data analysis

Principal component analysis (PCA) and partial least squares regression (PLS-R) were fitted based on NIR spectra (Figure 1).

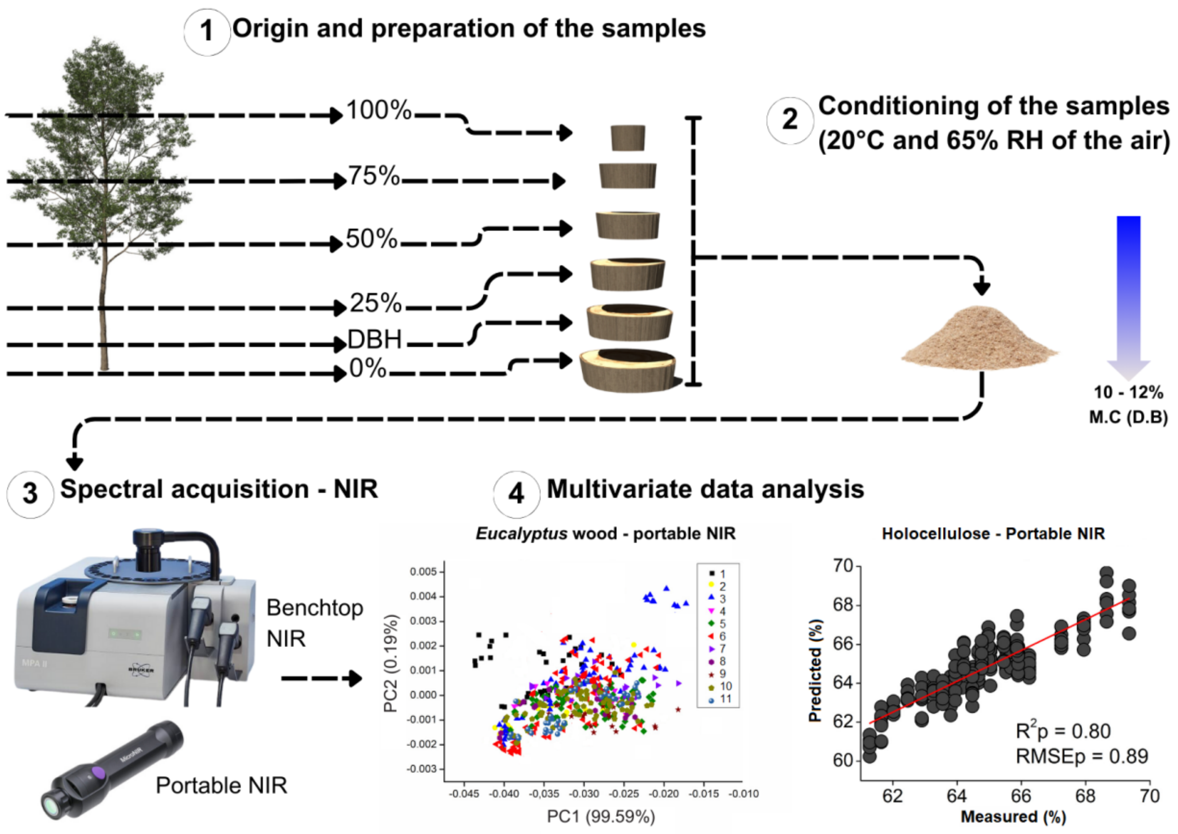

Figure 1 - Experimental scheme for data collection and processing using NIR spectroscopy.

Chemoface software version 1.63 (NUNES *et al*., 2012) was used for multivariate data analysis. PCA was applied to analyze the similarity of spectral data from wood clones of *Eucalyptus* and *Corymbia* within each genus. PLS-R models were fitted using wood spectra to predict the S/G ratio, cellulose crystallinity, structural chemical composition and wood basic density. A combination of cross-validation (leave-one-out) and independent validation (through a test set) was employed for model validation. Determining latent variables involved minimizing the standard error and maximizing the coefficient of determination during the validation phase. Consequently, the leave-one-out method was applied for cross-validations. For independent validations, the dataset was divided into calibration and validation sets, using 66.6% of the data for model calibration and the remaining 33.3% for validation, as recommended by Loureiro *et al*. (2022).

The original spectra and those mathematically treated with the 1st derivative (13-point filter and 2nd-order polynomial), normalization, and standard normal variation (SNV) were tested in constructing the models, aiming for better parameters and adjustments. The selection of the ideal models was based on statistical parameters, including the coefficient of determination for calibration (R^2c), root mean square error for calibration (RMSEc), coefficient of determination for cross-validation (R^2cv), root mean square error for cross-validation (RMSEcv), deviation performance ratio for cross-validation (RPDcv), root mean square error for prediction (RMSEp), deviation performance ratio for prediction (RPD), and latent variables (LV).

3. RESULTS AND DISCUSSION

3.1. Spectral signatures from NIR

The original spectral signatures and those treated with the 1st derivative for the wood dataset of *Eucalyptus* and *Corymbia* clones can be seen in Figure 2. The treatment of the spectra with the first derivative was performed to identify the spectral peaks clearly and succinctly. Thus, the spectral behavior of the two genera was observed to be similar because both belong to the Myrtaceae family, which justifies their proximity. Therefore, the differences observed in the spectral signatures are related only to the intensity of the peaks.

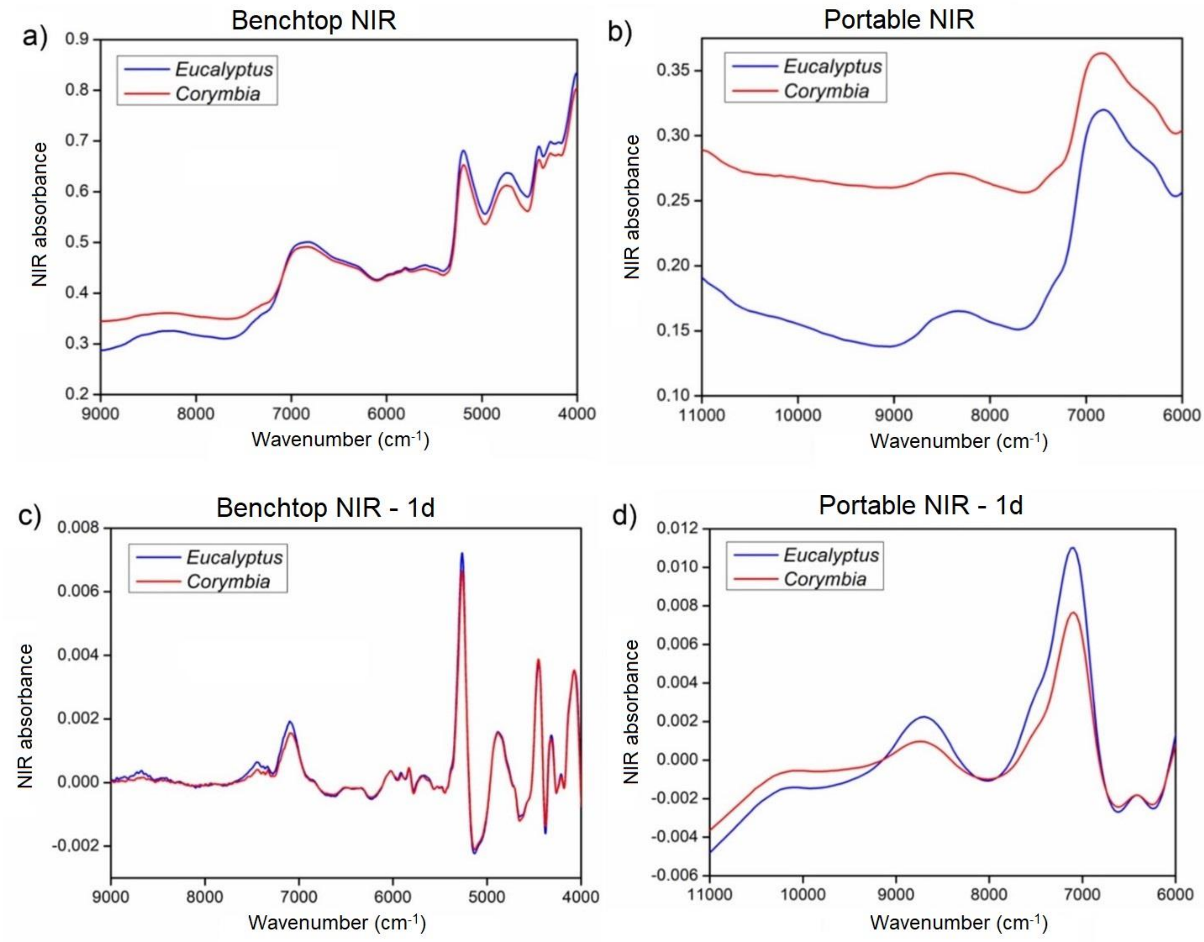

Figure 2 - Average spectral signatures of wood from *Eucalyptus* and *Corymbia* clones obtained with benchtop (a - untreated spectra; c - treated with 1st derivative) and portable (b - untreated spectra; d - treated with 1st derivative) NIR instruments.

Based on the spectral signatures provided by the NIR instruments, both species' absorbance values ranged from 0.3 to 0.9 for the benchtop NIR and 0.1 to 0.4 for the portable NIR. According to Medeiros *et al*. (2024), this result is consistent since characteristics such as the type of lamp, light output, radiation intensity, and spectral acquisition technology of the portable NIR are inferior to the characteristics provided by the benchtop NIR. Based on the hypothesis that the portable NIR can accurately estimate the chemical and physical properties of biological materials, such characteristics are expected to not reduce the information extracted from the multivariate statistical analyses.

According to Pasquini (2003), NIR radiation interacts with the chemical constituents' C-H, N-H, O-H and S-H bonds in materials of biological origin. Thus, for both *Eucalyptus* and *Corymbia*, the range between 7000 and 6287 cm^{-1} corresponds to the vibrational energy of cellulose's amorphous and crystalline regions (NIGOSKI *et* *al*., 2016; MEDEIROS *et al*., 2023). The high intensity of the peaks in this range may be associated with the reactivity of the hydroxyl groups in the cellulose chains, resulting in increased humidity in this region. Therefore, the interaction of electromagnetic radiation in the near-infrared range with the vibrations of the hydroxyl groups was intensified, increasing the absorbance and information about the material. The range between 8750 and 8540 cm^{-1} is related to the vibrational energy of the bonds of the aromatic groups of lignin (SCHWANNINGER; RODRIGUES; FACKLER, 2011). The range between 6000 and 5970 cm^{-1} was observed only in the benchtop NIR instrument due to the size of the wavelength and is related to the vibrational energy of the bonds of hemicellulose and extractive molecules (VIEIRA *et al*., 2021). Finally, the range between 4808 cm^{-1} and 4739 cm^{-1}, also observed only in the benchtop NIR wavelength, corresponds to the vibrational energy of the bonds of cellulose molecules (SCHWANNINGER; RODRIGUES; FACKLER, 2011).

Although the spectral peaks are related to the chemical properties of the wood, the complex composition of *Eucalyptus* and *Corymbia* wood makes visual analysis insufficient, requiring multivariate statistics to highlight possible differences between clones. It is worth noting that although the spectral range of the portable NIR instrument is smaller than that of the benchtop NIR, it was possible to identify some characteristic peaks of organic chemical constituents in this range, which allows the use of the NIR technique.

3.2. Principal component analysis (PCA)

Using benchtop and portable NIR instruments, principal component analysis (PCA) with the untreated and first-derivative-treated NIR spectra was performed to separate the *Eucalyptus* and *Corymbia* clones into distinct groups within each genus (Figure 3). In the present study, the benchtop NIR instrument could distinguish only 1 *Eucalyptus* clone (Figure 3a) and 2 *Corymbia* clones (Figure 3c). Regarding the portable NIR instrument, based on their spectral signatures, it was impossible to indicate the groups of clones within each genus (*Eucalyptus* and *Corymbia*). Although it did not distinguish all clones within each genus, the benchtop NIR instrument tended to group the clones more than the portable NIR.

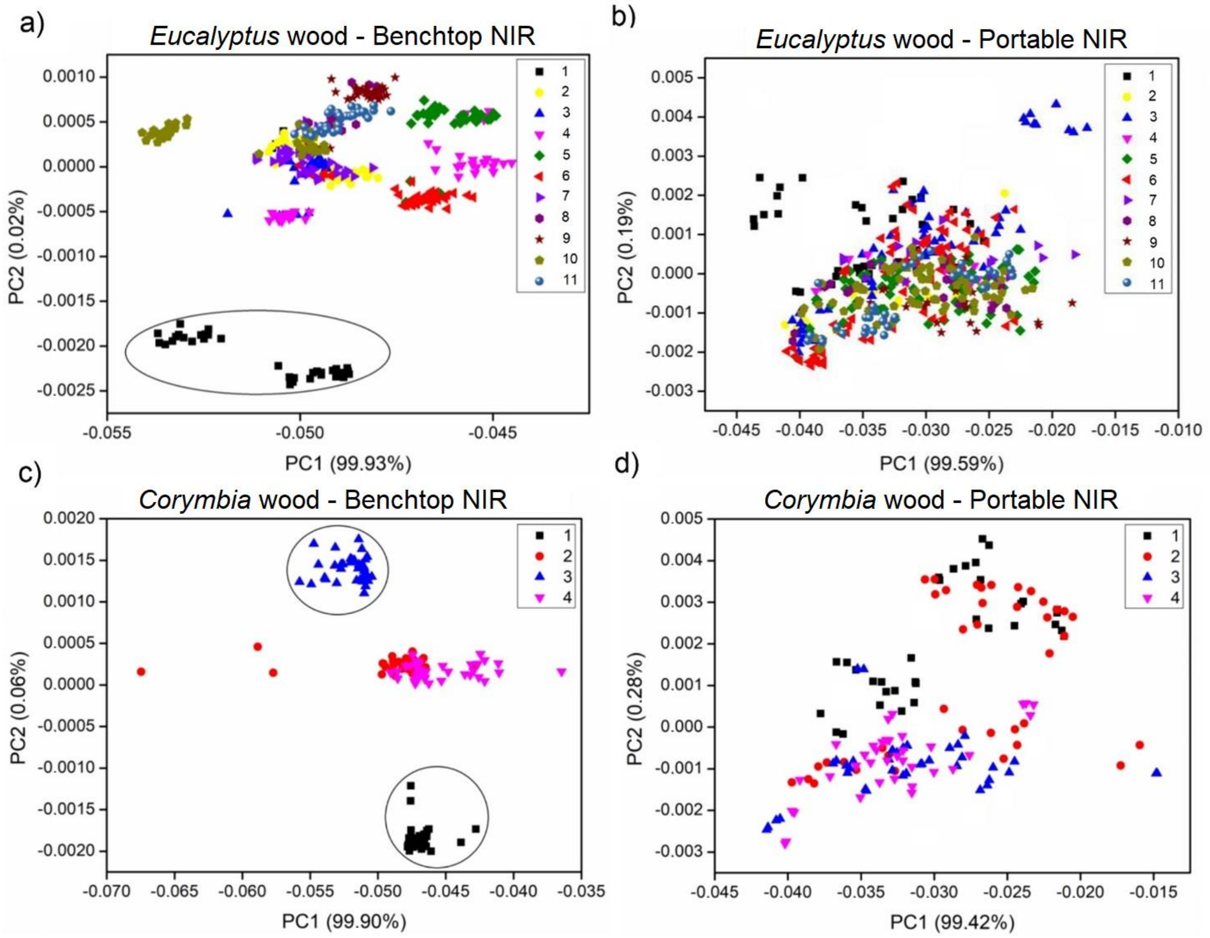

Figure 3 - Principal component analysis (PCA) of spectral data treated with 1st derivative obtained from *Eucalyptus* and *Corymbia* clones with benchtop (a and c) and portable (b and d) NIR instruments.

The spectra treated with the first derivative allowed linear combinations corresponding to the original variables of the wood samples from *Eucalyptus* and *Corymbia.* Thus, the sum of the principal components (PC1 + PC2) explained 99.95% and 99.78% of the variability of the raw spectral data of the wood from *Eucalyptus* clones with benchtop and portable NIR instruments, respectively, and 99.96% (benchtop NIR) and 99.70% (portable NIR) of the wood from *Corymbia* clones.

Although the tree's structural composition is heterogeneous, formed by several elements in different anatomical planes, the wood's chemical composition presents slight variation at the clone level for the same genus, as observed in the data in Table 1. This fact may explain the homogeneity of the spectra between the clones of each genus since the NIR spectra are closely associated with the vibrational patterns of the chemical groups present in wood composition (LOUREIRO *et al*., 2022).

Lima *et al*. (2022) evaluated residual wood from 12 Amazonian species by benchtop NIR spectroscopy and successfully distinguished species using PCA, demonstrating that differences in chemical composition between species are more evident when compared to the clone level. This result confirms that NIR spectroscopy is sensitive to the chemical composition of the wood and is also efficient in obtaining information through multivariate statistics.

Benchtop NIR showed a greater tendency to group clones than portable NIR due to the reduction in the spectral range of portable NIR compared to benchtop NIR, resulting in reduced information (Figure 2). The study by Vieira *et al*. (2019), when evaluating four native wood species using a benchtop NIR spectrometer, concluded that specific spectral ranges were significant for PC1. Similar results were found by Ramalho, Andrade and Hein (2018), who studied the discrimination of wood from native and planted forests using a benchtop spectrometer.

It is essential to highlight that the information that justified the absence of the formation of clone groups using PCA in this study was conclusive, specifically for the materials analyzed. This fact does not reduce the efficiency of the portable NIR instrument in distinguishing other organic materials.

3.3. Partial least squares regression (PLS-R)

Table 2 presents the statistics related to the PLS-R models used to estimate the chemical properties and basic wood density of *Eucalyptus* and *Corymbia* clones. Figs. 4 (*Eucalyptus* clones) and 5 (*Corymbia* clones) show the best cross-validation and independent models. The NIR spectra were subjected to various mathematical treatments (1st derivative, normalization and SNV) and the best models were selected, including those without spectra treatment.

Table 2 - Statistical parameters of the PLS-R models for predicting the chemical and physical properties of wood from *Eucalyptus* and *Corymbia* clones.

Genus	Parameter	Instrument	Treatament	R^2cv	RMSEcv	R^2p	RMSEp	RPD
				Cross-validation		Independent validation		
Eucalyptus	S/G	Benchtop	-	0.73	0.135	0.74	0.133	1.93
		Portable	-	0.60	0.137	0.58	0.141	1.58
	CRIST (%)	Benchtop	SNV	0.85	1.615	0.84	1.671	2.57
		Portable	SNV	0.75	2.031	0.77	2.033	2.03
	HOLO (%)	Benchtop	SNV	0.78	0.976	0.82	0.889	2.12
		Portable	SNV	0.80	0.881	0.80	0.892	2.23
	SL (%)	Benchtop	-	0.66	0.176	0.69	0.170	1.72
		Portable	-	0.65	0.138	0.65	0.140	1.69
	IL (%)	Benchtop	-	0.77	0.714	0.78	0.709	2.09
		Portable	-	0.69	0.607	0.72	0.586	1.81
	TL (%)	Benchtop	-	0.74	0.711	0.76	0.699	1.98
		Portable	-	0.71	0.574	0.74	0.545	1.86
	EXT (%)	Benchtop	-	0.85	0.679	0.86	0.655	2.55
		Portable	-	0.74	0.823	0.73	0.861	1.97
	BD (kg/m^3)	Benchtop	-	0.93	0.014	0.93	0.014	3.76
		Portable	-	0.76	0.021	0.75	0.024	1.93
Corymbia	S/G	Benchtop	-	0.94	0.067	0.96	0.057	4.28
		Portable	-	0.65	0.191	0.69	0.180	1.68
	CRIST (%)	Benchtop	SNV	0.87	0.779	0.91	0.674	2.82
		Portable	SNV	0.73	1.154	0.81	0.976	1.93
	HOLO (%)	Benchtop	SNV	0.93	0.484	0.93	0.485	3.71
		Portable	SNV	0.74	0.845	0.80	0.750	1.96
	SL (%)	Benchtop	-	0.85	0.103	0.82	0.114	2.63
		Portable	-	0.79	0.161	0.80	0.156	2.19
	IL (%)	Benchtop	-	0.91	0.391	0.90	0.418	3.39
		Portable	-	0.75	0.721	0.80	0.661	2.00
	TL (%)	Benchtop	-	0.88	0.437	0.87	0.466	2.94
		Portable	-	0.75	0.772	0.80	0.713	2.01
	EXT (%)	Benchtop	SNV	0.87	0.359	0.91	0.304	2.83
		Portable	SNV	0.76	0.614	0.73	0.651	2.06
	BD (kg/m^3)	Benchtop	SNV	0.91	0.006	0.94	0.005	3.28
		Portable	SNV	0.70	0.013	0.70	0.019	1.83

*SNV: Standard normal variation. R^2cv: Coefficient of determination for cross-validation. RMSEcv: Root mean square error for cross-validation. R^2p: Coefficient of determination for prediction. RMSEp: Root mean square error for prediction. RPD: Ratio performance to deviation. LV: Latent variables.

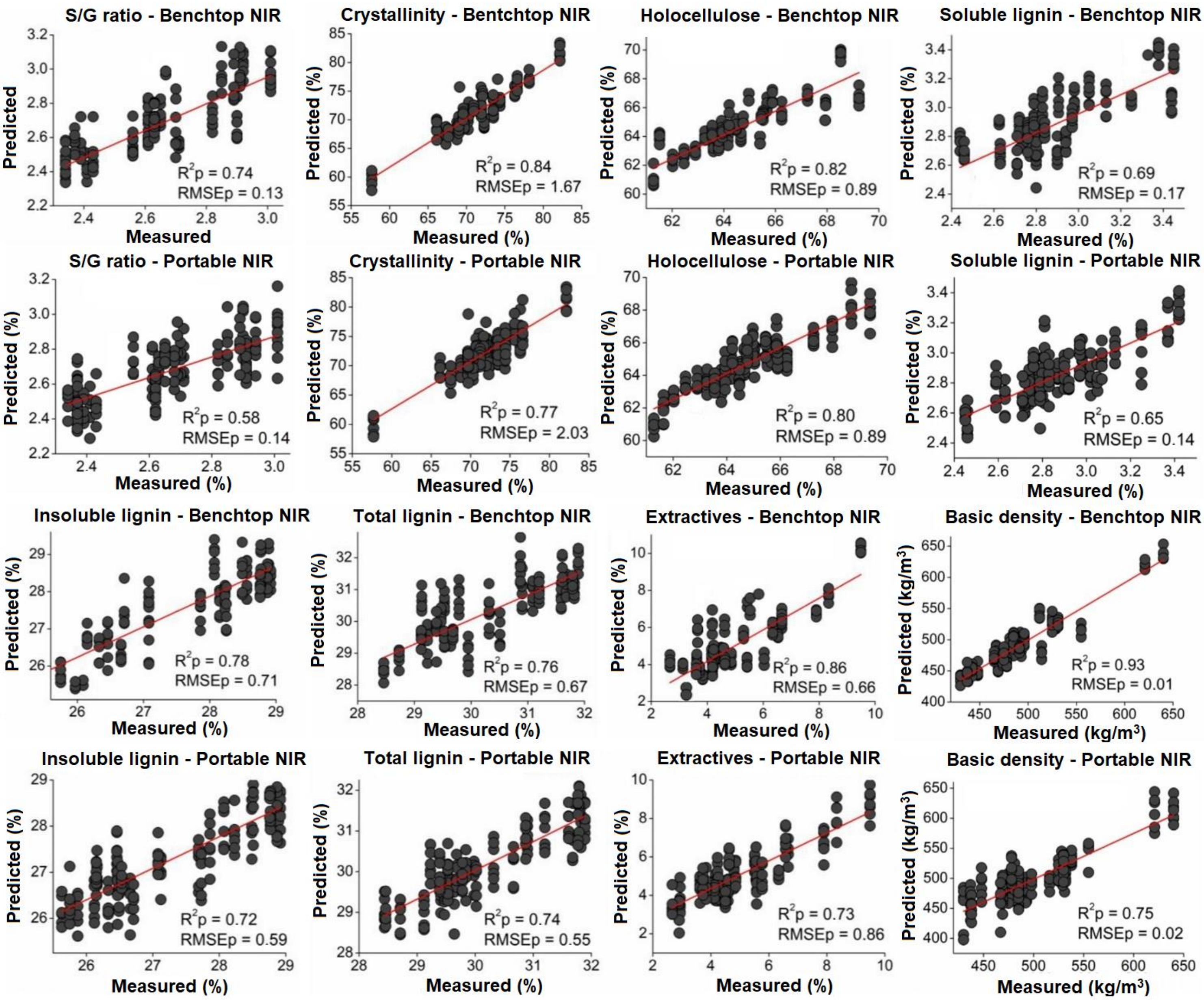

Figure 4 - Validations of PLS-R models for predicting wood properties of *Eucalyptus* clones with benchtop and portable NIR instruments.

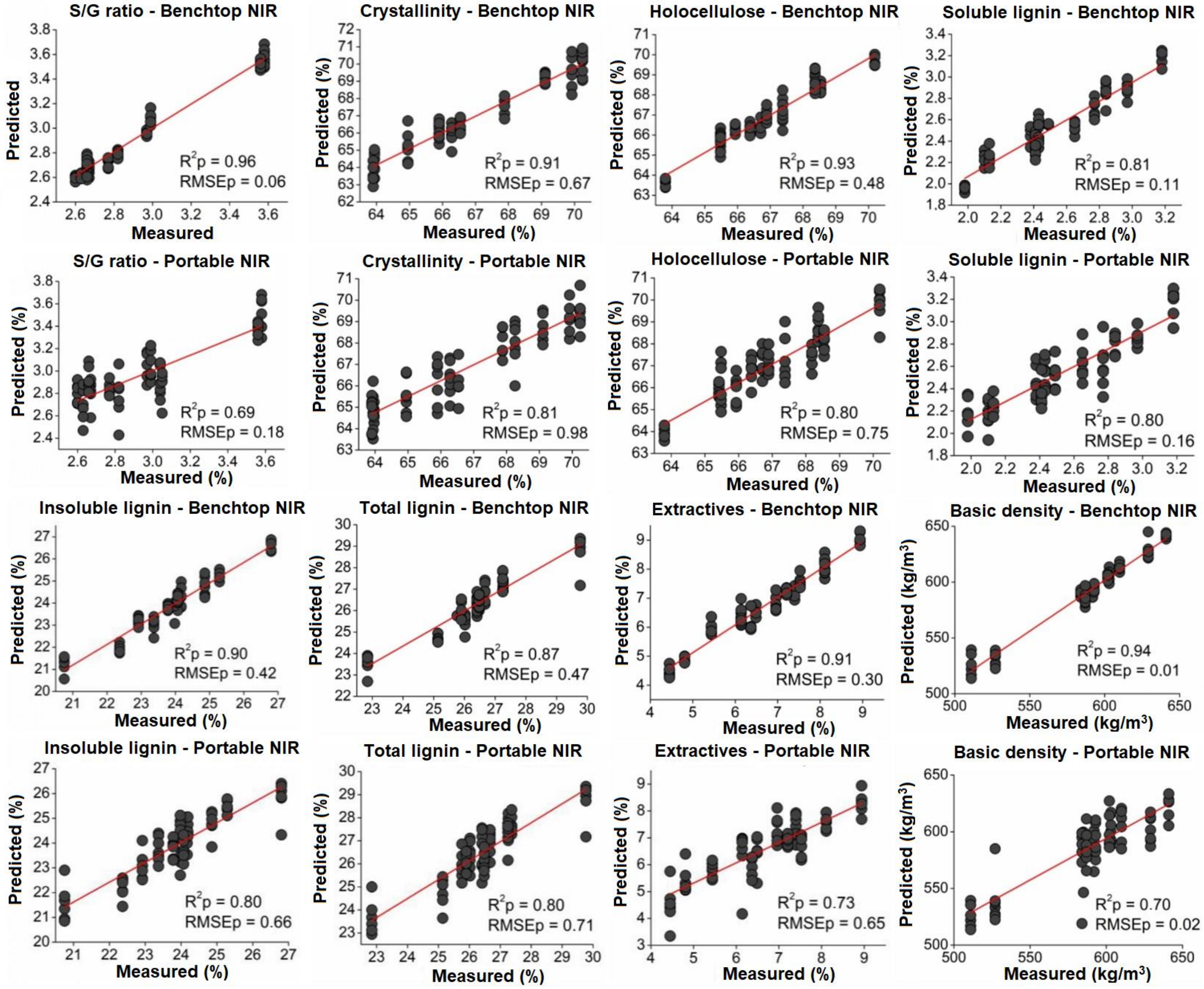

Figure 5 - Validations of PLS-R models for predicting wood properties of *Corymbia* clones with benchtop and portable NIR instruments.

Estimating the S/G ratio of lignin is a relevant parameter for charcoal production units, as it is directly associated with the gravimetric yield of the carbonization process. Protásio *et al*. (2021) reported that the lower the S/G ratio, the higher the gravimetric yield of charcoal after wood carbonization. As noted by Massuque *et al*. (2021), this trend can be attributed to the presence of an available aromatic position (C5) in the guaiacyl group, which facilitates the formation of carbon–carbon bonds during the lignin biosynthesis process. This leads to more condensed and thermally stable lignin structures. Consequently, the most accurate models for predicting the syringyl-to-guaiacyl (S/G) ratio of lignin achieved an R^2p of 0.74 and an RPD of 1.93 using benchtop NIR, and an R^2p of 0.58 and an RPD of 1.58 using portable NIR, for *Eucalyptus* wood samples with spectra preprocessed using SNV.

For *Corymbia* clones, the best models presented R^2p of 0.96 and RPD of 4.28 (benchtop NIR) and R^2p of 0.69 and RPD of 1.68 (portable NIR) with the spectra without mathematical treatment. The model for wood from *Corymbia* clones with bench NIR presented superior mathematical parameters in relation to the others, which indicates a good correlation between the genus and the variable of interest. In addition, the more significant amount of information provided by the wavelength of bench NIR was another factor that allowed the best fit of the model. However, the lower correlation of the other models corroborates the study by Miranda *et al*. (2024) when analyzing the phenotyping of wood from *Eucalyptus* and *Corymbia* clones using NIR spectroscopy. The authors found values of R^2cv of 0.66 and RPDcv of 1.70 for the S/G ratio for wood from *Eucalyptus* clones and R^2cv of 0.63 and RPDcv of 1.60 for wood from *Corymbia* clones.

Cellulose crystallinity is another important energy parameter since charcoal yield can be influenced by the crystallinity of wood cellulose. Studies have demonstrated that the amorphous regions of cellulose are more susceptible to thermal degradation and exhibit lower thermal stability compared to the crystalline regions (ISHIMARU *et al*., 2007; KIM; EOM; WADA, 2010). Consequently, a higher cellulose crystallinity index indicates a greater likelihood that a larger fraction of the cellulose will withstand thermal decomposition during the carbonization of wood.

The models with the most satisfactory results for this parameter presented R^2p of 0.84 and RPD of 2.57 (benchtop NIR) and R^2p of 0.77 and RPD of 2.03 (portable NIR) for wood from *Eucalyptus* clones with spectra treated with SNV. For *Corymbia* clone wood, the best models presented R^2p of 0.91 and RPD of 2.82 (benchtop NIR) and R^2p of 0.81 and RPD of 1.93 (portable NIR) with the spectra without mathematical treatment. Jiang *et al*. (2007), analyzing cellulose's crystallinity from *Pinus elliotti* wood, found R^2p of 0.86 and RMSEp of 3.90 with spectra treated with the 1st derivative.

It is important to emphasize that studies to estimate cellulose crystallinity are scarce. No studies were found in the literature on estimating this parameter for wood from *Corymbia* clones, highlighting the unprecedented nature of this information. Thus, it was found that the mathematical parameters of the models in this study to estimate cellulose crystallinity were considered promising for industrial use.

Woods with reduced holocellulose content are desirable for energy purposes since cellulose and hemicelluloses, when subjected to thermal degradation, present high instability and lower resistance, corroborating the high thermal degradation of these components during wood carbonization (SILVA; ATAÍDE, 2019; ZHAO *et al*., 2019). The results that stood out for the prediction of holocellulose content models presented R^2p of 0.82 and RPD of 2.12 (benchtop NIR) and R^2p of 0.80 and RPD of 2.23 (portable NIR) for wood from *Eucalyptus* clones with spectra treated with SNV.

For *Corymbia* clones, the best models presented R^2p of 0.93 and RPD of 3.71 (benchtop NIR) and R^2p of 0.80 and RPD of 1.96 (portable NIR) with the spectra treated with SNV. Similar results were reported in the study by Liang *et al*. (2020) analyzing the holocellulose content of *Acacia* and *Eucalyptus* woods for pulp production, finding R^2p values of 0.83 and RPD of 2.50 with the spectra treated with the 1st derivative.

The lignin content in wood is a key parameter in the selection of clones for bioenergy production, as it directly influences the gravimetric yield of charcoal. This is due to lignin's aromatic chemical structure and high molar mass, which confer greater thermal resistance compared to cellulose and hemicellulose molecules (SJÖSTRÖM 1992). Additionally, lignin contains between 61% and 67% carbon in its composition, thereby enhancing the calorific value of the resulting energy products (HATA *et al*., 2019). Accordingly, the predictive models that achieved the best performance for total lignin content yielded an R^2p of 0.76 and an RPD of 1.98 using benchtop NIR, and an R^2p of 0.74 and an RPD of 1.86 using portable NIR, based on spectra from *Eucalyptus* wood without mathematical preprocessing.

For *Corymbia* clones, the best models presented R^2p of 0.87 and RPD of 2.94 (benchtop NIR) and R^2p of 0.80 and RPD of 2.01 (portable NIR) with the spectra without mathematical treatment. Poke *et al*. (2006), analyzing the extractive, lignin and cellulose content of *Eucalyptus globulus* wood at 14 years of age, built a model to estimate the total lignin content with R2c 0.78 and RPD < 1.37. However, Tyson *et al*. (2009), using 45 trees of the *Eucalyptus* genus, found lower values for the total lignin content, with R^2cv of 0.64 and RPD of 1.19, which highlights the good mathematical parameters of the models developed in our study.

With regard to extractive content, wood with high levels of extractives—particularly phenolic compounds—is recommended for energy applications, provided that the components exhibit sufficient resistance to thermal degradation. These compounds can positively affect both the calorific value and the fixed carbon yield of charcoal due to their high carbon content (COUTO *et al*., 2023). Accordingly, the most accurate prediction models for extractive content achieved an R^2p of 0.86 and an RPD of 2.55 using benchtop NIR, and an R^2p of 0.73 and an RPD of 1.97 using portable NIR, based on spectra from *Eucalyptus* wood without mathematical preprocessing.

For *Corymbia* clone wood, the best models presented R^2p of 0.91 and RPD of 2.83 (benchtop NIR) and R^2p of 0.72 and RPD of 2.06 (portable NIR) with the spectra treated with SNV. Mancini *et al*. (2021) studied the extractive content of native and planted woods using NIR spectroscopy and found R^2p of 0.87 and RPD of 2.12 for powdered wood with equilibrium moisture content. Miranda et al. (2024), in turn, found lower values for this parameter, with R^2cv values of 0.65 and RPDcv of 1.70 for *Eucalyptus* clone wood and R^2cv of 0.37 and RPD of 1.20 for *Corymbia* clone wood. The models developed to estimate *Eucalyptus* and *Corymbia* clone wood extractive content using benchtop NIR presented superior mathematical parameters compared to the models that used portable NIR. This fact can be justified again by the longer wavelength provided by benchtop NIR, which encompasses the vibrational energy related to the extractive molecules, as demonstrated in Figures 2a and 2c.

Wood with higher basic density is advantageous for the steel sector, as it increases charcoal productivity by allowing a greater amount of wood material to be loaded into carbonization furnaces (MASSUQUE *et al*., 2023). Therefore, the predictive models that provided the most favorable results for basic density achieved an R^2p of 0.93 and an RPD of 3.76 with benchtop NIR, and an R^2p of 0.75 and an RPD of 1.93 with portable NIR, using spectra from *Eucalyptus* clones without mathematical preprocessing.

For wood from *Corymbia* clones, the best models presented R^2p of 0.94 and RPD of 3.28 (bench NIR) and R^2p of 0.70 and RPD of 1.83 (portable NIR) with spectra treated with SNV. Costa *et al*. (2018) employed PLS-R models to estimate the density of *Eucalyptus* sp. wood based on NIR spectra from the transverse surface machined by a band saw. They found an R^2p of 0.87 and an RPD of 3.0 using an integrating sphere, and an R^2p of 0.78 and an RPD of 2.10 using optical fiber for spectra collection. Similarly, Medeiros *et al*. (2024), investigating the basic density of *Eucalyptus* grandis wood chips at different moisture levels, reported an R^2cv of 0.82 and an RMSEcv of 0.038 using benchtop NIR, and an R^2cv of 0.82 and an RMSEcv of 0.038 using portable NIR, both on the radial surface with spectra unprocessed.

The models obtained via PLS-R for wood from *Eucalyptus* and *Corymbia* clones showed promising results. Nevertheless, it was observed that the mathematical parameters resulting from the models that used wood from *Corymbia* clones were superior to those from *Eucalyptus* clones in almost all variables analyzed, regardless of whether the NIR instrument was benchtop or portable. This fact may be associated with the spectral behavior of both genera. The spectral range covers the interval between 8750 and 8540 cm^{-1}, with the vibrational energy of the aromatic groups of lignin (SCHWANNINGER; RODRIGUES; FACKLER, 2011) and the spectral range between 7000 and 6287 cm^{-1}, with the vibrational energy of the amorphous and crystalline regions of cellulose (NISGOSKI *et al*., 2016) stood out in the spectral signatures, both in the wood from *Eucalyptus* and *Corymbia* clones. However, Figure 2 revealed that for the genus *Corymbia*, these spectral peaks were even more pronounced at the wavelength encompassing both benchtop and portable NIR.

Furthermore, the data in Table 1 showed that wood from *Corymbia* clones had higher density values than wood from *Eucalyptus* clones. The greater the amount of mass in the same volume, the greater the amount of structural components of the cell wall (MASSUQUE *et al*., 2023). Thus, more cell wall components became susceptible to changes, such as forming more hydrogen bonds due to the greater amount of free hydroxyls available. Wang *et al*. (2022) states that NIR spectroscopy is very sensitive in identifying water molecules, which can influence the obtaining of models with better mathematical parameters.

Regarding the portable NIR instrument, the models showed a reduction in mathematical parameters in certain correlation adjustments compared to the results found by the benchtop NIR. According to Medeiros *et al*. (2024), the spectral reading area may have influenced the reduced performance of the models, as benchtop instruments collect spectra using an integrating sphere with an approximate diameter of 10 mm. In contrast, through the optical reading system, the portable NIR has a punctual collection area with less surface representation. In addition, the smaller spectral range and, consequently, the reduction in the vibrational energy of the chemical components of the wood and the decrease in the range of the emitted light may be other factors that influenced the reduction in mathematical parameters. Despite this, the models of this instrument showed good performance and could be used by bioenergy-producing industries. It is worth mentioning that this study has limitations regarding the environmental conditions in which it was carried out.

The samples evaluated were controlled at the laboratory level, presenting significant differences in wood storage yards, where the raw material is exposed to adverse weather conditions and the action of xylophagous agents. Therefore, further studies are needed to consider these sources of variation to better understand the influence of these factors in predicting the chemical and physical properties of wood. Considering that the chemical and physical properties vary between clones and between different longitudinal positions of the tree, the plantation management itself, such as silvicultural treatments, nutritional parameters and water availability, may result in different spectral responses that can influence the parameters of the predictive models using NIR spectroscopy.

3.4. Implications and limitations of the study

This study demonstrates the potential of portable NIR instruments to predict wood quality for energy purposes, especially in clones of *Corymbia* and *Eucalyptus*. Spectral acquisition was performed using wood powder under controlled conditions, which standardized the samples but does not fully reproduce field variables such as temperature and humidity. The number of trees sampled was limited, and the focus was on the DBH region, although wood properties can vary along the stem. Future studies should evaluate the effects of real field conditions and include more trees and additional stem positions. Despite these limitations, the results provide an initial reference for the development of broader predictive models.

4. CONCLUSIONS

NIR spectroscopy, associated with multivariate statistics, was able to predict the chemical properties and basic density of wood from *Eucalyptus* and *Corymbia* clones and may be useful in the selection of superior clones in genetic improvement programs and, consequently, optimizing the process since the time and cost of evaluations are reduced.

Principal component analysis (PCA) of the spectra discriminated >99.0% of the data variation for both instruments. However, using the benchtop NIR, it was possible to group only 1 clone of *Eucalyptus* wood and 2 clones of *Corymbia* wood. No clone was correctly grouped within each genus with the portable NIR spectra.

According to the predetermined parameters to evaluate the reliability of the models, it was observed that the models, both benchtop NIR and portable NIR, presented good predictive capacity, with the best model reaching R^2p of 0.96. Although portable NIR presents a reduction in mathematical parameters compared to benchtop NIR, the results found were considered promising. Portable NIR presents a lower cost and simplified operation compared to benchtop NIR, which can be a differentiator in the choice of the instrument.

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CHAPTER 3

PREDICTION OF THE ENERGY PROPERTIES OF CHARCOAL OBTAINED FROM *Eucalyptus* AND *Corymbia* BIOMASS USING PORTABLE AND BENCHTOP NIR SPECTROMETERS

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ABSTRACT

Monitoring charcoal quality is essential for the industry. Near-infrared (NIR) spectroscopy enables fast and accurate predictions of key properties. This study evaluated the use of benchtop and portable NIR sensors to predict charcoal characteristics from woody biomass of 15 commercial clones (11 *Eucalyptus* and 4 *Corymbia*). Two trees per clone were sampled at six stem positions, generating 30 composite wood samples. After carbonization and grinding, spectral data were collected, totaling 600 spectra per sensor. Partial least squares regression was used to develop models for gravimetric yield (GY), apparent relative density (ARD), fines content (FC), volatile matter content (VMC), ash content (AC), and fixed carbon content (FCC). For *Eucalyptus* clones, the benchtop sensor outperformed the portable one for GY (R^2p = 0.74; RPD = 2.02), ARD (R^2p = 0.87; RPD = 2.82), VMC (R^2p = 0.72; RPD = 1.92), AC (R^2p = 0.72; RPD = 1.92), and FCC (R^2p = 0.63; RPD = 1.64). The portable sensor was better only for FC (R^2p = 0.64; RPD = 1.60). Similarly, for *Corymbia* clones, the benchtop sensor performed better for GY (R^2p = 0.79; RPD = 2.15), ARD (R^2p = 0.87; RPD = 2.77), FC (R^2p = 0.69; RPD = 1.73), and AC (R^2p = 0.61; RPD = 1.62). The portable sensor showed better results for FCC (R^2p = 0.61; RPD = 1.48) and VMC (R^2p = 0.64; RPD = 1.40). Overall, benchtop and portable NIR spectrometers showed similar performance in estimating charcoal parameters.

Keywords: Bioenergy. Forest biomass. Immediate Chemical analysis Multivariate statistics. Wood pyrolysis.

1. INTRODUCTION

Brazil stands out on the world stage for being the largest producer and consumer of charcoal. According to the IBÁ report (IBÁ, 2025), Brazilian production was 6.6 million tons in 2024, almost entirely destined to supply the domestic market, emphasizing the steel and iron and steel sectors. The report also points out that of this total, 1.12 million hectares of planted forests were destined for the production of charcoal, mainly with the use of clones of the *Eucalyptus* genus (IBÁ, 2025; PROTÁSIO *et al*., 2021; TEIXEIRA *et al*., 2024), in addition to the use of clones of the *Corymbia* genus (LOUREIRO *et al*., 2019; MASSUQUE *et al*., 2023), indicating advances in clonal silviculture practiced by forestry companies and a reduction in the use of native woods from deforestation.

As it is a versatile energy material, charcoal offers various applications. In the steel industry, it is used as a source of energy and a bioreducing agent, in addition to supporting a load of iron ore (COSTA; TRUGILHO; HEIN, 2018). This material, in turn, is used as a raw material for pig iron production, and its destination is steel production (ABREU NETO *et al*., 2020). Therefore, charcoal improves the quality of pig iron and steel due to the absence of sulfur and lower ash content when compared to coal, making the process environmentally cleaner (LIMA *et al*., 2020).

To increase the quality of charcoal, carbonization plants use the strategy of selecting wood with desirable characteristics for energy purposes and controlling the pyrolysis process to improve gravimetric yield and conversion efficiency (TAZEBEW *et al*., 2024). Therefore, at the end of the wood carbonization process, it is necessary to monitor charcoal's chemical, physical, and energetic characteristics, such as apparent relative density and immediate chemistry, since homogeneous materials are desirable to maintain the quality of products from the steel sector.

Variables such as gravimetric yield, apparent relative density, fines content, volatile matter content, ash content, and fixed carbon content are indicators of charcoal quality, depending on the parameters of the carbonization process and the classification of the raw material (ASSIS *et al*., 2015; PROTÁSIO *et al*., 2021). In other words, this information makes it possible to optimize final carbonization temperatures (COSTA; TRUGILHO; HEIN, 2018), furnace loading adjustments to improve carbonization efficiency (LIMA *et al*., 2020), the particle size of the biomass used for charcoal production (SOMERVILLE; DEEV, 2020), and heating rates (LIANGMENG *et* *al*., 2022). However, the production dynamics of charcoal in industrial settings are highly intense and often demand speed and accuracy in the results. This, in turn, is not always achievable through laboratory procedures which, although precise, are time-consuming, costly, and require high implementation and maintenance investments.

A possible alternative to optimize the charcoal characterization process is the NIR technique, which is fast and reliable (LI *et al*., 2020; WANG *et al*., 2022). In the forestry sector, several studies have shown that this technique can contribute to the monitoring and classifying of raw lignocellulosic material and can also help characterize its products, such as charcoal (MUNIZ *et al*., 2013; REIS *et al*., 2019).

For example, Ramalho *et al*. (2017) developed predictive models to classify charcoal produced from native and planted wood and analyze the influence of the final carbonization temperature on the differentiation. The researchers' results were satisfactory, so the percentage of correct classifications ranged from 66 to 100%. Abreu Neto *et al*. (2021) applied NIR spectroscopy to estimate the mechanical properties of charcoal. The authors found suitable parameters for the model to estimate the friability of charcoal, with R^2c of 0.91 for dynamic hardness with a final carbonization temperature of 750°C. Therefore, the studies reported in the literature addressing the use of NIR spectroscopy in charcoal used the benchtop instrument.

As observed, although scarce, the available studies in literature using NIR spectroscopy on charcoal have provided relevant information regarding the quantitative and qualitative analyses of this material. However, these studies were conducted using benchtop equipment and, as far as we know, no studies have been carried out on the characterization and classification of charcoal from different sources using portable NIR spectrometers. This represents a gap in scientific knowledge, given that benchtop instruments are calibrated and developed to provide higher resolution and more detailed spectral information, which makes them more expensive. In addition, benchtop devices are more sensitive and require specific operating conditions, which may hinder their use in the field, unlike portable NIR devices (RAMALHO *et al*., 2019; MEDEIROS *et al*., 2025), which can make the charcoal characterization process more dynamic, optimizing decision-making in the control of the production process.

The portable NIR instrument thus presents itself as a promising alternative, as it offers, in addition to the functionalities provided by benchtop equipment, advantages such as reduced size, lower commercial cost, and the ability to evaluate the desired parameter at the point of use (SCHIMLECK *et al*., 2018; TOSCANO *et al*., 2022; ZHANG *et al*., 2025). Despite the narrower spectral range of the portable NIR instrument (11.000–6.000 cm^{-1}) compared to most benchtop instruments (12.500–3.500 cm^{-1}), the spectra resulting from the interaction between the emitted light beam and the analyzed material provide the necessary information to enable the construction of multivariate statistical models (SANTOS *et al*., 2013; ZHU *et al*., 2022).

Therefore, this study proposes, as an innovative approach to address scientific gaps, the analysis of *Eucalyptus* and *Corymbia* charcoal parameters using portable NIR spectroscopy to assess charcoal quality. Furthermore, no studies were found that independently use portable NIR spectrometers for the characterization of charcoal derived from *Corymbia* clones. Thus, the hypotheses of this work are: (i) portable NIR spectrometers provide accuracy comparable to benchtop instruments in evaluating charcoal properties; and (ii) both portable and benchtop instruments can accurately estimate the chemical, physical, and energetic properties of charcoal produced from *Eucalyptus* and *Corymbia* clones.

In this context, this study aimed to predict the gravimetric yield, apparent density, fines content, and immediate chemical composition of *Eucalyptus* and *Corymbia* charcoal using benchtop and portable NIR spectrometers. Once the predictive potential of these instruments for such parameters is confirmed, their use could be recommended to the charcoal production industry for quality control of the manufactured material.

2. MATERIAL AND METHODS

2.1. Obtainment and preparation of vegetal material

Fifteen commercial clones (11 from the genus *Eucalyptus* and 4 from the genus *Corymbia*) were collected, planted at a spacing of 3 x 3 meters and 84 months of age, from plantations located in the city of Itamarandiba, Minas Gerais (latitude 17º 44’ 45” S; longitude 42º 45’ 11” W; and altitude 1000 m). Then, the stems of each sampling unit were sectioned to obtain discs in six different longitudinal positions (0, DBH, 25, 50, 75, and 100%), obtaining a composite sample for each clone. Posteriorly, the material was sent for qualitative analyses and carbonization.

2.2. Wood basic density

Samples were collected at 1.30 m above ground level (DBH) , and the resulting average of the basic density of two opposite wedges passing through the disc pith with a thickness of 2.5 cm was calculated, following the ABNT NBR 11941 standard (ABNT, 2003).

2.3. Wood carbonization

After obtaining samples from each clone, the wood was sectioned and dried in an oven at 103 ± 2°C for 72 h until constant mass. Carbonization was performed in an electric muffle furnace, with approximately 400 g of wood in each cycle, and the sample from each clone was carbonized individually.

The wood samples were inserted into a metal container with nominal dimensions of 0.3 m in length, 0.12 m in diameter, and a volume of 0.003 m³, and the container was subsequently fixed to the muffle. The heating system was manually controlled, with an average heating rate of 4.17°C/min, as shown in Table 1 (COSTA *et al*., 2024). The initial and final temperatures were set at 150 and 450°C, respectively, remaining stabilized at the latter for 60 min, totaling 4 h and 30 min of carbonization. Subsequently, the samples were cooled by natural convection for 16 h.

Table 1 - Heating rate used in the carbonization of genotypes of *Eucalyptus* and *Corymbia.*

Steps	Temperature (ºC)	Heating rate (ºC/min)
1	150	-
2	200	3.33
3	250	4.17
4	350	3.89
5	400	4.44
6	450	5.00

After each carbonization cycle, the gravimetric yield of charcoal was determined by the ratio between the mass of dry charcoal produced and the mass of dry wood, as shown by Equation 1:

$$GYC = \frac{mdc}{mdw} x\ 100 \qquad Eq. (1)$$

Where *GYC* is the gravimetric yield of charcoal (%), *mdc* is the mass of dry charcoal (kg), and *mdw* is the mass of dry wood (kg).

2.4. Characteristics of charcoal

The preparation of the samples to determine the immediate chemical composition (volatile materials content, ash, and fixed carbon) and the collection of the spectra were similar. The samples were crushed manually and then classified with 0.42 mm and 0.25 mm sieves. The material analyzed was retained on the sieve with 0.25 mm (ASTM, 1982). The immediate chemical composition of the charcoal was determined according to the ABNT NBR 8112 standard (ASTM, 1986). To determine the volatile material content of the charcoal, the samples were deposited in covered porcelain crucibles and subjected to a muffle furnace stabilized at 950°C, with 2 and 3 min of acclimatization at the entrance and edge of the muffle, respectively, and 6 min inside the muffle, totaling 11 min of exposure.

The ash content was obtained after the complete combustion of the charcoal after the material was exposed to a temperature of 600°C for 6 h. The fixed carbon content was obtained by difference, subtracting the volatile material and ash contents from 100. The apparent relative density of charcoal was determined by the hydrostatic method, in which the samples were immersed in mercury, as reported by Vital (1984). The test was performed on charcoal samples with 5% moisture, with seven replicates for each carbonization, so that the average apparent relative density was obtained by the arithmetic average.

The determination of friability was performed with approximately 20 g of charcoal samples, which were subjected to a friabilometer for 14 min at a speed of 35.5 RPM, following the protocol established by the Technological Center of Minas Gerais (CETEC), as mentioned by Oliveira *et al*. (1982). Subsequently, the charcoal was sieved through 9.5 mm, and the mass loss was calculated.

2.5. Description of the chemical, physical and energetic properties of charcoal

The charcoal from *Eucalyptus* and *Corymbia* clones were subjected to physical and energy laboratory analyses following the standards and methodologies presented and the results obtained can be seen in Table 2.

Table 2 - Chemical, physical and energetic characteristics of charcoal from clones of *Eucalyptus* and *Corymbia.*

*CL	GY (%)	ARD (kg/m^3)	FC (%)	VMC (%, bs)	AC (%, db)	FCC (%, db)
C1	33.37 ± 0.79	408.96 ± 8.31	5.60 ± 1.10	22.81 ± 0.15	1.33 ± 0.05	75.86 ± 0.11
C2	36.17 ± 0.39	424.07 ± 4.59	8.57 ± 0.40	23.90 ± 0.23	0.51 ± 0.09	75.60 ± 0.28
C3	34.56 ± 0.15	386.61 ± 4.69	7.92 ± 0.53	21.86 ± 0.87	1.54 ± 0.17	76.60 ± 0.71
C4	33.68 ± 0.30	455.59 ± 14.11	7.55 ± 0.63	22.38 ± 1.69	1.29 ± 0.02	76.34 ± 1.71
E1	33.40 ± 0.94	362.61 ± 4.55	7.57 ± 0.41	21.99 ± 0.83	1.52 ± 0.11	76.49 ± 0.94
E2	34.33 ± 1.43	408.49 ± 13.19	8.80 ± 0.56	21.97 ± 1.56	0.72 ± 0.13	77.32 ± 1.43
E3	33.84 ± 0.92	301.22 ± 13.50	12.54 ± 0.91	23.96 ± 0.93	0.61 ± 0.02	75.43 ± 0.92
E4	35.12 ± 0.19	287.77 ± 10.11	9.90 ± 1.41	24.37 ± 1.42	0.77 ± 0.33	74.86 ± 1.09
E5	34.88 ± 0.52	332.54 ± 3.13	7.77 ± 0.38	23.16 ± 0.58	0.61 ± 0.16	76.23 ± 0.52
E6	35.07 ± 0.02	345.62 ± 47.92	8.85 ± 0.34	22.79 ± 0.61	0.91 ± 0.06	76.29 ± 0.57
E7	34.34 ± 0.03	222.59 ± 6.11	6.51 ± 1.16	23.70 ± 0.28	0.62 ± 0.06	75.68 ± 0.35
E8	34.64 ± 1.13	339.76 ± 11.86	6.79 ± 1.28	22.57 ± 0.22	0.87 ± 0.28	76.57 ± 0.32
E9	35.06 ± 0.45	312.95 ± 2.84	8.40 ± 0.56	21.33 ± 0.43	1.01 ± 0.04	77.66 ± 0.44
E10	34.97 ± 0.05	362.71 ± 7.87	8.21 ± 0.80	23.16 ± 1.24	0.71 ± 0.14	76.13 ± 1.37
E11	34.74 ± 0.42	288.64 ± 34.72	7.98 ± 0.93	24.54 ± 0.42	0.85 ± 0.06	74.61 ± 0.43

*CL = Clone; C = *Corymbia*; E = *Eucalyptus*; GY = Gravimetric yield; ARD= Apparent relative density; FC = Fines content; VMC = Volatile material content; AC = Ash content; FCC = Fixed carbon content.

2.6. Sample preparation for spectra collection

Ground charcoal samples for each clone (positions 0, DBH, 25, 50, 75, and 100%) were classified using 0.42 mm and 0.25 mm sieves, using the material retained on the 0.25 mm. Afterward, the samples were kept in a room with a temperature of 20°C and relative humidity of around 65% until they reached an equilibrium moisture of approximately 6% (dry basis).

After adequate sample conditioning, spectral analyses were performed using benchtop and portable NIR spectrometers. In the benchtop equipment, measurements were performed with samples deposited in specific cuvettes compatible with the spectrometer sensor. In the portable equipment, acquisitions were made directly on the material deposited in translucent containers (Petri dishes).

2.7. Spectra acquisition

The spectra in the NIR region were obtained with a portable and benchtop instrument, according to the procedures described by Medeiros *et al*. (2025). The benchtop instrument used for the analysis was a Fourier transform NIR spectrometer, model MPA, manufactured by Bruker Optik GmbH (Ettlingen, Germany), operating with the OPUS software version 7.0. The spectra were obtained through diffuse reflection in the integration sphere (12.500-3.500 cm^{-1}), with a resolution of 8 cm^{-1}, resulting in 1.300 spectral variables. Sixteen scans were performed for each spectrum collected, and the averages of these scans were calculated and compared with the standard to generate the specimen's absorption spectrum. Background compensation was performed every 10 min during the spectral acquisition, and the light emission from the MPA window was shielded. The 9.000-4.000 cm^{-1} spectral range was used for the calculations after applying a band selection method to eliminate possible noise.

The portable instrument used was the MicroNIR On-site (Viavi Solutions Inc., CA, United States), connected to a computer to store the spectral data collected in the Spectral Solutions program (Viavi Solutions Inc., CA, USA). The acquisition range was 11.000-6.000 cm^{-1} with a resolution of 5.6 nm and 125 spectral variables. Each spectra results from an average of 16 scans in diffuse reflectance mode. Twenty readings were performed per sample so that the sample was homogenized in the interval between each reading, totaling 600 spectra. The NIR spectral signatures were associated with the laboratory analysis data, and multivariate models were developed.

2.8. Multivariate data analysis

Principal component analysis (PCA) and partial least squares regression (PLS-R) were fitted based on NIR spectra (Figure 1).

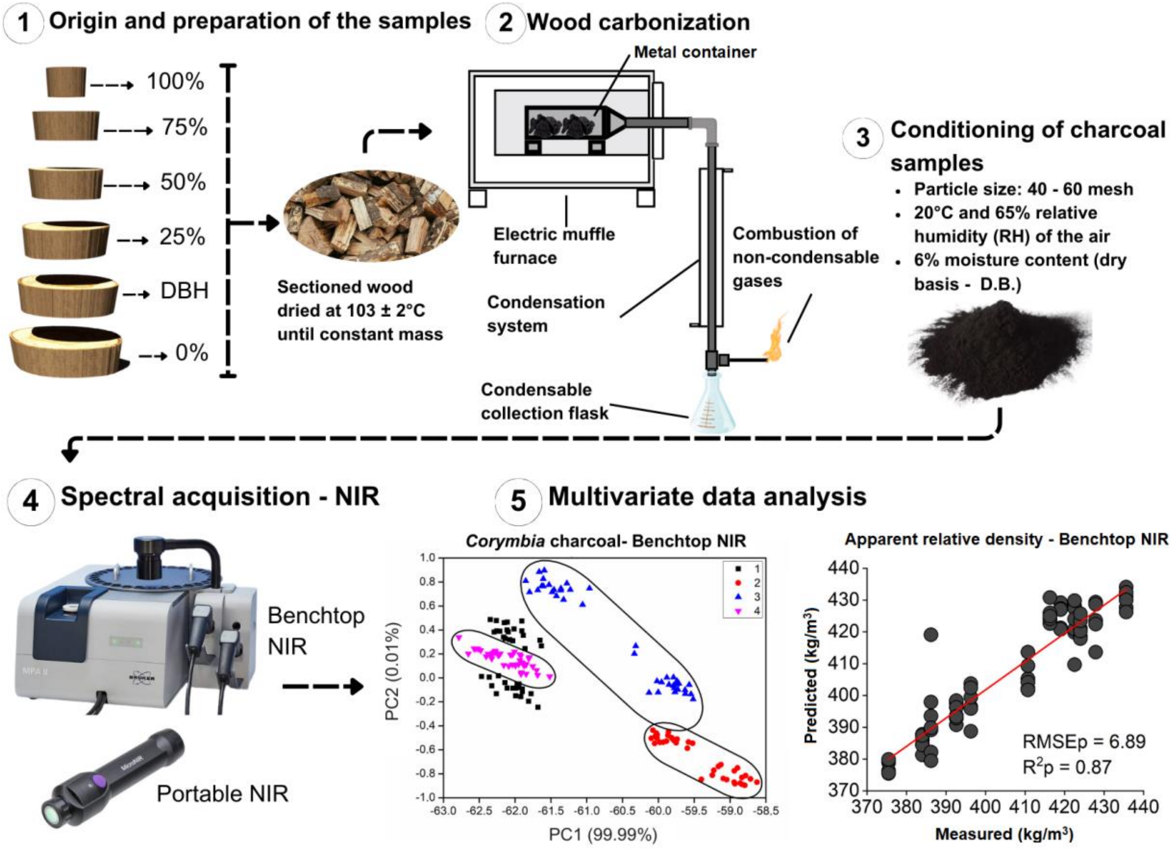

Figure 1 – Experimental scheme for data collection and processing using NIR spectroscopy.

Chemoface software version 1.63 was used for multivariate data analysis. PCA was applied to evaluate the clustering of charcoal data from *Eucalyptus* and *Corymbia* clones within each genus.

The PLS-R models were adjusted using wood spectra to predict gravimetric yield, apparent relative density, fines content, volatile matter content, ash content, and fixed carbon content. Cross-validation and independent validation (through a set of tests) were used to validate the models. The number of latent variables was defined based on minimizing the standard error and maximizing the coefficient of determination of the validation, resulting in the selection of 8 to 11 latent variables in the adjusted models. The leave-one-out method was applied for cross-validation. The data set was divided into calibration and validation sets for independent validations, using 66.6% of the data for model calibration and the remaining 33.3% for validation, according to the data selection process proposed by Medeiros *et al*. (2025).

The original spectra and those mathematically treated with first derivative (13-point filter and second-order polynomial), normalization, and standard normal variation (SNV) were used to improve the mathematical parameters of the models. The statistical parameters used to select the best prediction models were the calibration coefficient of determination (R^2c), mean square error of calibration (RMSEC), cross-validation coefficient of determination (R^2cv), root mean square error of cross-validation (RMSEcv), cross-validation deviation performance ratio (RPDcv), root mean square error of prediction (RMSEp) and prediction deviation performance ratio (RPD).

3. RESULTS AND DISCUSSION

3.1. NIR spectral signatures

Figure 2 shows the original and first derivative (1d) treated average spectral signatures for the charcoal dataset of *Eucalyptus* and *Corymbia* clones. The spectra were treated with the first derivative (Fig. 2c and 2d) for better visualization and identification of the spectral peaks. Thus, similarity was observed between the spectral behavior of the two genus, so the differences found correspond to the intensity of the peaks.

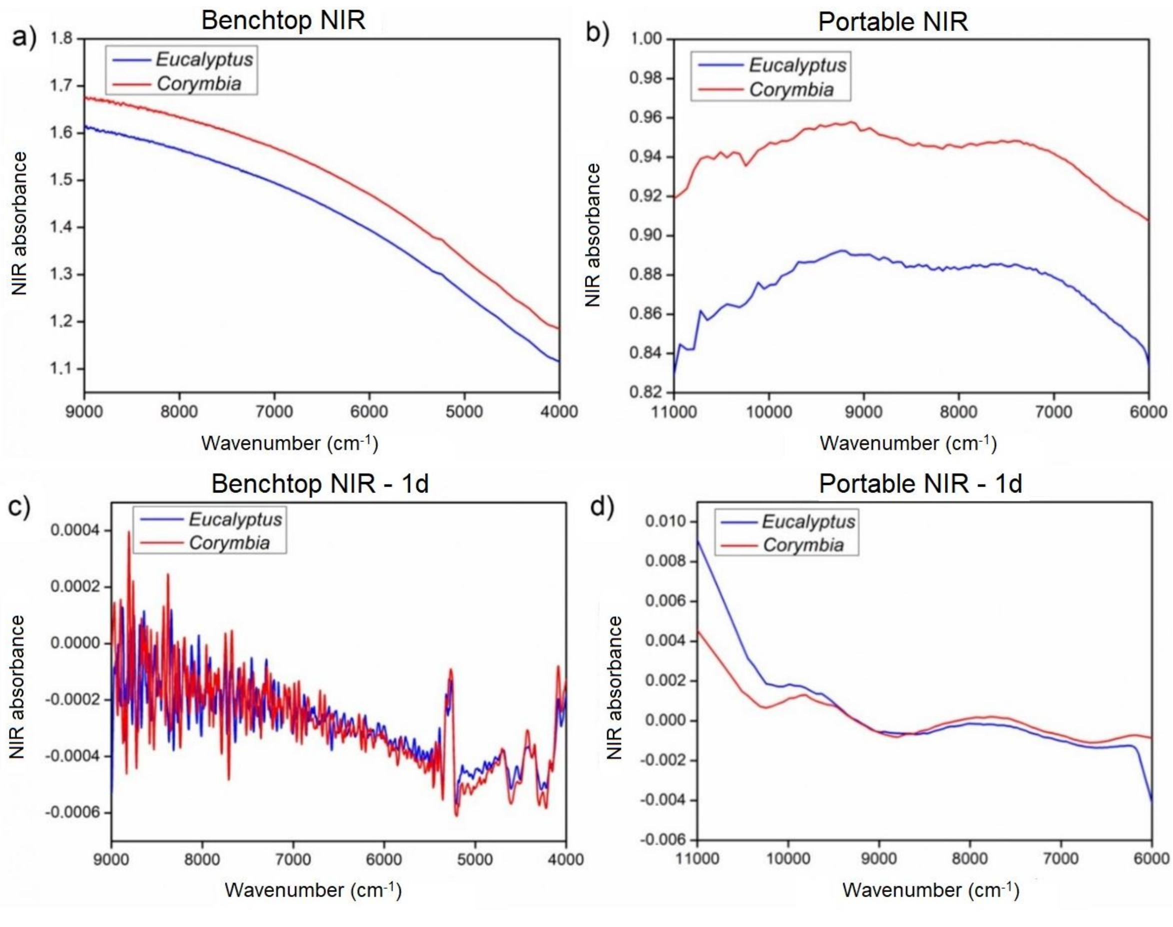

Figure 2 - Average spectral signatures of *Eucalyptus* and *Corymbia* charcoal obtained with benchtop (a - untreated spectra; c - treated with 1st derivative) and portable (b - untreated spectra; d - treated with 1st derivative) NIR instruments.

Absorption bands are more intense at specific wavenumbers (COSTA; TRUGILHO; HEIN, 2018). These wavenumbers vary according to the chemical components present in the material, whether wood or charcoal. In this study, it was possible to observe that charcoal provided lower NIR absorbance intensity, resulting in greater homogeneity of the spectra and reduction of informative peaks. Similar results were found in the study by Abreu Neto *et al*. (2021) when analyzing the spectral behavior of *Eucalyptus* charcoal using a final carbonization temperature of 450°C.

After the wood pyrolysis stage, a significant fraction of the structural components are thermally degraded, resulting in more homogeneous charcoal with a higher concentration of carbon in its composition. The study by Ramalho *et al*. (2017) demonstrated that the final carbonization temperature directly influences the spectral behavior of charcoal since the higher the final carbonization temperature, the smaller the absorption bands in the NIR. This fact can be associated with the thermochemical conversion of the main components of wood (cellulose, hemicelluloses, lignin, and extractives), which occurs in different temperature ranges (ZHANG; ZHANG, 2019; WANG; WU, 2023). The final carbonization temperature adopted in this study was 450°C, resulting in the thermal degradation of a large part of the carbohydrates in the wood.

Figures 2a and 2c correspond to the benchtop NIR spectra (untreated and treated with 1st derivative, respectively). The spectra in Figure 2a showed homogeneous behavior, so that it was not possible to identify peaks related to the organic chemical components of charcoal. However, after treating the spectra with the first derivative (Figure 2c), it was possible to observe peaks between 7.200 cm^{-1} and 5.300 cm^{-1} more clearly, which can be associated with the vibrational energy of OH stretching (WORKMAN; WEYER, 2007). The peak around 9.800 cm^{-1}, evidenced by Figures 2b and 2d (portable NIR spectra), can be related to the second overtone of vibrations of C-H and N-H bonds (SANTOS *et al*., 2021).

Despite the greater homogeneity of the spectral signatures of charcoal of both types, it was possible to observe that the absorbance bands presented interaction in certain absorption bands. Furthermore, although the spectral range of the benchtop and portable NIR presented different intervals, it was possible to identify characteristic peaks of organic chemical constituents in both instruments, which allowed the exploration of various information through appropriate multivariate statistical analyses.

3.2. Principal component analysis (PCA)

The results indicated variations among charcoals from clones of the same genus since many samples did not overlap (Figure 3). The benchtop NIR instrument was able to group 1 charcoal from *Eucalyptus* clone (Figure 3a) and 3 charcoal from *Corymbia* (Figure 3c). In Figures 3a and 3c, a subtle separation of the groups was observed for the same clone in *Eucalyptus* and *Corymbia* (highlighted in black). Several explanations can be attributed to this behavior, one of which is related to the method of sampling wood from the base to the top for charcoal production, indicating greater sensitivity of the benchtop NIR, whose spectral range is 12.500-3.500 cm^{-1}, compared to portable NIR (9.000-4.000 cm^{-1}), as reported by other studies using NIR for the classification of other wood products (MEDEIROS *et al*., 2025).

Another aspect is that the differences in the structural molecular composition in the base-top direction of the woods that originated the charcoal are probably more discrepant in relation to the other clones evaluated. These differences, at the time of carbonization, may have generated different chemical structures and/or variations in the amount of compounds, promoting variations in the spectral response in NIR (COSTA; TRUGILHO; HEIN, 2018; RAMALHO *et al*., 2017).

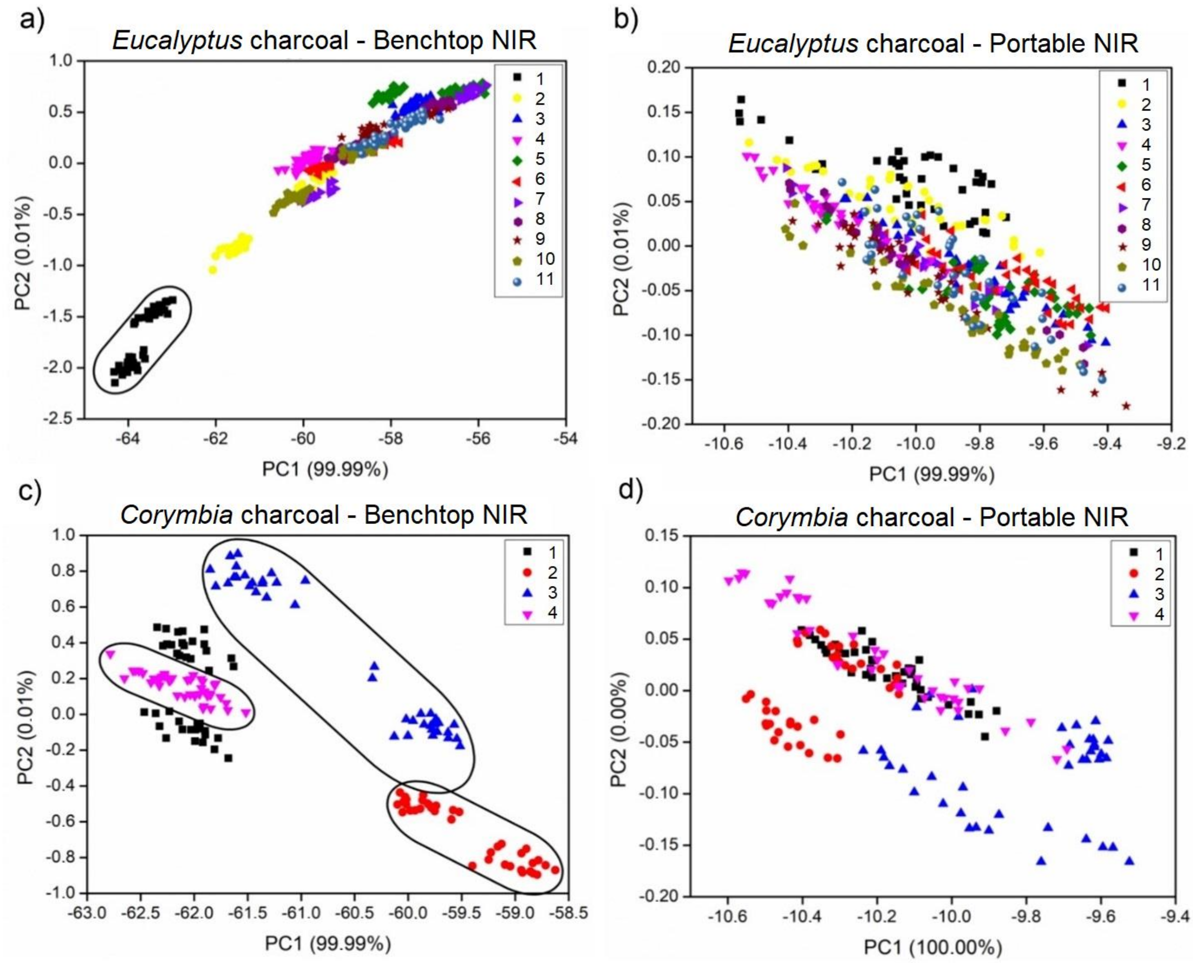

Figure 3 - Principal component analysis (PCA) of treated and untreated spectral data obtained from charcoal of *Eucalyptus* and *Corymbia* clones with benchtop (a and c) and portable (b and d) NIR instruments.

The untreated and first derivative-treated spectra allowed the formation of linear combinations corresponding to the original variables of the charcoal samples of *Eucalyptus* and *Corymbia* clones. The sum of the principal components (PC1 + PC2) explained 100% of the variability of the raw spectral data of *Eucalyptus* and *Corymbia* charcoal with both instruments.

The greater tendency for charcoal grouping from *Corymbia* clones in relation to *Eucalyptus* clones may be related to the apparent relative density (ARD) values (see Table 1). The ARD values of charcoals from *Corymbia* clones are higher than those of *Eucalyptus* clones, resulting in a greater quantity of carbonized woody material in the same volume. Thus, it is likely that a greater amount of organic chemical constituents are present in charcoals from this genus, which made it possible to group almost all these clones using benchtop NIR.

Regarding the portable NIR instrument, it was not possible to identify the formation of charcoal groups within each genus (*Eucalyptus* and *Corymbia*) based on their spectral signatures. The hypothesis raised to justify this behavior involves the smaller spectral range of the portable NIR about the benchtop one, which may have influenced the smaller amount of information in the spectra available for the multivariate analyses. It is worth noting that the portable NIR instrument was not effective specifically for this analysis, which does not prevent its effectiveness for other materials and/or different objectives.

As common aspects for both instruments, it is essential to highlight that a large part of the structural and chemical components of the wood are thermally degraded during the carbonization process, which makes the spectra more homogeneous, with a reduced amount of informative bands and peaks (RAMALHO *et al*., 2017). In addition, the release of water from the wood in the form of vapor during the drying phase of carbonization is another factor that can influence the grouping process of the materials. According to Wang *et al*. (2022), the NIR absorbance is intensified by the greater amount of water since the vibrational energy of the hydroxyl groups is intensified through electromagnetic radiation in regions of higher moisture content. Therefore, the information available in the spectral signatures is reduced after the carbonization of the wood, which may have made it challenging to group similar materials.

3.3. Partial least square regression (PLS-R)

Table 3 shows the PLS-R models used to estimate the chemical, physical, and energetic characteristics of charcoal from *Eucalyptus* and *Corymbia* clones with benchtop and portable NIR instruments. Figure 4 (*Eucalyptus* clones) and Figure 5 (*Corymbia* clones) represent the best calibration and independent validation models. The NIR spectra were treated mathematically (1^{st} derivative, normalization, and SNV), and the best models were selected, including those without spectra treatment.

Table 3 - Statistical parameters of PLS-R models for predicting the chemical, physical and energetic characteristics of charcoal from clones of *Eucalyptus* and *Corymbia.*

Genus	Characteristics	Instrument	Treatment	R^2cv	RMSEcv	R^2p	RMSEp	RPD
				Cross-validation		Independent validation		
Eucalyptus	GY (%)	Benchtop	-	0.67	0.259	0.74	0.213	2.02
		Portable	-	0.65	0.243	0.65	0.244	1.70
	ARD (kg/m^3)	Benchtop	-	0.82	10.855	0.87	9.160	2.82
		Portable	-	0.78	11.633	0.78	11.385	2.12
	FC (%)	Benchtop	-	0.56	0.476	0.60	0.448	1.60
		Portable	-	0.61	0.523	0.64	0.495	1.60
	VMC (%)	Benchtop	-	0.71	0.159	0.72	0.154	1.92
		Portable	-	0.71	0.203	0.70	0.223	2.03
	AC (%)	Benchtop	*SNV	0.69	0.094	0.72	0.088	1.92
		Portable	SNV	0.68	0.103	0.65	0.107	1.76
	FCC (%)	Benchtop	-	0.63	0.155	0.63	0.155	1.64
		Portable	-	0.66	0.218	0.63	0.225	1.71
Corymbia	GY (%)	Benchtop	-	0.74	0.187	0.79	0.165	2.15
		Portable	-	0.61	0.222	0.58	0.232	1.60
	ARD (kg/m^3)	Benchtop	-	0.82	8.122	0.87	6.893	2.77
		Portable	-	0.67	12.033	0.62	14.615	2.45
	FC (%)	Benchtop	-	0.72	0.613	0.69	0.645	1.73
		Portable	-	0.65	0.662	0.63	0.692	1.68
	VMC (%)	Benchtop	-	0.53	0.215	0.54	0.214	1.47
		Portable	-	0.50	0.336	0.64	0.371	1.40
	AC (%)	Benchtop	SNV	0.60	0.050	0.61	0.048	1.62
		Portable	SNV	0.57	0.058	0.57	0.067	1.52
	FCC (%)	Benchtop	-	0.54	0.227	0.58	0.251	1.33
		Portable	-	0.55	0.348	0.61	0.374	1.48

*GY: Gravimetric yield. ARD: Apparent relative density. FC: Fines content. VMC: Volatile material content. AC: Ash content. FCC: Fixed carbon content.SNV: Standard normal variation. R^2cv: Coefficient of determination for cross-validation. RMSEcv: Mean squared error for cross-validation. R^2p: Coefficient of determination for independent validation. RMSEp: Mean squared error for independent validation. RPD: ratio performance to deviation.

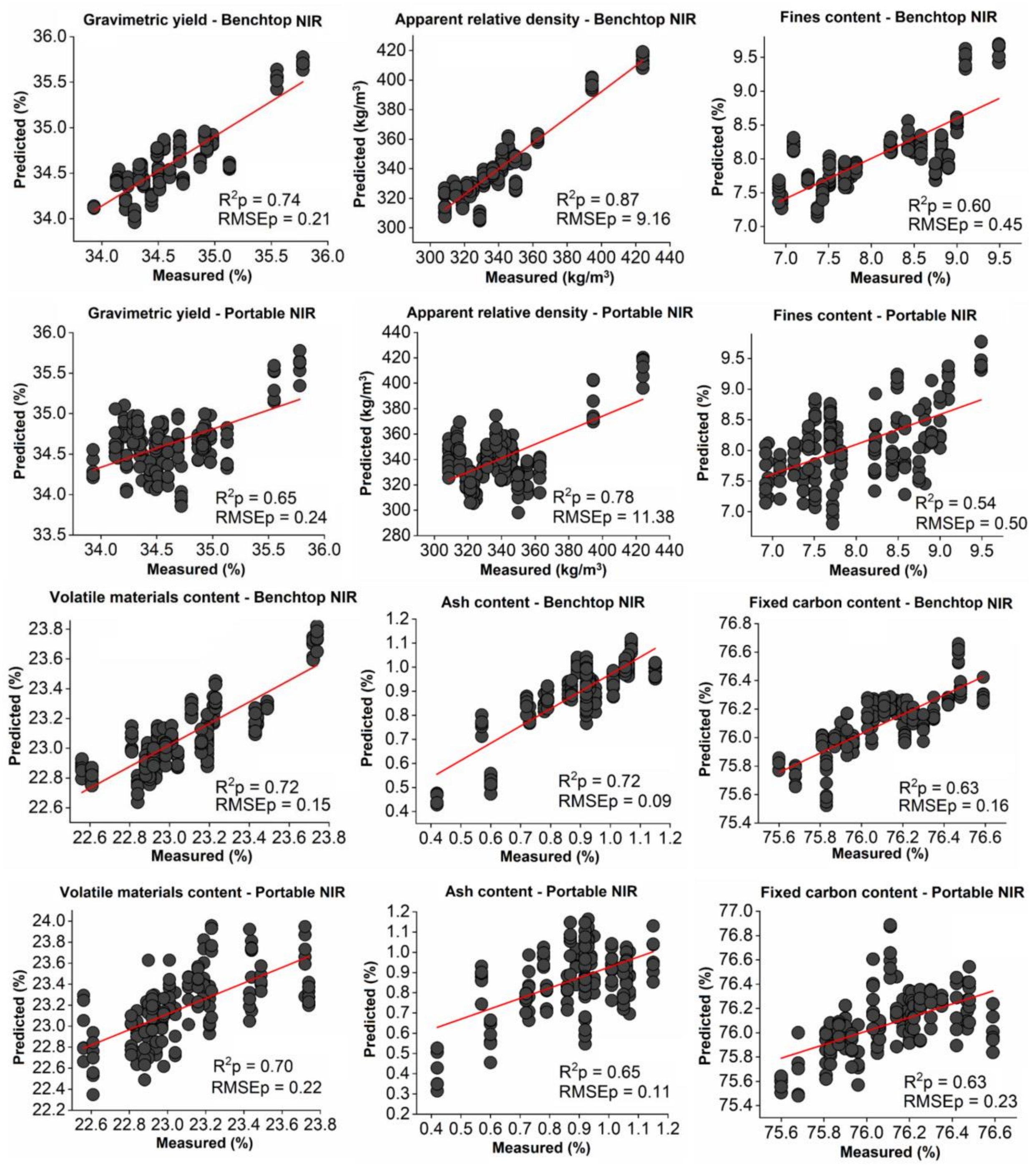

Figure 4 - PLS-R validation graphs for predicting charcoal characteristics from *Eucalyptus* clones using benchtop and portable NIR instruments.

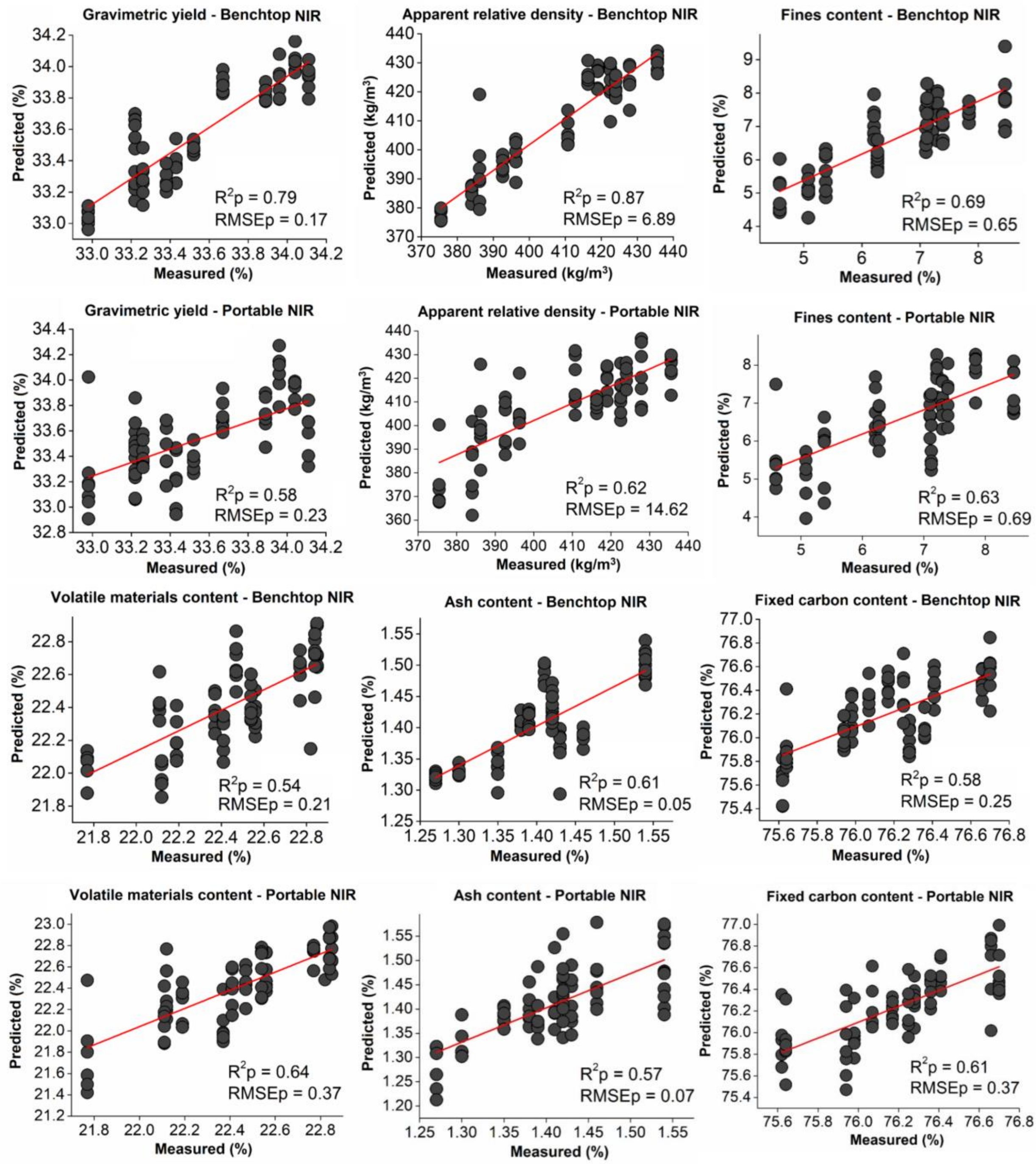

Figure 5 – PLS-R validation graphs for predicting charcoal characteristics from *Corymbia* clones with benchtop and portable NIR instruments.

Gravimetric yield (GY) is a fundamental parameter for optimizing charcoal production, as it is directly related to the efficiency of the thermochemical conversion of wood into charcoal (PROTÁSIO *et al*., 2021). Characteristics such as process efficiency, economic impact, sustainability, quality of the final product, and process control are directly influenced by the GY of the wood carbonization process

(LOUREIRO *et al*., 2021). Thus, maximizing this parameter is desirable to ensure the efficiency and profitability of charcoal production units. The best models for predicting GY presented an R^2p of 0.74 and an RPD of 2.02 (benchtop NIR), an R^2p of 0.65, and an RPD of 1.70 (portable NIR) for charcoal from *Eucalyptus* clones with spectra without mathematical treatment.

The best models for charcoal from *Corymbia* clones presented R^2p of 0.79 and RPD of 2.15 (benchtop NIR) and R^2p of 0.58 and RPD of 1.60 (portable NIR) with the spectra without mathematical treatment. The study by Costa, Trugilho and Hein (2018), when evaluating the quality of *Eucalyptus* charcoal by NIR spectroscopy, found superior results for GY about this study, with R^2cv values of 0.85 and RPD of 2.57 for the original spectral data and varied final carbonization temperatures (400, 500, 600, and 700°C). Despite this, the results found in our study were satisfactory, except for charcoal from *Corymbia* clones using portable NIR.

The apparent relative density (ARD) directly affects the industrial processes that use charcoal as a source of raw material. The higher the apparent density, the higher the relative density. The mechanical resistance and the amount of charcoal that can be stored in a smaller space are greater, facilitating the storage and transportation of these materials (DUFOURNY *et al*., 2019). Furthermore, the higher ADR improves the quality of the charcoal because it generally presents a greater amount of fixed carbon, resulting in a greater amount of energy released during the burning process and optimizing the production of pig iron and steel (LIMA *et al*., 2020). Thus, the best models for predicting ADR presented R^2p of 0.87 and RPD of 2.82 (benchtop NIR) and R^2p of 0.78 and RPD of 2.12 (portable NIR) for charcoal from *Eucalyptus* clones with spectra without mathematical treatment.

The best models for charcoal from *Corymbia* clones presented R^2p of 0.87 and RPD of 2.77 (benchtop NIR) and R^2p of 0.62 and RPD of 2.45 (portable NIR) with spectra without mathematical treatment. Abreu Neto *et al*. (2021), when analyzing the hardness and apparent density of charcoal from clones of *Eucalyptus* sp. and *Corymbia citriodora* together, did not find satisfactory values for apparent density (R^2cv of 0.49 and RPD of 1.40) with original spectral data and a final carbonization temperature of 450°C. These results reinforce the promising results found in our study for the models of this variable.

In the wood carbonization process, charcoal is desirable to be less friable to reduce the amount of fine particles generated during handling and transportation to the steel and steel companies, which can increase the energy released in the form of heat (MASSUQUE *et al*., 2023). In addition, charcoal's low fine content (FC) can increase the permeability of the charge bed in the blast furnace, positively influencing the efficiency of the steelmaking process (SILVA; ATAÍDE, 2019; PADILHA *et al*., 2020). Therefore, the best models for predicting the FC presented R^2p of 0.60 and RPD of 1.60 (benchtop NIR) and R^2p of 0.64 and RPD of 1.60 (portable NIR) for charcoal from *Eucalyptus* clones with spectra without mathematical treatment.

For charcoal from *Corymbia* clones, the best models presented R^2p of 0.69 and RPD of 1.73 (benchtop NIR) and R^2p of 0.63 and RPD of 1.68 (portable NIR) with the spectra without mathematical treatment. Although no study registered in the literature has developed statistical models to predict this parameter based on the NIR spectra, the statistics found in this study were considered satisfactory for both the genus and the instruments tested. This result was considered one of the differentials of this study due to the novelty of the information, which may be of interest to charcoal-producing units, given the relevance of this parameter within the charcoal production and transportation chain.

The volatile material content (VMC) is another fundamental parameter in charcoal production. The literature recommends that charcoal should present VMC between 22-25% by mass for steelmaking use. Levels above this range result in lower fixed carbon contents, directly affecting charcoal's energy availability (SURUP; TRUBETSKAYA; TANGSTAD, 2020; KHAESO; SUKHUNA; KATEKAEW, 2024). Thus, the best models for predicting TMV presented R^2p of 0.72, RPD of 1.92 (benchtop NIR) and R^2p of 0.70, and RPD of 2.03 (portable NIR) for charcoal from *Eucalyptus* clones with spectra without mathematical treatment.

The best models for charcoal from *Corymbia* clones presented R^2p of 0.54 and RPD of 1.47 (benchtop NIR) and R^2p of 0.64 and RPD of 1.40 (portable NIR) with spectra without mathematical treatment. Andrade *et al*. (2012) analyzed the properties of charcoal from *Eucalyptus* using NIR spectroscopy. They found superior results in relation to those found in this study, with R^2p values of 0.91 and RPD of 2.94 with spectra treated with 1st derivative and final carbonization temperatures of 350, 450, 550, and 900°C. However, the results found in our study were satisfactory, except for the charcoal from *Corymbia* clones using benchtop NIR.

Lower ash content (AC) is desirable for charcoal since the higher the ash content, the lower the calorific value (KUMAR *et al*., 2021). Thus, selecting clones with lower AC can be an essential factor in charcoal production since it can corroborate the increase in energy per volume of charcoal (MASSUQUE *et al*., 2021). Thus, the best models for predicting AC presented R^2p of 0.72, RPD of 1.92 (benchtop NIR) and R^2p of 0.65, and RPD of 1.76 (portable NIR) for charcoal from *Eucalyptus* clones with spectra treated with SNV.

For charcoal from *Corymbia* clones, the best models presented R^2p of 0.61 and RPD of 1.62 (benchtop NIR) and R^2p of 0.57 and RPD of 1.52 (portable NIR) with spectra treated with SNV. The results found in this study for AC were acceptable, although the model did not present a high correlation. However, Ramalho *et al*. (2019), when evaluating the influence of particle size on the estimates of the properties of charcoal from *Eucalyptus* sp., did not find satisfactory results for this parameter, with R^2c values of 0.38 and RMSEcv of 0.058 for fine charcoal powder, with spectra without mathematical treatment and a final carbonization temperature of 450°C. The authors highlighted that the difficulty in finding satisfactory results for this parameter may be associated with the composition of the ash since these materials are inorganic, and NIR spectroscopy is recommended for organic materials.

The fixed carbon content (FCC) directly influences charcoal's efficiency, quality, and sustainability since the higher the FCC, the greater the energy efficiency and durability of the charcoal due to the increased combustion process time (TRAN *et al*., 2017). From a sustainability point of view, charcoals with a higher FCC tend to emit fewer polluting gases during combustion because burning is more efficient, releasing fewer substances such as carbon monoxide (CO), carbon dioxide (CO_2), and other volatile compounds (ANTAL; GRØNLI, 2003). Thus, the best models for predicting the FCC presented R^2p of 0.63 and RPD of 1.64 (benchtop NIR) and R^2p of 0.63 and RPD of 1.71 (portable NIR) for charcoal from *Eucalyptus* clones with spectra without mathematical treatment.

For charcoal from *Corymbia* clones, the best models presented R^2p of 0.58, RPD of 1.33 (benchtop NIR), R^2p of 0.61, and RPD of 1.48 (portable NIR) with the spectra without mathematical treatment. Similar results were found in Ramalho *et al*. (2019). The authors found the FCC values of R^2cv of 0.60 and RMSEcv of 1.402 for charcoals retained in the 0.25 mm screen. Spectra were treated with normalization, and the final carbonization temperature was 450°C.

In the general context, it was observed that the models of charcoals from *Eucalyptus* clones presented superior results to those of *Corymbia*. Despite the same carbonization conditions of both genus, the structural chemical composition becomes more homogeneous due to the thermodegradation of a significant fraction of the components. Differences concerning the statistical parameters of the models were observed. A possible explanation may be associated with the number of clones used in constructing the models. The models estimated that the genus *Eucalyptus* used eleven different clones, while only four were used for the genus *Corymbia*. According to Zhu *et al*. (2022), the greater the variability between the components and the number of samples available, the better the statistical parameters of the models.

Regarding the portable NIR instrument, it was observed that some parameters were higher and others lower than the benchtop one. The same trend was observed when comparing the results of other studies reported in the literature. As previously stated, studies on charcoal using NIR spectroscopy are scarce, and no study has been carried out using portable NIR instruments. Despite this, most of the models generated were classified as adjusted and would be suitable for use. It should be noted that this study has some limitations regarding the environmental conditions in which it was carried out.

The samples evaluated were controlled at the laboratory level, presenting significant differences in relation to the charcoal-producing units. Another important aspect is related to the particle size of charcoal. This study used ground and sieved charcoal (0.42 mm and 0.25 mm), presenting significant differences in relation to the charcoal commercialized by the charcoal-producing industries. Therefore, future studies are necessary to fill these gaps in scientific knowledge.

4. CONCLUSIONS

The benchtop and portable NIR instruments showed promising results in almost all the chemical, physical, and energetic characteristics of the charcoal of both genera analyzed. Thus, these instruments can be valuable tools for charcoal-producing units since the evaluation of charcoal quality can be optimized, resulting in time and operating cost savings.

The PCA allowed the distinction of one clone of *Eucalyptus* and three clones of *Corymbia* using the benchtop NIR. With the portable NIR instrument, no charcoal clone was grouped within each genus through this analysis. Following the pre-established parameters to evaluate the models' predictive capacity for both instruments, it was observed that the models presented variation in precision, with the best model presenting an R^2p of 0.87.

The models obtained for charcoal from *Eucalyptus* clones showed similar results with both instruments, which may favor the portable NIR due to its lower cost and easier operation. However, for *Corymbia* charcoals, the portable NIR models showed poorer performance compared to the benchtop.

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CHAPTER 4

PREDICTION OF THE APPARENT DENSITY OF WOOD AND CHARCOAL USING BENCHTOP AND PORTABLE NIR INSTRUMENTS BASED ON X-RAY DENSITOMETRY

PREDICTION OF THE APPARENT DENSITY OF WOOD AND CHARCOAL USING BENCHTOP AND PORTABLE NIR INSTRUMENTS BASED ON X-RAY DENSITOMETRY

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PREDICTION OF THE APPARENT DENSITY OF WOOD AND CHARCOAL USING BENCHTOP AND PORTABLE NIR INSTRUMENTS BASED ON X-RAY DENSITOMETRY

ABSTRACT

The increasing demand for high-quality wood and charcoal highlights the need to monitor key properties such as density. In this context, near-infrared (NIR) spectroscopy and X-ray densitometry represent a promising approach for rapid and non-destructive density estimation. This study aimed to predict the apparent density of wood and charcoal from 15 *Eucalyptus* and *Corymbia* clones (84 months old) using NIR spectroscopy with benchtop (MPA) and portable (MicroNIR and Trinamix) instruments, combined with X-ray densitometry. From each tree, a wood disc 10 cm thick was collected at breast height (DBH). From this disc, ten subsamples 2 mm thick were sectioned in the radial direction, from pith to bark. Five subsamples were analyzed in natura, while the remaining five were subjected to the carbonization process. X-ray images and NIR spectra were acquired for all samples previously and after carbonization in a muffle furnace. Five equidistant positions were defined per sample for densitometric and spectral data collection, totalling 375 variables per instrument for both materials. Principal component analysis (PCA) showed an accumulated variance above 99% for all instruments and materials. Partial least squares regression (PLS-R) models for wood showed prediction coefficients (R^2p) of 0.87 for the MPA, 0.75 for the MicroNIR, and 0.67 for the Trinamix. For charcoal, the best models showed R^2p values of 0.71 (MPA), 0.62 (MicroNIR), and 0.60 (Trinamix). Overall, NIR spectroscopy demonstrated high potential for estimating apparent density, with better predictive performance for wood and some limitations for charcoal. Moreover, the benchtop instrument outperformed the portable ones for both materials. These results reinforce the potential of integrating NIR spectroscopy and X-ray densitometry for the rapid, non-destructive, and efficient characterization of lignocellulosic materials.

Keywords: Forest biomass. Quality control. Multivariate statistics. Non-destructive evaluation. Wood pyrolysis.

1. INTRODUCTION

Wood from tree cultivation constitutes the main source of raw material for the forestry industry. Due to its rapid growth, high productivity, and favorable anatomical and chemical characteristics, such as high lignin content and low ash and extractives contents, eucalyptus wood presents significant advantages for charcoal production (MASSUQUE *et al*., 2023; TEIXEIRA *et al*., 2024). Among these attributes, its higher lignin content stands out as an important component in the production of high-quality charcoal, as it promotes increased gravimetric yield, raises the fixed carbon content, and enhances the energetic properties of the product (PROTÁSIO *et al*., 2021; IBÁ, 2025).

Similarly, *Corymbia* wood becoming a promising alternative, since its high density and rapid biomass accumulation confer substantial potential this genus to produce charcoal intended to supply the steel industry (MELO *et al*., 2024; MARTINS *et al*., 2025a). Thus, industries systematically monitor the quality of raw materials and final products with the purpose of optimizing production efficiency and, consequently, maximize economic returns.

Among the properties of wood and charcoal, density is one of the most relevant attributes, as it directly influences the structural, energetic, and technological characteristics of these materials. This property shows a strong correlation with anatomical and chemical parameters of wood, such as cell wall thickness, especially of the S2 layer, carbon content, and the proportion of latewood, establishing itself as an essential parameter for energy applications (GENDVILAS *et al*., 2024). In addition, density is a variable influenced by genetic material and plantation management practices, reflecting the interaction between genetic and environmental factors (MANIA; KUPFERNAGEL; CURLING, 2024).

For charcoal production, wood density directly influences the pyrolysis process and the quality of the final product, as it affects heat transfer, the kinetics of thermal degradation, and the formation of the charcoal structure (PADILLA *et al*., 2020). Higher-density woods, due to their lower porosity and greater cell wall thickness, hinder heat diffusion into the interior of the material, requiring more controlled heating rates and longer residence times to ensure homogeneous carbonization (SILVA *et al*., 2024).

In addition, density is associated with the chemical composition of wood, particularly lignin content, which provides greater thermal stability and results in a more gradual release of volatile compounds during pyrolysis (PROTÁSIO *et al*., 2019). As a consequence, higher-density woods tend to produce charcoal with higher apparent density, higher fixed carbon content, better mechanical strength, and greater gravimetric and energy yields, provided that the process is properly adjusted to the characteristics of the material (RIBEIRO *et al*., 2024). Therefore, the development of rapid and accurate methods for estimating this variable can contribute to optimizing genetic materials selection, as well as ensuring the quality of products, thereby promoting greater productive and economic efficiency throughout the forestry production chain.

In this context, near-infrared (NIR) spectroscopy is a non-destructive, rapid, and low-cost technique capable of effectively assisting in the characterization of these materials (ZHU *et al*. 2022; MEDEIROS *et al*., 2025) and available in both benchtop and portable versions. The first type of instrument provides high spectral resolution and a broader spectral range, enabling the acquisition of detailed data for the calibration of robust predictive models (MANCINI *et al*., 2021; LIMA *et al*., 2022a).

In contrast, portable instruments offer greater flexibility and mobility, allowing in situ analyses and direct field monitoring, although they are limited regarding sensitivity for having a narrower spectral range than benchtop devices (TOSCANO *et al*., 2022; GOMES *et al*., 2024). Therefore, the comparison between these two types of instruments is essential to assess the applicability of NIR spectroscopy in different industrial and research contexts, aiming to balance analytical accuracy with operational practicality.

However, NIR spectroscopy relies on laboratory data for the calibration of predictive models. In the case of density, conventional laboratory methods are characterized by their destructive nature, high cost, and long processing times required to obtain accurate results (MEDEIROS *et al*., 2023a). In this context, X-ray densitometry emerges as an alternative for obtaining apparent density data. This technique allows the assessment of a material’s apparent density without damaging the sample, offering high precision and reproducibility (BARBOSA *et al*., 2024).

Moreover, it enables the generation of detailed densitometric profiles, identifying variations along the longitudinal axis of wood or charcoal, which is particularly relevant for studies on growth, quality, and structural characteristics (JACQUIN *et al*., 2017;

GAITAN-ALVAREZ; MOYA; BERROCAL, 2019). Additional advantages include faster data acquisition and processing, reduced operational costs, and the potential for integration with other analytical techniques, such as NIR spectroscopy, for the development of robust and efficient predictive models.

Previous studies have employed NIR spectroscopy to estimate density in the forestry sector (LI; BRIAN; YAOXIANG, 2020; DEEPA; SHUKLA, 2024; MEDEIROS *et al*., 2024; YUAN *et al*., 2025). However, most of these studies were based on data obtained through conventional laboratory methods to build predictive models. To date, there is no information regarding the estimation of apparent density of wood and charcoal by integrating NIR spectroscopy with X-ray densitometry, both of which are non-destructive techniques. In addition, data on the efficiency of portable NIR instruments considering the approach adopted in this study are still scarce, which further reinforces its innovative character.

Accordingly, this study was guided by two main hypotheses. The first one establishes that portable NIR spectrometers can deliver precision levels comparable to those obtained with benchtop equipment when predicting the apparent density of wood and charcoal. The second hypothesis assumes that both categories of instruments can reliably estimate the apparent density of materials derived from *Eucalyptus* and *Corymbia* clones. By confirming the effectiveness of integrating near-infrared spectroscopy with X-ray densitometry for this purpose, the combined approach emerges as a fast, non-destructive, and feasible alternative for evaluating this key quality attribute.

2. MATERIAL AND METHODS

2.1. Obtainment and preparation of wood samples

A total of fifteen commercial clones were assessed, including eleven belonging to the genus *Eucalyptus* and four to *Corymbia*. All clones were grown at a 3 m × 3 m spacing and were 84 months old, originating from plantations located in Itamarandiba, Minas Gerais, Brazil (17º 44’ 45” S; 42º 45’ 11” W; 1000 m of altitude at sea level).

The stems of the sample units were sectioned to obtain disks at the longitudinal position corresponding to the diameter at breast height (DBH) with a thickness of 10.0 cm. From these disks, samples with dimensions of 10 × 2 cm (width × thickness) were extracted in the pith-to-bark direction using a vertical band saw. From these samples, ten 2 mm-thick subsamples were obtained for each clone using a table saw. Five subsamples were evaluated as green wood, while the remaining five were subjected to the carbonization process in a muffle furnace.

2.2. Wood carbonization

The wood subsamples destined for carbonization were first oven-dried at 103 ± 2°C for 72 h, ensuring stabilization at constant mass. After drying, each subsample was carbonized individually in an electric muffle furnace. For this process, the specimens were positioned between two metallic sieves and placed inside a cylindrical metallic container measuring 0.30 cm in length and 0.12 cm in diameter, with an internal volume of 3.000 cm³. The remaining internal space was filled with wood chips to ensure a more uniform thermal environment.

The loaded container was inserted into the muffle furnace, whose heating was manually regulated to produce an average temperature increase of 4.17 °C/min, in accordance with the procedure described by Martins *et al*. (2025a). The carbonization protocol consisted of heating from an initial temperature of 150°C to a final temperature of 450°C, followed by a 60-min holding period at the maximum temperature. The complete thermal cycle lasted 4 h and 30 min. Upon completion, the samples were allowed to cool naturally under room conditions for 16 h.

2.3. Apparent density and X-ray densitometry

Before the imaging procedures, both wood and charcoal subsamples were conditioned for 24 h in a controlled environment set at 20°C and 65% relative humidity, as described by Martins *et al*. (2025b).

Digital image acquisition was performed using a Faxitron LX-60 system (Faxitron, Lincolnshire, England). Each specimen was positioned together with a cellulose acetate calibration scale, and the equipment, previously adjusted for automatic measurement, operated at 26 kV with an exposure time of 19 seconds. The radiographic images were saved in DICOM format (FAXITRON, 2009).

The DICOM files were subsequently analyzed in ImageJ software, where mean apparent density values were extracted based on measurements taken along the entire length of each sample.

Each subsample was subdivided into five equally spaced regions, and densitometric profiles were constructed for each region, allowing determination of the mean apparent density in each specified position.

2.4. Spectra acquisition

The wood and charcoal subsamples were first equilibrated in a climate-controlled environment maintained at approximately 20°C and 65% relative humidity, until reaching a moisture content between 10% and 12% on a dry basis. Following conditioning, spectral measurements were obtained using both benchtop and portable near-infrared (NIR) spectrometers. For all instruments, spectra were collected directly on the surface of the subsamples, at the same positions previously established for the X-ray densitometry assessments.

The benchtop instrument employed was an FT-NIR MPA spectrometer (Bruker Optik GmbH, Ettlingen, Germany), operated via OPUS 7.0 software. Spectra were acquired in diffuse reflectance mode using a fiber-optic probe, covering the spectral range of 12.500–3.500 cm^{-1} with an 8 cm^{-1} resolution, and averaging 16 scans per measurement. Background correction was performed at 10-min intervals, and the emission from the MPA optical window was appropriately shielded. For subsequent chemometric analyses, the spectral interval was restricted to 9.000–4.000 cm^{-1} through band selection to minimize noise.

Two portable NIR instruments were also used. The first was the MicroNIR On-site (Viavi Solutions Inc., CA, USA), with data acquisition controlled through Spectral

Solutions software. Measurements were taken in diffuse reflectance mode across 11.000–6.000 cm^{-1}, with a resolution of 5.6 nm, resulting in 125 spectral variables per sample, and each spectrum obtained from 16 averaged scans.

The second portable device was the Mobile NIR developed by Trinamix GmbH (Ludwigshafen, Germany). Spectra were recorded over the range of 6.896–4.080 cm^{-1}, at a resolution of 10 nm, generating 353 spectral variables per spectrum, with storage performed via direct computer connection.

For each instrument, five measurements were performed per subsample, considering five samples per clone and a total of 15 clones evaluated. Thus, 375 spectra were obtained per instrument for the wood, with an equivalent number acquired for the charcoal.

2.5. Multivariate data analysis

Multivariate analyses were conducted using Chemoface version 1.63 (Nunes *et al*., 2012). Principal Component Analysis (PCA) was employed to examine the spectral relationships and clustering patterns among wood and charcoal samples from *Eucalyptus* and *Corymbia* wood. In addition, Partial Least Squares Regression (PLS-R) models were constructed from the spectral datasets to prediction the apparent density of both materials, using the reference values obtained through X-ray densitometry (Figure 1).

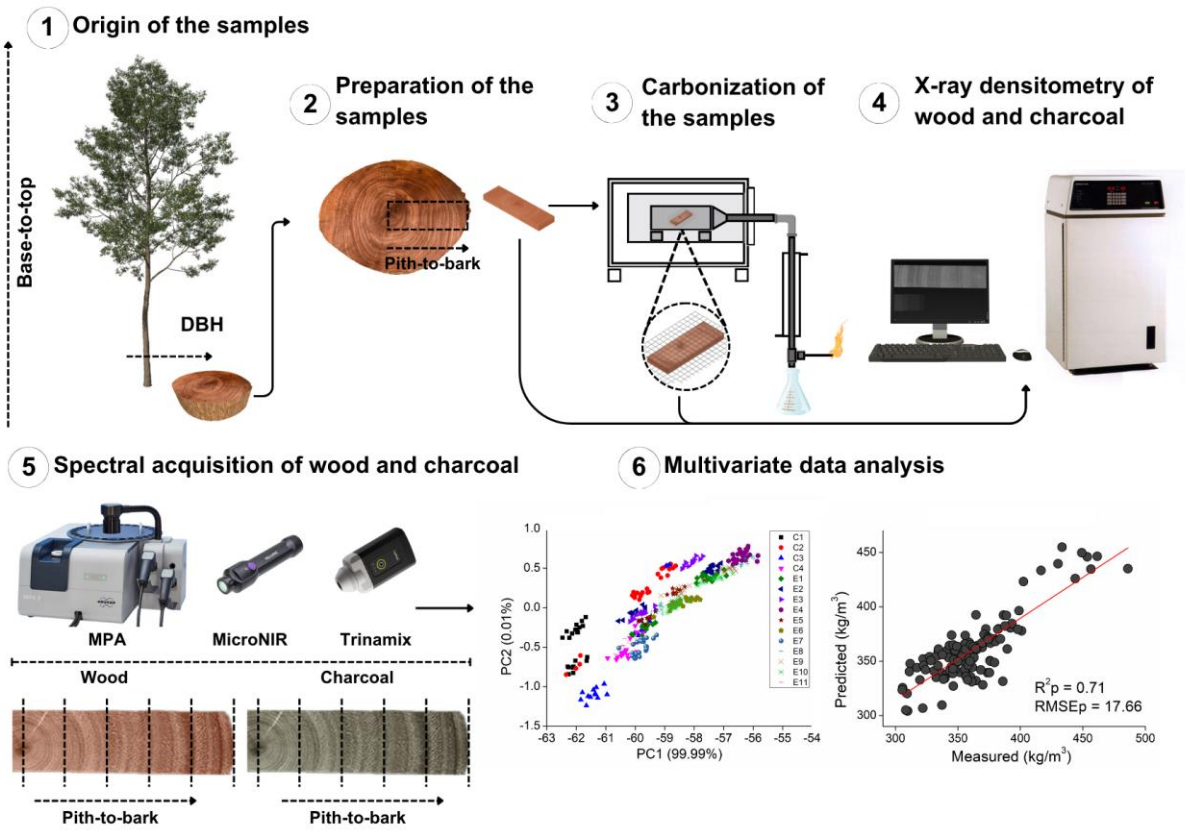

Figure 1 – Experimental schematic for data collection and processing using NIR spectroscopy and X-ray densitometry.

Model validation employed two complementary approaches: cross-validation using the leave-one-out (LOOCV) procedure and independent validation through an external test set. The selection of the optimal number of latent variables was based on achieving the lowest standard error and the highest determination coefficient during the validation stage. In the LOOCV procedure, each sample was sequentially omitted and predicted, whereas in the independent validation approach the dataset was partitioned into a calibration subset (66.6% of the samples) and an external validation subset (33.3%), following the methodology proposed by Martins *et al*. (2026).

To refine model performance, both the raw spectral data and spectra subjected to mathematical preprocessing were evaluated. The preprocessing techniques included the first derivative (13-point smoothing window with a 2nd-order polynomial), the second derivative, and the standard normal variate (SNV). The final PLS-R models were selected considering the combination of lowest root mean square error (RMSE), highest ratio of performance to deviation (RPD), and coefficients of determination (R^2) closest to 1.0, ensuring superior predictive accuracy and robustness.

3. RESULTS AND DISCUSSION

3.1. Spectral signatures from NIR

Regardless of the type of NIR instrument (benchtop or portable), the spectral behavior of both genera was similar for both wood and charcoal, differing only in peak intensity (Figure 2a and 2b). This similarity can be attributed to the phylogenetic proximity between the genera, since both belong to the Myrtaceae family and therefore share closely related genetic characteristics (MELO et al., 2024).

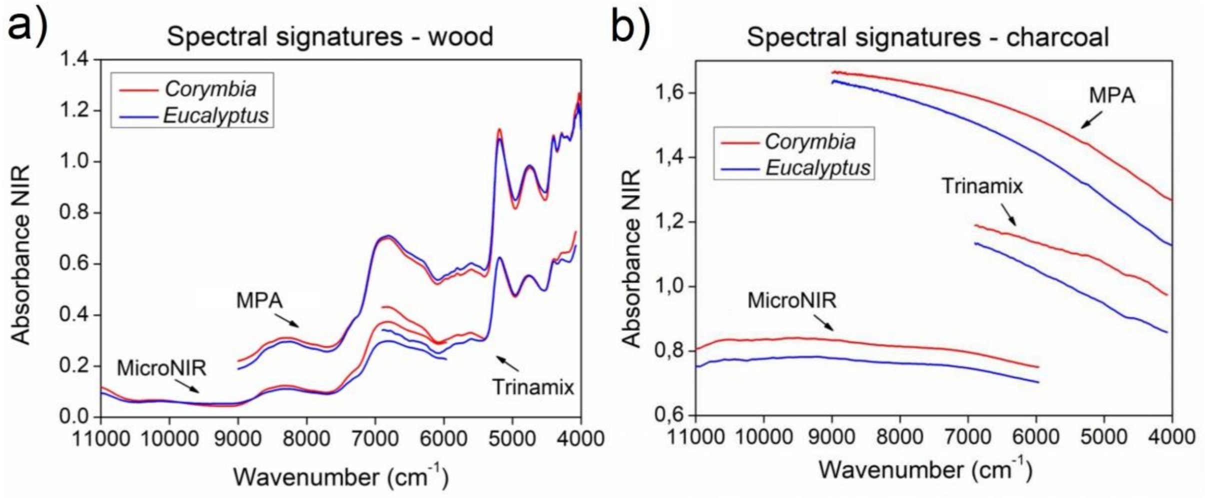

Figure 2 - Average spectral signatures of wood (a) and charcoal (b) from *Eucalyptus* and *Corymbia* obtained using benchtop and portable NIR instruments.

For the spectral signatures between the NIR instruments, variations were observed across the entire spectral range, especially in terms of peak prominence and absorbance values for both materials. Such differences may be associated with the technological specifications of each device, including radiation intensity, light power, and the spectral range covered (MEDEIROS et al., 2025; MARTINS et al., 2026). For wood, the minimum and maximum absorbance values recorded were 0.2 and 1.3 for the MPA; 0.3 and 0.6 for the Trinamix; and 0.1 and 0.3 for the MicroNIR, respectively.

For charcoal, the minimum and maximum absorbance values were 1.1 and 1.7 for the MPA, 0.9 and 1.2 for the Trinamix, and 0.7 and 0.8 for the MicroNIR. The results indicate that, for both wood and charcoal, the MPA instrument provided a higher density of spectral information, consequently presenting a broader absorbance range. This behavior can be attributed to the spectral acquisition mode, since the MPA is equipped with an integrating sphere, which allows it to capture a greater amount of electromagnetic radiation and perform a more comprehensive wavelength scan (GOMES *et al*., 2025).

Among the portable instruments, the Trinamix exhibited higher maximum absorbance values compared to those observed for the MicroNIR. This difference may be related to the spectral regions covered by each device: the Trinamix spectral range extends from 6.896 to 4.080 cm^{-1}, while the MicroNIR covers from 11.000 to 6.000 cm^{-1}. Although the MicroNIR has a broader spectral range, it covers regions with lower-intensity peaks for both materials when compared to the peaks within the range covered by the Trinamix. Thus, the more prominent and characteristic peaks found within the Trinamix spectral range may have contributed to the higher absorbance values obtained in comparison with the MicroNIR.

In *Eucalyptus* and *Corymbia* woods, the spectral ranges between 7.000 and 6.287 cm^{-1} correspond to the amorphous and crystalline regions of cellulose (MEDEIROS *et al*., 2024), while the bands between 8.750 and 8.540 cm^{-1} are associated with aromatic groups of lignin (SCHWANNINGER *et al*., 2011). The peak intensity in this region reflects the reactivity of hydroxyl groups, increasing the interaction of radiation with O–H vibrations and, consequently, raising the absorbance values (MEDEIROS *et al*., 2023b).

Mathematical preprocessing methods were applied to the spectral matrix to improve spectral signal quality and minimize noise interference. In this study, the first and second derivatives, as well as the Standard Normal Variate (SNV), were employed. The models resulting from the spectra obtained using the MPA and MicroNIR instruments did not show significant statistical improvements after preprocessing. However, for the model generated from Trinamix data, the SNV proved effective in improving statistical parameters, as suggested by Martens and Tormod (1989).

The carbonization of *Eucalyptus* and *Corymbia* woods resulted in the thermal degradation of structural components, producing a more homogeneous charcoal with a higher carbon content compared to the wood. The final carbonization temperature has a direct influence on the spectral behavior of charcoal, as it affects the intensity of absorption bands according to the thermochemical conversion of wood constituents (COSTA *et al*., 2019; LIMA *et al*., 2022b). In this study, the carbonization at 450°C promoted the degradation of most carbohydrates, causing significant changes in spectral signatures compared to raw wood. Consequently, peaks between 7.200 and 5.300 cm^{-1} were observed, attributed to O–H stretching (MARTINS *et al*., 2025a), and in the MicroNIR, peaks near 9.800 cm^{-1} are related to the second overtone of C–H and N–H vibrations (SANTOS *et al*., 2021).

The same preprocessing methods applied to the wood spectral matrix were also used for the charcoal matrix. However, none of them produced significant improvements in the statistical parameters of the models developed from the spectra obtained by both benchtop and portable instruments. Similar results were reported by Ramalho *et al*. (2017) and Costa, Trugilho and Hein (2018) when evaluating intrinsic properties of charcoal.

3.2. Principal component analysis (PCA)

The PCA was applied to the wood and charcoal samples to evaluate the ability to separate the *Eucalyptus* and *Corymbia* clones into distinct groups within each genus, using both the benchtop instrument (MPA) and the portable ones (MicroNIR and Trinamix) (Figure 3).

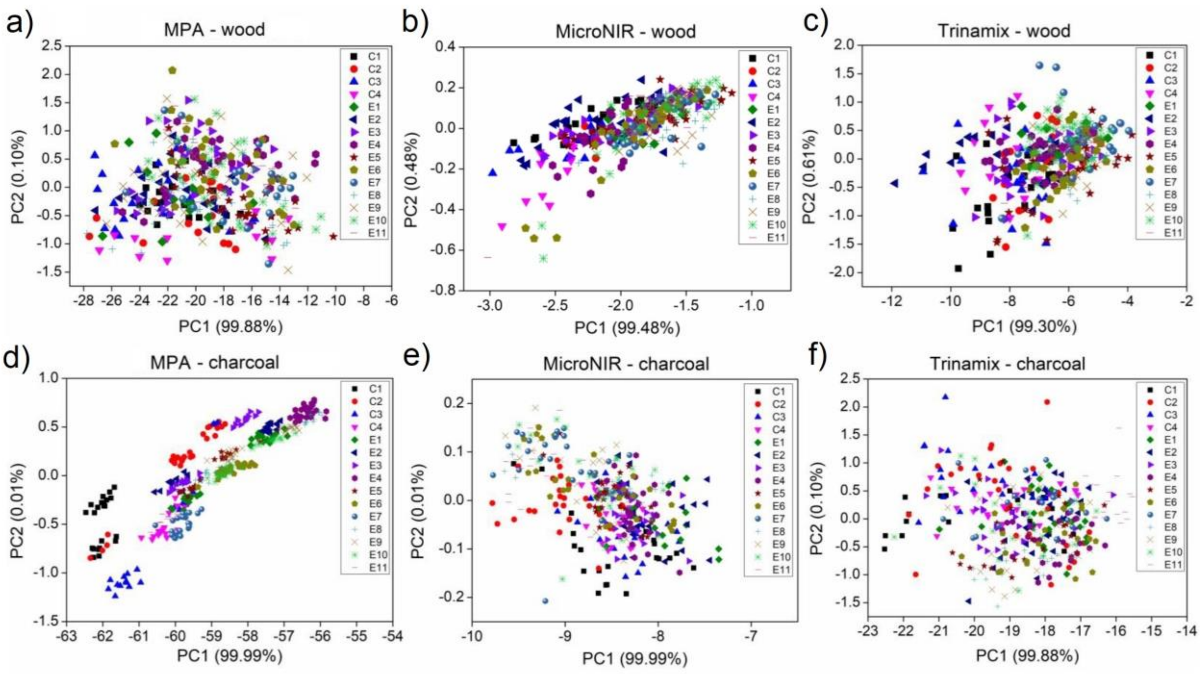

Figure 3 – Principal Component Analysis (PCA) of untreated spectral data obtained from wood (a, b, and c) and charcoal (d, e, and f) of *Eucalyptus* and *Corymbia* clones using benchtop and portable NIR instruments.

The raw spectra of the *Eucalyptus* and *Corymbia* wood and charcoal samples exhibited similar behavior, resulting in linear combinations that predominantly reflected the original spectral variations. Accordingly, the sum of the first two principal components (PC1 + PC2) explained more than 99.0% of the spectral variability of both materials for both the benchtop instrument and the portable devices.

In this study, it was not possible to identify consistent groupings among the clones of each genus based on their spectral signatures, regardless of the material analyzed and the instrument used. This lack of discrimination may be associated with the sampling method adopted, since the wood samples were obtained from discs collected at the same height along the trunk (DBH) and at the same reference age (84 months), a condition that likely resulted in greater spectral homogeneity. Moreover, the similarity in chemical composition among the clones may have contributed to the reduced variability observed in the spectral distribution. Consequently, NIR spectroscopy, through PCA, did not exhibit sufficient sensitivity to discriminate the clones into distinct groups.

Specifically for charcoal, another factor that may be related to the absence of distinction among clones within each genus is its more homogeneous structure, resulting from the significant changes in chemical composition after the carbonization process. During this stage, the chemical components most susceptible to high temperatures, such as cellulose and hemicelluloses, are degraded, while water is released in the form of vapor (SILVA *et al*., 2024; SOUZA BARROS *et al*., 2025).

These phenomena promote structural rearrangements and chemical transformations in the carbonized material, resulting in less informative spectra and, consequently, reducing the potential for discrimination among the clones (RAMALHO *et al*., 2017). Similar results were reported by Lima *et al*. (2025), who, when applying PCA, were not successful in differentiating tropical species based on spectral data from charcoal. In that study, the authors employed PLS-DA to classify the charcoals according to their fixed carbon content, demonstrating that supervised methods may be more effective than exploratory approaches for this type of material.

Despite this, it was observed that the MPA showed a greater tendency to cluster the clones compared with the portable instruments for the charcoal samples. This superior performance may be associated with the higher sensitivity of the MPA to the chemical variations resulting from the carbonization process, particularly those related to changes in carbon chains (COSTA *et al*., 2019; MARTINS *et al*., 2025). Furthermore, its broader spectral range compared with that of the portable instruments, may also have contributed to this behavior.

3.3. Apparent density prediction by PLS-R

NIR spectra subjected to different mathematical treatments (first derivative, second derivative and SNV), as well as untreated spectra, were used in the construction of global models aimed at estimating the apparent density of wood and charcoal from *Eucalyptus* and *Corymbia* clones using benchtop and portable NIR instruments. Table 1 summarizes the statistical parameters of all evaluated models, while Figure 4 presents those that showed the best performance in terms of calibration and independent validation for each instrument analyzed.

Table 1 – Statistical parameters of global PLS-R models for predicting the apparent density of wood and charcoal from *Eucalyptus* and *Corymbia* clones.

Material	Instrument	Treatment	R^2cv	RMSEcv	R^2p	RMSEp	RPD
			Cross-validation		Independent validation		
Wood	MPA	Untreated	0.86	18.31	0.87	18.27	2.67
		1°D	0.73	25.51	0.80	22.63	2.16
		2°D	0.67	28.53	0.72	26.55	1.84
		SNV	0.81	21.32	0.81	22.27	2.19
	MicroNIR	Untreated	0.76	37.27	0.75	38.69	1.94
		1°D	0.64	45.05	0.71	41.67	1.80
		2°D	0.70	41.39	0.73	39.97	1.88
		SNV	0.75	37.84	0.72	40.87	1.84
	Trinamix	Untreated	0.68	36.64	0.65	42.20	1.92
		1°D	0.63	41.62	0.66	43.73	1.86
		2°D	0.64	41.80	0.64	43.91	1.84
		SNV	0.70	37.53	0.67	40.39	2.02
Charcoal	MPA	Untreated	0.71	18.10	0.71	17.66	1.94
		1°D	0.63	23.46	0.70	17.97	1.91
		2°D	0.59	32.86	0.67	24.45	1.70
		SNV	0.67	22.61	0.69	20.97	1.63
	MicroNIR	Untreated	0.61	11.97	0.62	12.35	1.51
		1°D	0.57	12.52	0.59	12.94	1.44
		2°D	0.58	12.89	0.59	13.22	1.46
		SNV	0.57	12.54	0.58	13.31	1.40
	Trinamix	Untreated	0.60	14.33	0.60	14.88	1.43

1°D	0.59	16.71	0.59	15.04	1.41
2°D	0.60	18.87	0.59	15.08	1.41
SNV	0.59	18.27	0.60	15.03	1.42

* SNV: Standard normal variation. 1°D: First derivative. 2°D: Second derivative. RMSEcv: Mean squared error for cross-validation. R^2cv: Coefficient of determination for cross-validation. RMSEp: Mean squared error for independent validation. R^2p: Coefficient of determination for independent validation. RPD: Ratio performance to deviation.

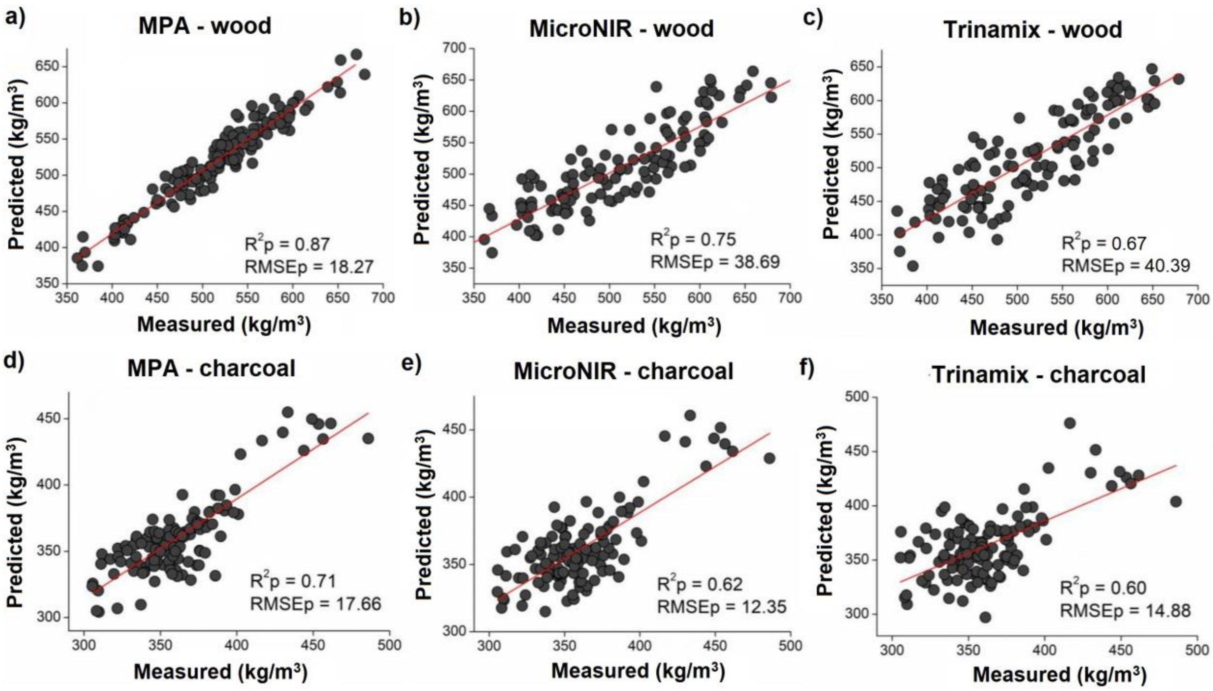

Figure 4 – Superior global PLS-R models for predicting the apparent density of wood (a, b and c) and charcoal (d, e and f) from *Eucalyptus* and *Corymbia* clones using benchtop and portable NIR instruments.

The apparent density of wood directly influences the performance of steel industries, since denser woods tend to provide higher gravimetric yields, more stable pyrolysis processes, and better physicochemical quality of the charcoal produced (CHARVET *et al*., 2021; YANG *et al*., 2024). The best global models for predicting apparent density showed satisfactory performance, with R^2p values of 0.87 and RMSEp of 18.27 for the MPA instrument. For the MicroNIR, the models resulted in an R^2p of 0.75 and an RMSEp of 38.69. The Trinamix, in turn, presented an R^2p of 0.67 and an RMSEp of 40.39. These prediction models refer to wood from *Eucalyptus* and *Corymbia* clones, for which untreated spectra were used for the MPA and MicroNIR, whereas spectra processed with SNV were employed in the case of the Trinamix.

Despite the lack of studies in the literature using NIR spectroscopy to estimate the apparent density of wood, it is noteworthy that this property exhibits a strong correlation with basic density, since both reflect the amount of mass per unit volume and are directly related to anatomical structure and the content of cell wall components (CURVO *et al*., 2024). Accordingly, the results observed in this study are consistent with the PLS-R models developed by Medeiros *et al*. (2024), which reported R^2 values ranging from 0.77 to 0.85 for the prediction of basic density in *Eucalyptus grandis* wood at different moisture levels.

Regarding charcoal, apparent density directly influences its behavior, since denser charcoals exhibit greater mechanical strength, higher fixed-carbon content, and more efficient combustion, resulting in improved performance in blast furnaces and increased operational efficiency (COUTO *et al*., 2023). The best global models presented an R^2p of 0.71 and an RMSEp of 17.66 (MPA), an R^2p of 0.62 and an RMSEp of 12.35 (MicroNIR), as well as an R^2p of 0.60 and an RMSEp of 14.88 (Trinamix), using spectra without mathematical preprocessing for all instruments.

The results obtained were considered satisfactory, especially for the MPA instrument, although a reduction in the statistical parameters of all models was observed when compared to those generated from wood. This behavior was expected, given that the carbonization process tends to promote greater spectral homogeneity, thereby reducing the ability of the spectra to capture relevant chemical variations (MARTINS *et al*., 2025a). The influence of this effect can also be verified in the results presented by Abreu Neto *et al*. (2021), who, when evaluating the apparent density of charcoal produced from clones of *Eucalyptus* sp. and *Corymbia citriodora*, reported R^2cv values of 0.49 and an RPD of 1.40 using original spectra and a final carbonization temperature of 450°C.

When analyzing the models resulting from the spectra obtained by each instrument, a similar behavior was observed for both evaluated materials (wood and charcoal). The MPA instrument yielded the models with the best statistical parameters, demonstrating higher accuracy and predictive capability, and is therefore the most suitable for estimating apparent density through NIR spectroscopy associated with X-ray densitometry.

This superior performance can be attributed to intrinsic characteristics of benchtop instruments. In general, the MPA operates with higher spectral resolution, an elevated signal-to-noise ratio and superior optical stability, factors that enhance its ability to detect subtle chemical and structural variations in the materials (MEDEIROS *et al*., 2025). Additionally, the MPA covers broader spectral ranges and uses more sensitive detectors, enabling the capture of more informative absorption bands relevant to statistical modeling. Thus, the more robust instrumental configuration of the MPA likely contributed to the superior performance observed in comparison to portable instruments for estimating the variable under study.

Regarding the portable instruments (MicroNIR and Trinamix), it was observed that the models generated from the spectra obtained by the MicroNIR for wood showed superior statistical parameters compared to those obtained by the Trinamix. This behavior may be associated with the broader spectral range of the MicroNIR (11.000 to 6.000 cm^{-1}), which, although it includes spectrally more homogeneous regions, covers a wider interval than the Trinamix (6.896 to 4.080 cm^{-1}). The greater spectral extension may have enabled the detection of additional peaks, such as those related to the aromatic groups of lignin (8.750–8.540 cm^{-1}) and the second overtone of C–H and N–H vibrations (approximately 9.800 cm^{-1}), which may be potentially more informative for modeling wood properties (SCHWANNINGER *et al*., 2011; SANTOS *et al*., 2021).

For charcoal, however, a different pattern was observed. Due to the thermal degradation of the chemical constituents of wood during the carbonization process, the spectra became more homogeneous, resulting in lower spectral variability available for the models (LIMA *et al*., 2025). Thus, the statistical parameters obtained by both instruments were similar, making it impossible to state that one of them performed statistically better in predicting this variable.

3.4. Implications and limitations of the study

This study demonstrates the potential of benchtop and portable NIR instruments to predict the apparent density of wood and charcoal, especially in *Corymbia* and *Eucalyptus* clones. Despite these contributions, some limitations must be highlighted. The predictive capacity of NIR spectroscopy depends on the quality and representativeness of the calibration dataset, which may vary according to species, clone, or processing conditions. Thus, the sample size used in this study, although representative, may have limited the performance of the mathematical models.

Furthermore, both NIR spectroscopy and X-ray densitometry are considered alternative techniques compared to conventional laboratory methods. Therefore, the combination of two indirect methodologies may have contributed to the reduction in model accuracy, as potential deviations inherent to each technique can accumulate during data acquisition.

Environmental and physical factors, such as temperature, moisture, and surface roughness of the samples, can also significantly influence spectral responses. Surface roughness is a especially critical aspect for charcoal, since the contraction and shrinkage movements inherent to the carbonization process result in more pronounced surface irregularities. These structural alterations can intensify the scattering of incident radiation and compromise the optical interaction between the beam and the material, resulting in greater spectral variability. Consequently, such effects may have contributed to the reduction of the mathematical parameters of the models obtained for this material.

Hence, future studies should focus on expanding calibration datasets, evaluating a greater diversity of species and materials, and standardizing acquisition protocols to enhance the robustness and reproducibility of the models.

4. CONCLUSIONS

The data obtained through near-infrared (NIR) spectroscopy, combined with information from X-ray densitometry, enabled the prediction of the apparent density of wood and charcoal from *Eucalyptus* and *Corymbia* clones. This approach proves to be promising for optimizing the selection of superior clones intended for energy production, standing out for its non-destructive nature, low cost, and rapid data acquisition.

Principal component analysis (PCA) applied to the spectra explained more than 99.0% of the total data variability for all instruments evaluated. However, it was not possible to adequately distinguish the clones within each genus due to the high similarity in apparent density values among the analyzed materials.

The multivariate models developed using partial least squares regression (PLS-R) showed a high predictive capacity for wood, based on spectra obtained from both the benchtop NIR equipment and portable devices. The best model achieved a coefficient of determination for prediction (R^2p) of 0.87. In the case of charcoal, however, only the benchtop NIR presented satisfactory performance, with an R^2p of 0.71 for the best model, while models generated from spectra obtained with portable instruments exhibited lower performance.

The benchtop NIR equipment produced models with superior statistical parameters; however, its high cost and limitation to laboratory use restrict its applicability. On the other hand, portable instruments, although yielding models with lower statistical parameters, stand out for their lower cost and greater ease of operation. Thus, the choice of the most suitable instrument should consider the required level of accuracy, as both present inherent advantages and limitations.

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FINAL CONCLUSIONS OF THE THESIS

In summary, the bibliometric analysis and literature review presented in Chapter 1 highlight the high potential of near-infrared (NIR) spectroscopy as a promising analytical tool for the wood sector, especially in light of technological innovations associated with the development of portable instruments. Although benchtop instruments still predominate in scientific research and show superior statistical performance, there is a growing trend toward the expansion and improvement of portable NIR devices, which offer significant advantages such as lower cost, ease of operation, portability, and the possibility of in situ, real-time analyses with minimal sample preparation.

Furthermore, studies reported in the literature indicate that intrinsic sample factors such as particle size, moisture content, surface roughness, and structural heterogeneity, directly influence the quality of the spectra and, consequently, the robustness and accuracy of the predictive models generated. Since NIR spectroscopy is based on the interaction of electromagnetic radiation with the molecular vibrations of the sample's chemical constituents, controlling and standardizing these experimental variables is essential to ensure consistent and reproducible results under laboratory conditions. In industrial and/or field environments, the explicit inclusion of these variables in the models is crucial to enhance the ability of multivariate algorithms to distinguish and compensate for variations associated with real operating conditions, such as environmental, operational, or sample preparation differences.

Chapter 2 demonstrated that NIR spectroscopy was effective in predicting the chemical properties and basic density of wood from *Eucalyptus* and *Corymbia* clones. The spectral analysis revealed high quality and consistency of the data obtained with both instruments. However, the benchtop instrument showed better performance in clone discrimination, whereas spectra obtained with the portable NIR showed lower grouping capacity, possibly due to its lower spectral resolution and greater sensitivity to environmental and surface conditions of the samples. Overall, both instruments showed satisfactory predictive performance, confirming the applicability of NIR spectroscopy for rapid and reliable estimation of wood properties. Despite slightly lower results, the portable NIR stands out for its practicality, lower cost, and potential for in situ use.

In Chapter 3, both benchtop and portable NIR instruments showed satisfactory performance in predicting the chemical, physical, and energetic properties of charcoal produced from *Eucalyptus* and *Corymbia* clones. Exploratory spectral analysis revealed that the benchtop instrument showed greater discriminatory power among clones, whereas the portable NIR showed limitations in distinguishing samples from different genetic materials. This performance difference may be associated with instrument configuration limitations of the portable device itself. The models developed for charcoal from *Eucalyptus* clones showed equivalent performance between benchtop and portable instruments, indicating that the use of the portable NIR may be a viable alternative, especially due to its lower cost and ease of operation in field conditions. In contrast, for charcoal from *Corymbia* clones, the models based on portable NIR spectral signatures showed lower performance compared to the benchtop instrument.

Finally, Chapter 4 demonstrated that the integration of NIR spectroscopy with X-ray densitometry can be an alternative approach for predicting the apparent density of wood and charcoal from *Eucalyptus* and *Corymbia* clones. Exploratory spectral analysis indicated high consistency and representativeness of the data obtained, although it was not possible to adequately distinguish clones within each genus, likely due to the high similarity in apparent density values among the evaluated clones. The multivariate models developed showed high predictive potential for wood, using both benchtop and portable NIR instruments. In the case of charcoal, the benchtop instrument showed superior performance, while the portable instruments exhibited lower predictive capacity.

In this context, the study developed in this thesis demonstrated that strengthening research focused on robust multivariate calibration and validation represents a strategic advance toward consolidating NIR spectroscopy as a reference technology. When combined with emerging approaches such as advanced chemometric modeling, machine learning, and integration with digital process monitoring and control systems, NIR spectroscopy has the potential to significantly expand its applicability in the rapid, sustainable, and non-destructive characterization of wood and its derivatives.

This technological integration contributes to improving production efficiency and strengthening sustainable practices in forestry and industrial systems. Therefore, the choice between benchtop and portable instruments should be guided by the required level of accuracy and operational conditions of use, as both offer complementary advantages and play a fundamental role in advancing innovative and environmentally responsible analytical methodologies within the forestry sector.