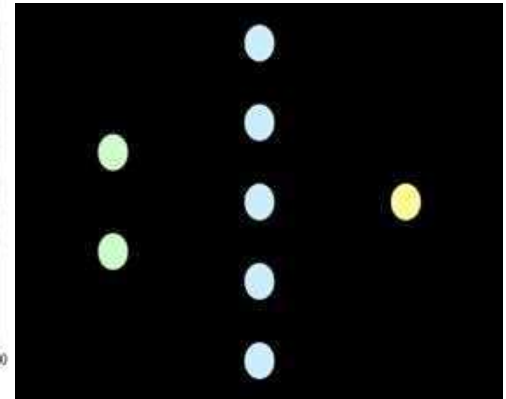




From the lab to the field: How much does moisture affect NIR readings in wood?



Paulo Hein (DCF/UFLA)

Universidade Federal de Lavras

UFLA in numbers

30 undergraduate courses
13,500 undergraduate students
34 academic PG programs
9 Professional PG Programs
3,000 postgraduate students

How do you adjust the
amount of coffee and milk?

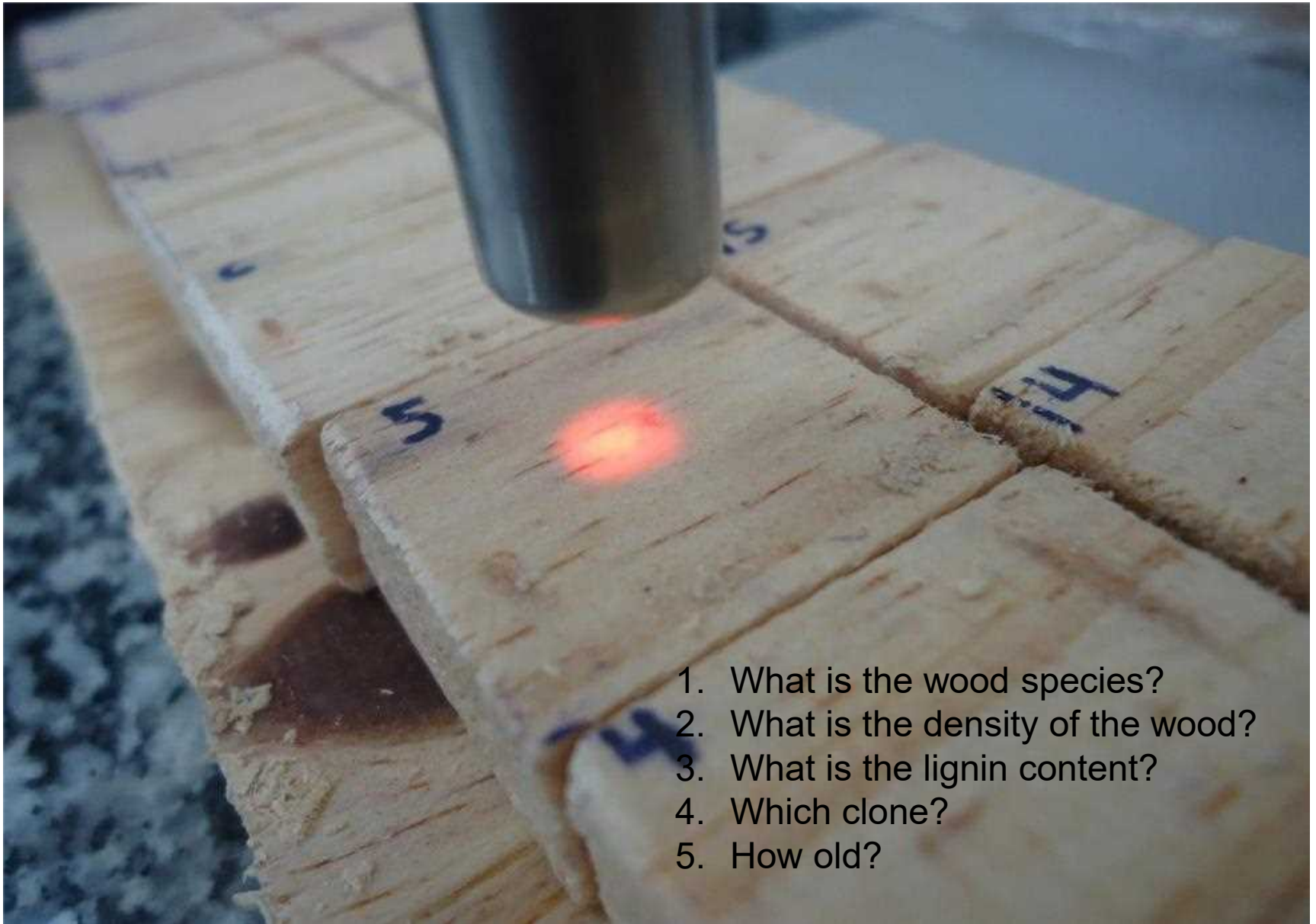


What are these wood species?



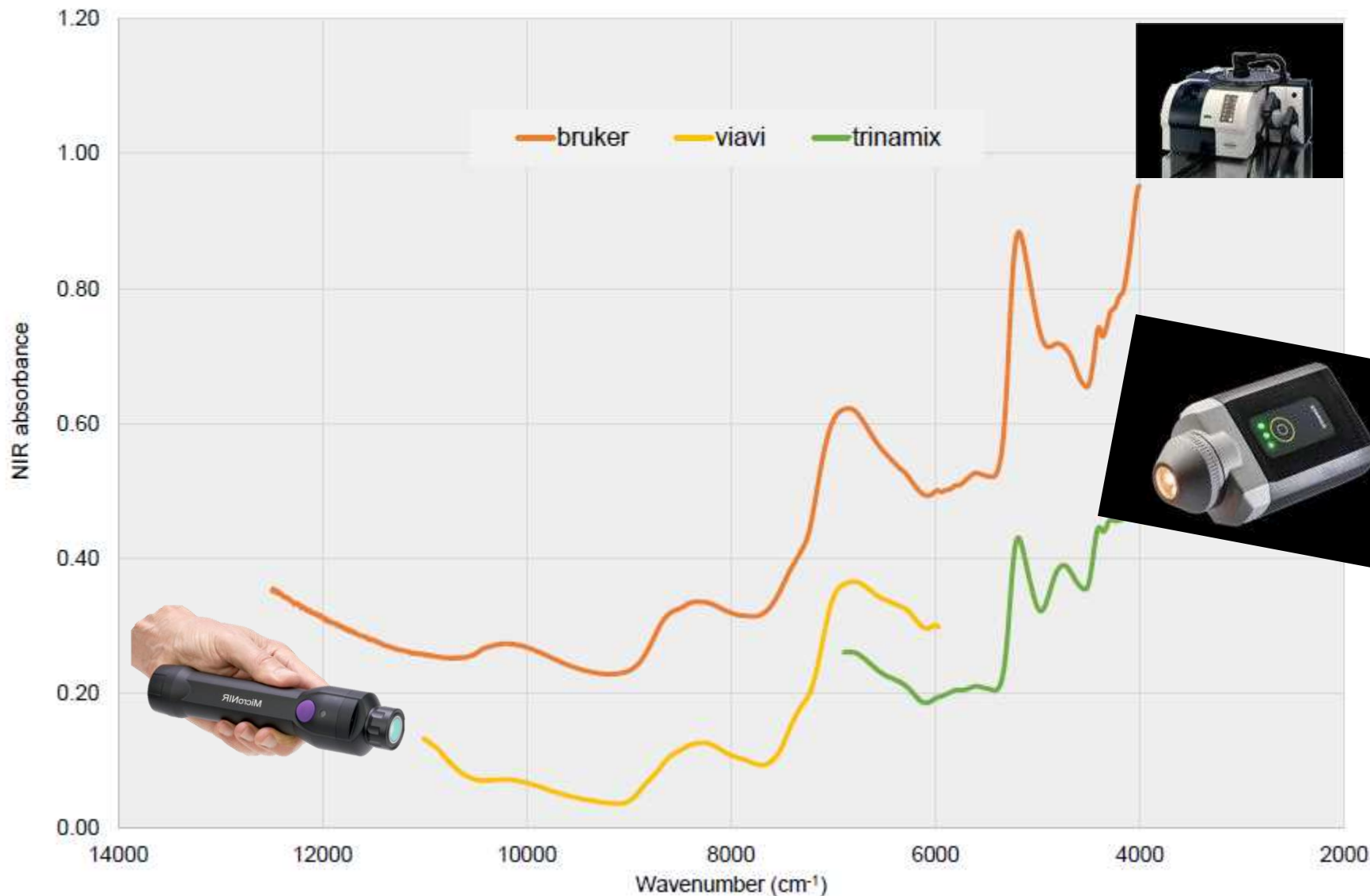
1) Marupa, 3) Castanheira, 4) Guajará, 5) Aroeira, 6) Itaúba, 7) Angelim, 8) Jatobá, 9) Sucupira, 11) Muiracatiara, 12) Cumaru, 13) Roxinho

NIR analysis of wood samples for industrial purposes



1. What is the wood species?
2. What is the density of the wood?
3. What is the lignin content?
4. Which clone?
5. How old?

NIR spectrometers



FT-NIR spectrometer (MPA, Bruker)

Spectral range: 750 a 2.500 nm.

Scan mode: transmittance and reflectance

Scan time: 15 seconds.

€ 80.000,00 (R\$500.000,00)



MicroNIR (Viavi Solutions)

Spectral range: 950 a 1.650 nm

Scan mode: reflectance

Scan time: 0.25 - 4 seconds

U\$ 25.000,00 (R\$120.000,00)



TrinamiX (BASF)



Spectral range: 1.450 a 2.450 nm
Scan mode: reflectance
Scan time: 1 - 2 seconds
€ 11.000,00 (R\$70.000,00)



Hyperspectral Camera SWIR



FX10 (VNIR: 400-1000 nm)



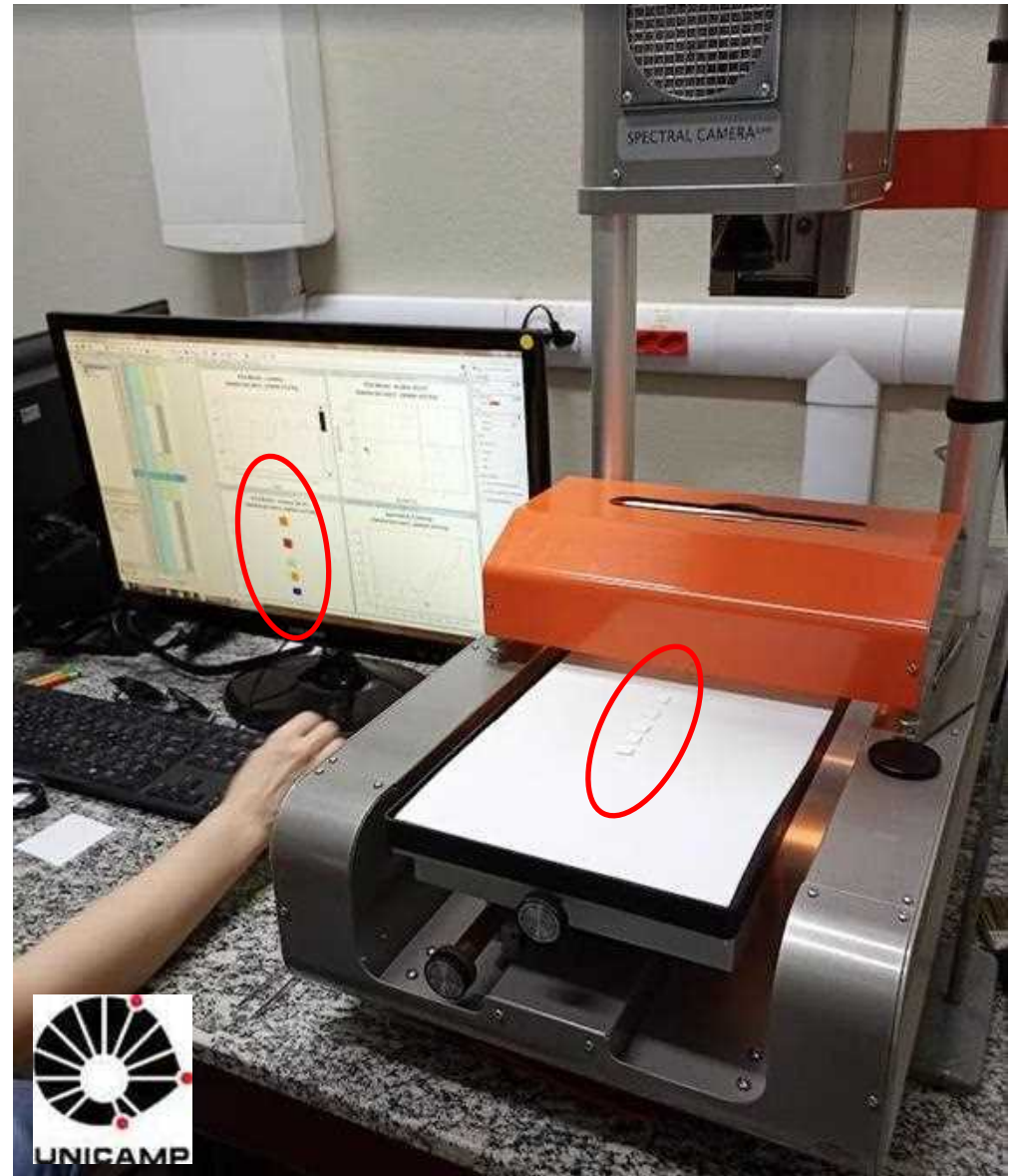
SWIR (1000 - 2500 nm)

Spectral range: 400 a 2.500 nm

Pixel size: 24 x 24 μm

Frame ratio: 450 fps

€ 271.298,33 (R\$1.745.807,24)



Hyperspectral Camera SWIR



FX10 (VNIR: 400-1000 nm)



SWIR (1000 - 2500 nm)

Spectral range: 400 a 2.500 nm

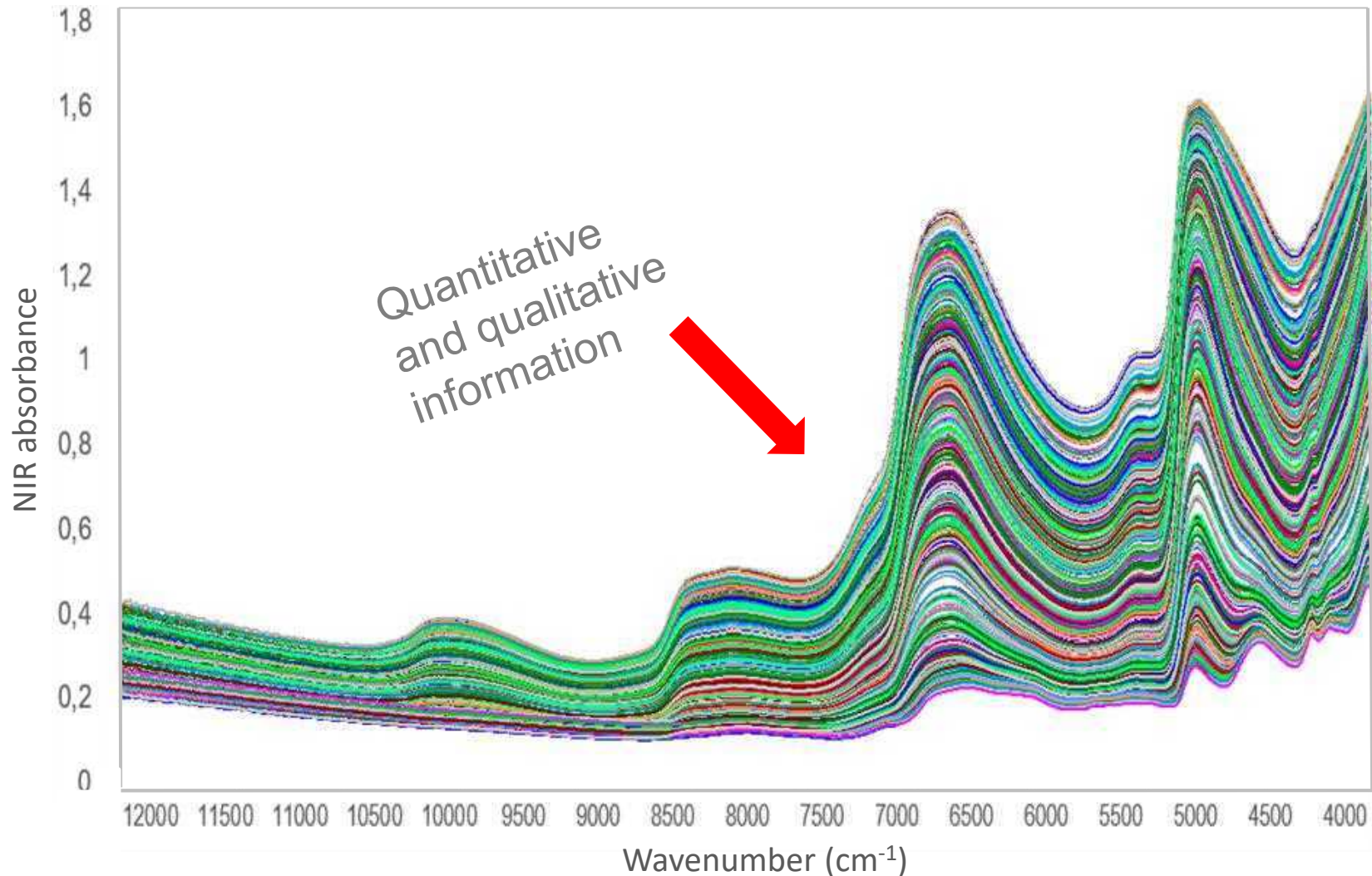
Pixel size: 24 x 24 μm

Frame ratio: 450 fps

€ 271.298,33 (R\$1.745.807,24)



NIR spectra in cellulose pulp at different moisture conditions

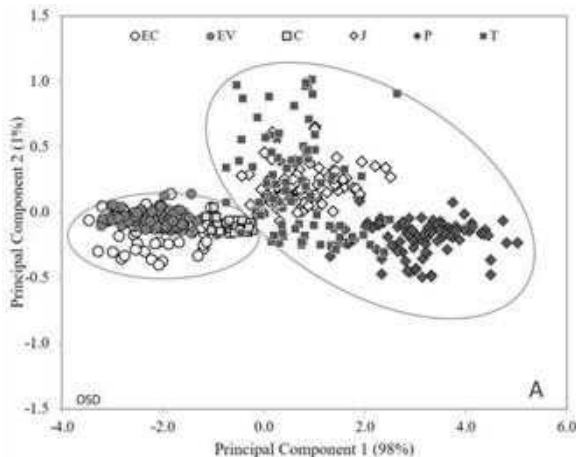


Chemometrics: qualitative and quantitative analysis

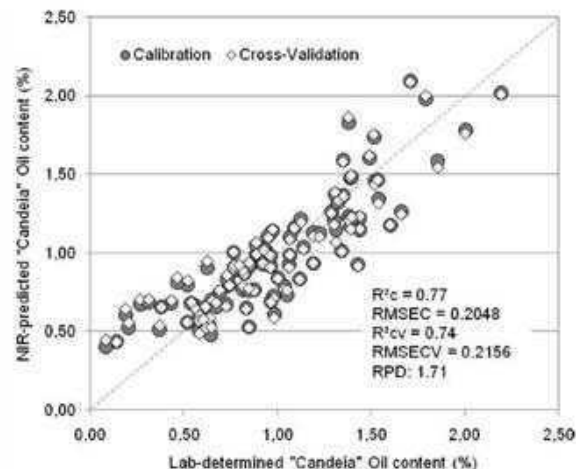
1. Exploring data
separating
wood species,
clones, ages

2. Predicting
properties:
wood density,
lignin content, oil
content, wood
natural durability,
energetic density

3. Classifying
materials:
wood species,
charcoal quality,
density or
moisture level



PCA

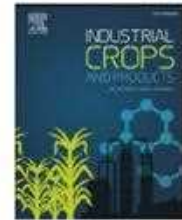


PLS-R

Table 3. Classification of wood samples according to vegetal material by means of PLS-DA using cross-validation and test set from untreated NIR spectra.

Validation	Material	Class of vegetal material predicted by NIR						N°	% Success
		EC	EV	C	J	P	T		
Cross-validation	EC	63	27					90	70
	EV	17	73					90	81
	C		1	44				45	99
	J				89		1	90	99
	P					87	1	88	99
	T					7	80	87	92
Test set	EC	21	9					30	70
	EV	7	23					30	77
	C			15				15	100
	J				30			30	100
	P					29		29	100
	T					4	25	29	86

PLS-DA



Estimation of the basic density of *Eucalyptus grandis* wood chips at different moisture levels using benchtop and handheld NIR instruments

Dayane Targino de Medeiros^{a,*}, Jhennyfer Nayara Nogueira Gomes^{a,2},
Felipe Gomes Batista^{a,3}, Adriano Reis Prazeres Mascarenhas^{b,4},
Emanuella Mesquita Pimenta^{c,5}, Gilles Chaix^{d,e,f,6}, Paulo Ricardo Gherardi Hein^{a,7}

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^d CIRAD - UMR AGAP Institut, Montpellier, France

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^f ChemHouse Research Group, Montpellier, France

ARTICLE INFO

Keywords:

Fiber saturation point
Pulp and paper industry
Multivariate statistics
Quality control
Real-time evaluation

ABSTRACT

With the increasing demand for productivity and quality in the forestry sector, near-infrared (NIR) spectroscopy is promising in the monitoring of wood properties, such as density. However, most predictive models are based on spectra acquired in wood at equilibrium moisture content using benchtop equipment. The objective of this study was to evaluate the performance of the NIR instruments in predicting the basic density of *Eucalyptus grandis* wood at different moisture contents. The wood chips were evaluated from saturated conditions (freshly felled) to hygroscopic equilibrium conditions using benchtop and portable NIR instruments. Principal component analysis (PCA) was performed to verify the behavior of spectral data, partial least squares discriminant analysis (PLS-DA) to classify density categories, and partial least squares regression (PLS-R) to develop predictive models. The moisture gradient was not the limiting factor for the statistical modeling. PCA discriminated 99.50% of the variation in the data, while the PLS-DA correctly categorized in the range of 0–94% the density classes. The models developed by PLS-R with the benchtop instrument showed a prediction coefficient (R^2) ranging from 0.79 to 0.85 and those with the portable instrument ranged from 0.77 to 0.82; the ratios of prediction deviation (RPD) were 2.20 and 2.45, respectively. Thus, NIR spectroscopy has shown potential application in wood under saturated conditions, regardless of the type of instrument. In the industrial context, the use of a portable NIR instrument could streamline wood characterization without the need for drying and transporting samples to the laboratories.

Challenges:
Surface effect
MC effect

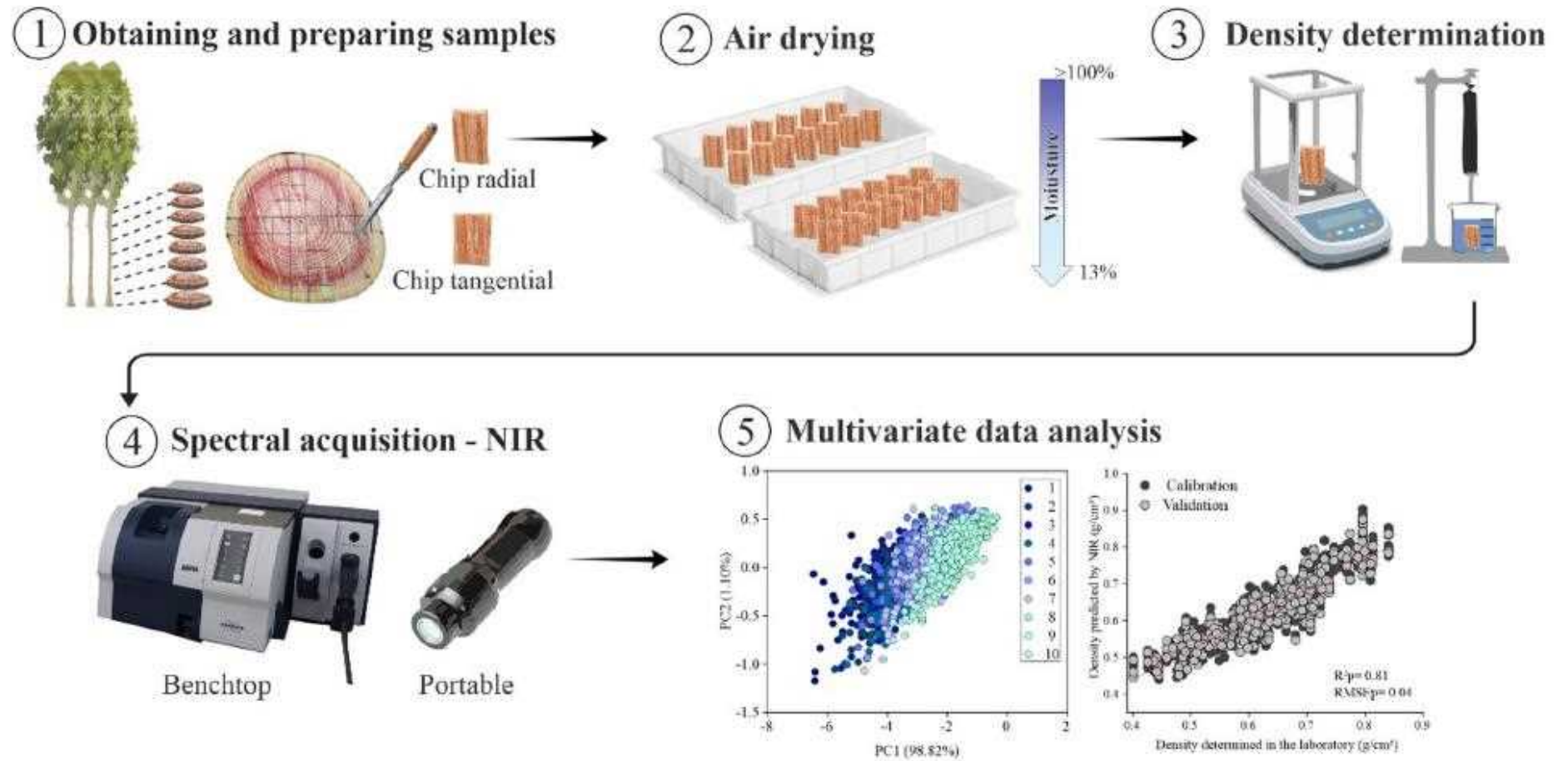


Fig. 1. Flowchart of the study stages.

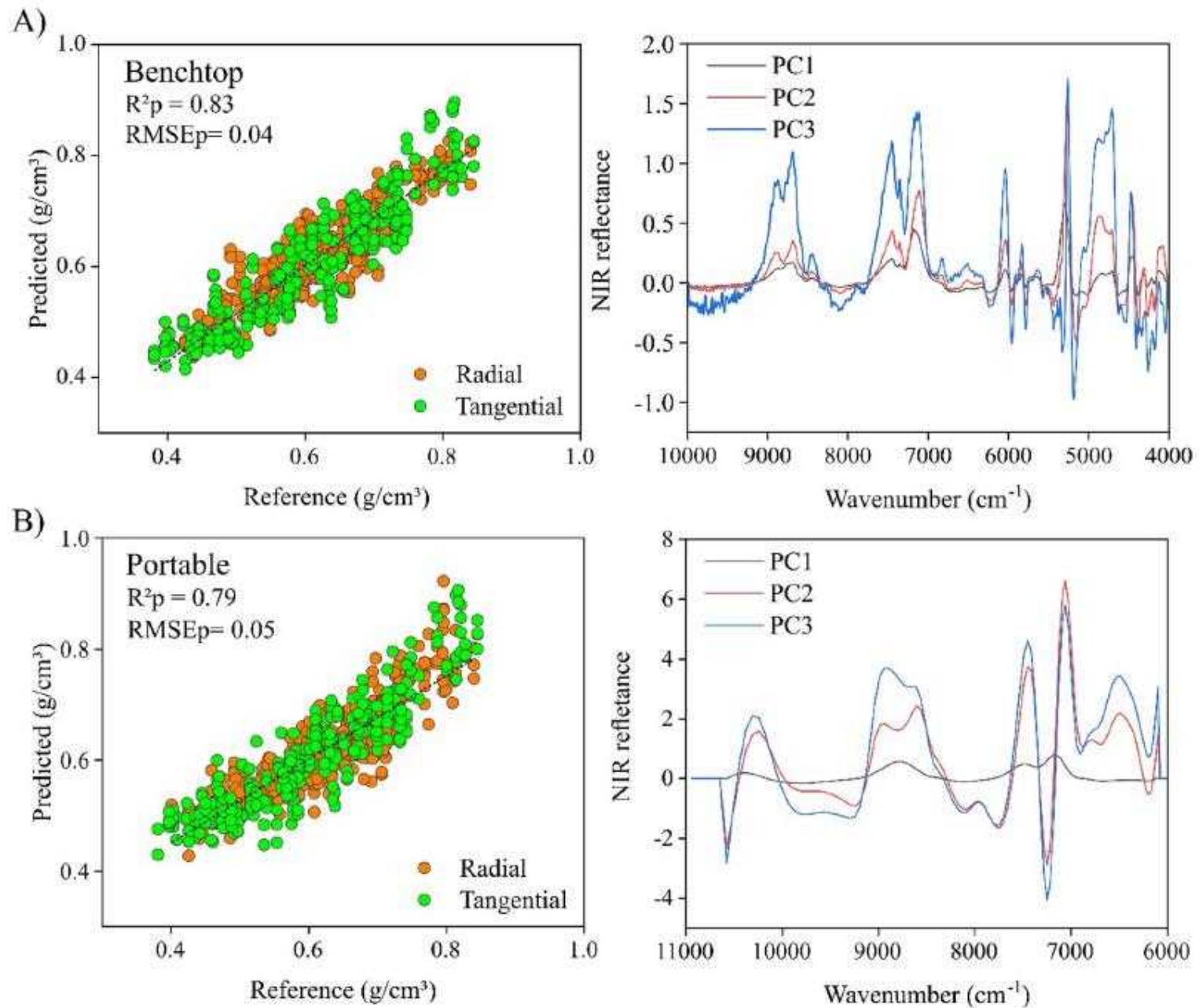


Fig. 7. Global model for the basic density of *Eucalyptus grandis* wood in benchtop (A) and portable (B) NIR instruments, with spectra treated with first derivative.

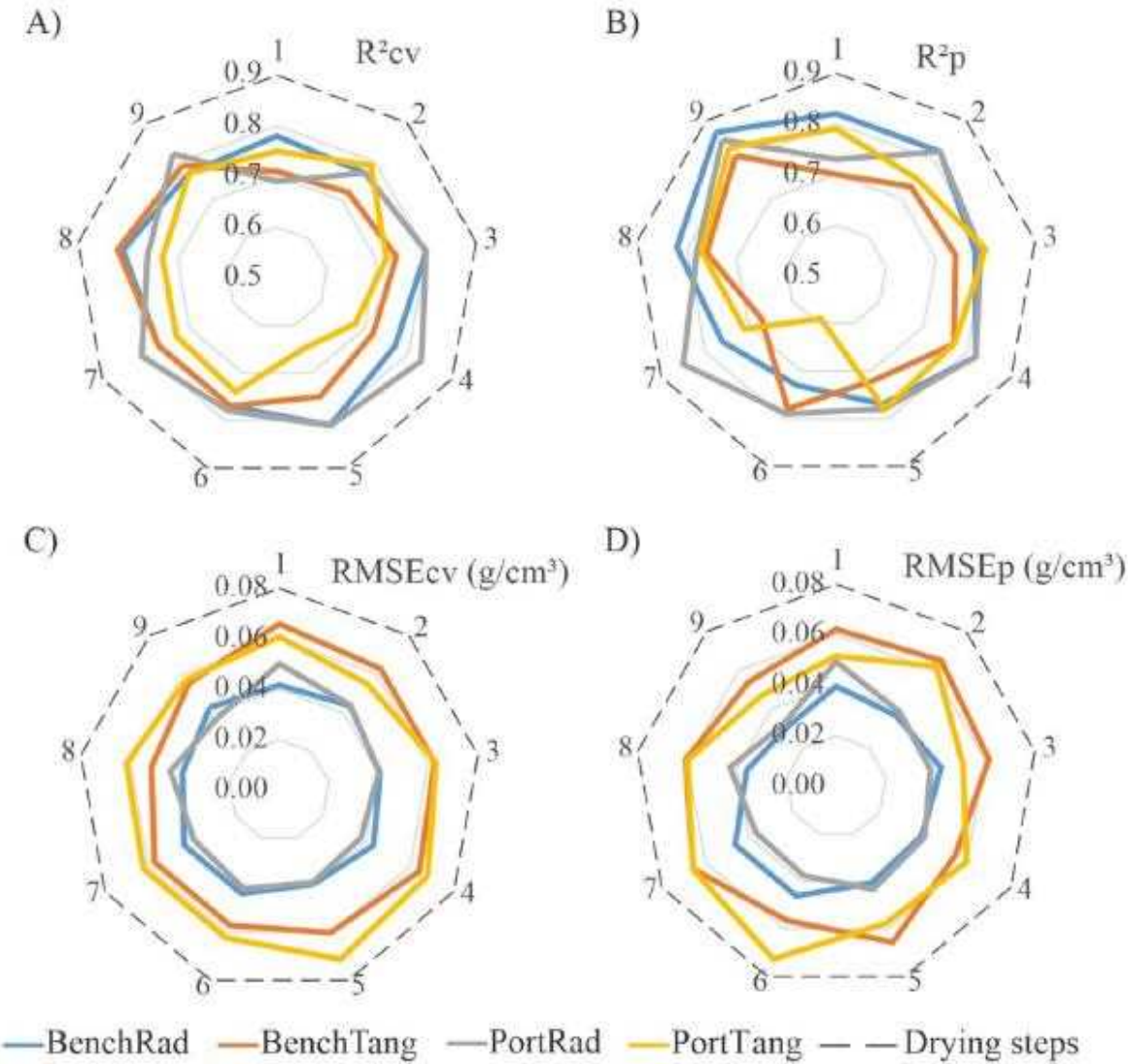


Fig. 6. Graphs of the prediction of the basic density per drying stage (stage 1 - wetter to stage 9 - drier) in different surfaces and instruments in the cross-validation (A) and in the independent validation (B) and their respective errors (C and D).

Wood Chemistry

Jhenyfer Nayara Nogueira Gomes, Dayane Targino Medeiros, Lívia Cássia Viana and Paulo Ricardo Gherardi Hein*

Influence of moisture on the identification of tropical wood species by NIR spectroscopy

<https://doi.org/10.1515/hf-2024-0111>

Received December 3, 2024; accepted March 11, 2025;

published online March 25, 2025

Keywords: forestry inspection; native woods; multivariate statistics; principal component analysis; partial least squares regression

Abstract: Solutions for species discrimination are important for monitoring native timber harvesting. Near-infrared (NIR) spectroscopy has shown promise for identifying wood species in real time. The influence of moisture content on the model's performance for classifying wood is not well known. The objective was to evaluate the effect of wood moisture on the predictive capacity of the models for species discrimination based on NIR spectra using a benchtop and a portable spectrometer. First, NIR signatures were collected on the radial face of wood specimens at equilibrium moisture content (EMC) of 11 native species from Amazonia using both equipments. After saturation, new spectra were collected at the maximum moisture condition and subsequently at every 10 % of the water mass loss during drying. Partial least squares discriminant analysis (PLS-DA) was developed to discriminate the timber species according to their spectral signatures. Principal component analysis of the spectral data obtained in EMC was able to discriminate the species depending on the density gradient of the specimens. Moisture had no significant impact on the spectral signal. The PLS-DA models successfully classified unknown wood samples by species with over 91 % accuracy, regardless of moisture content. Both NIR devices show strong potential for use in forest inspections.

1 Introduction

The Amazon region is one of the world's leading producers of timber and non-timber products from native forests. The high diversity of species available in this region has attracted the attention of the foreign market due to the superior quality of the wood used in construction and in various other sectors that use wood as a raw material. The constant demand for wood associated with the high similarity between species has contributed to the occurrence of fraud and illegal exploitation of these woods (Rocha et al. 2019). Forestry activities in Brazil are monitored by federal and state agencies, which follow the guidelines of the Brazilian Forestry Code (Federal Law 12,651/2012). However, the scientific and technological limitations of inspection bodies pose significant challenges for the sector, as the rapid and efficient identification of species remains a critical unmet need (Soares et al. 2017).

Near infrared (NIR) spectroscopy is a non-destructive analysis methodology associated with the chemical information of materials (Pasquini 2003). Using multivariate analysis, NIR directly measures absorbance, identifying

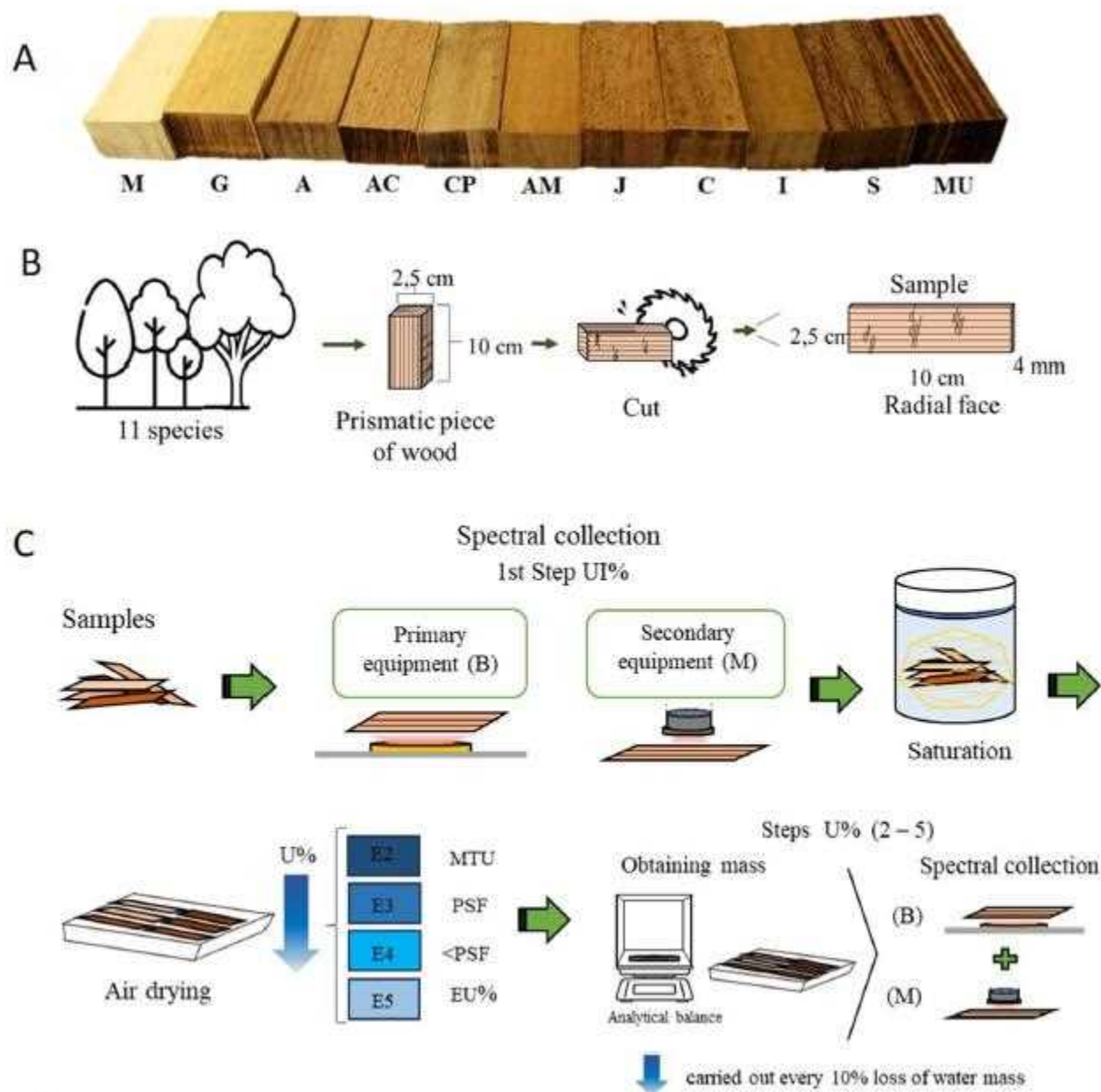


Figure 1: Amazonian species investigated in this study (A), sample preparation diagram (B), and methodological flowchart used for measuring NIR spectra at different moisture content (C).

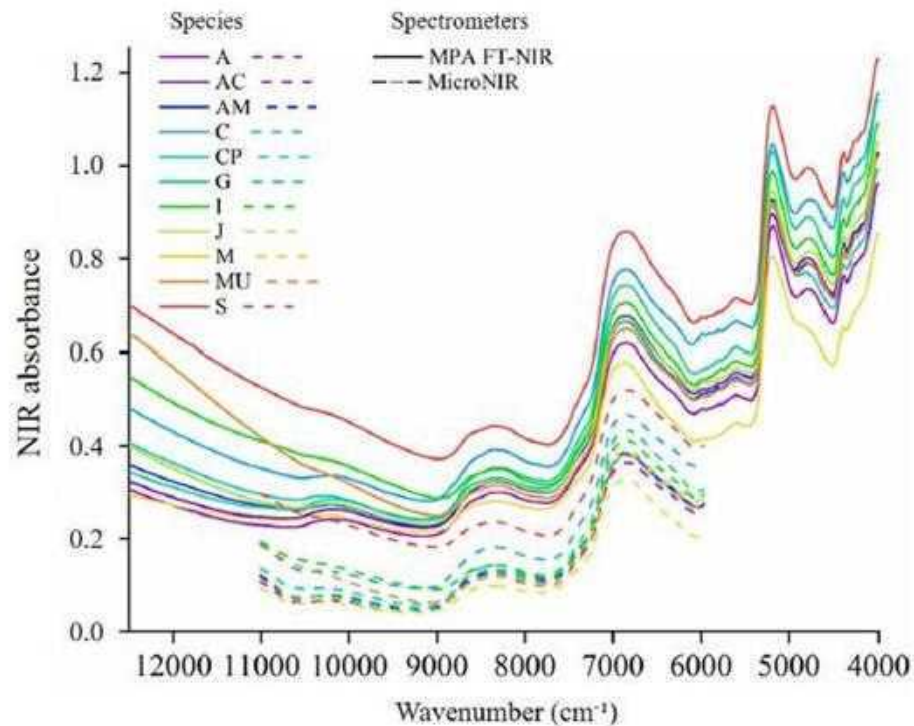


Figure 3: Average spectral signature obtained with the benchtop (MPA FT-NIR) and portable (MicroNIR) spectrometer for the wood species.

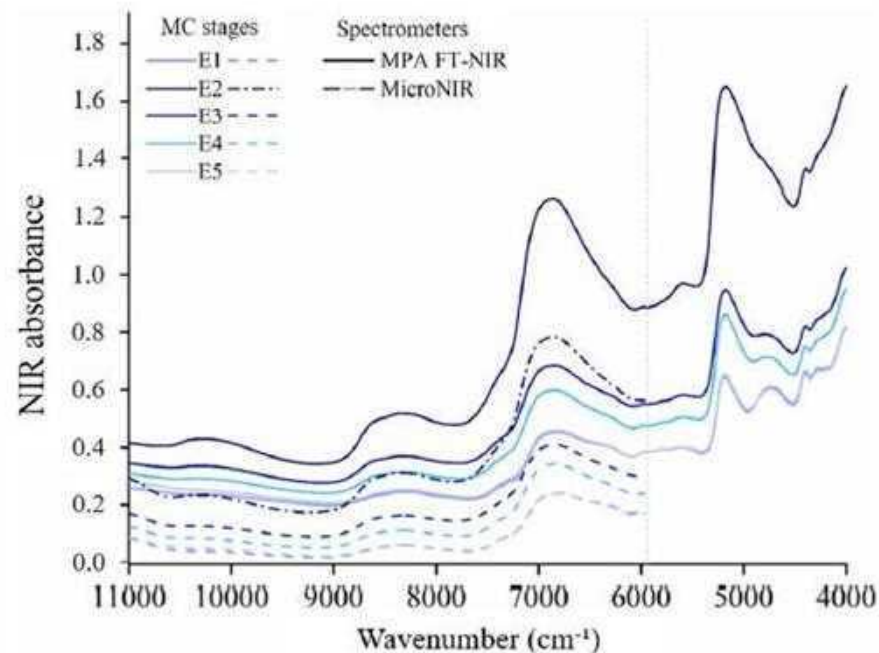


Figure 4: Averaged spectral signature (all species) per drying stage obtained with the benchtop spectrometer, considering the initial moisture content (Stage E1) to the equilibrium moisture content after saturation (Stage E5).

Table 5: PLS-DA models developed for classifying wood species from NIR spectra recorded using benchtop and portable NIR equipment at different wood moisture contents.

Equipment	Drying stage	MC %	Spectral range (cm ⁻¹)	Treatment	Nc	Np	LV	Hits %	
								Ccv	Cp ¹
MPA FT-NIR	E1	12	11,013–4,000	1D 25.2.1	88	22	9	100	100
	E2	42		MSC	88	22	9	99	91
	E3	32		MSC	88	22	9	92	95
	E4	23		1D 25.2.1	88	22	9	95	86
	E5	12		MSC	88	22	9	99	100
MicroNIR	E1	12	11,008–5,967	–	88	22	9	94	91
	E2	42		2D 15.2.2	88	22	9	97	91
	E3	32		2D 15.2.2	88	22	9	97	95
	E4	23		SNV + 2D	88	22	9	97	95
	E5	12		–	88	22	9	97	100

1D, 1st derivative of Savitzky and Golay (25.2.1); 2D, 2nd derivative of Savitzky and Golay (15.2.2); MSC, multiplicative scatter correction; SNV, standard normal variate; LV, latent variables; Nc, number of samples in calibration, Np, number of species in test set validation; Ccv, percentage of the cross-validation hits; and Cp, percentage of the correct answers in independent test set validation.

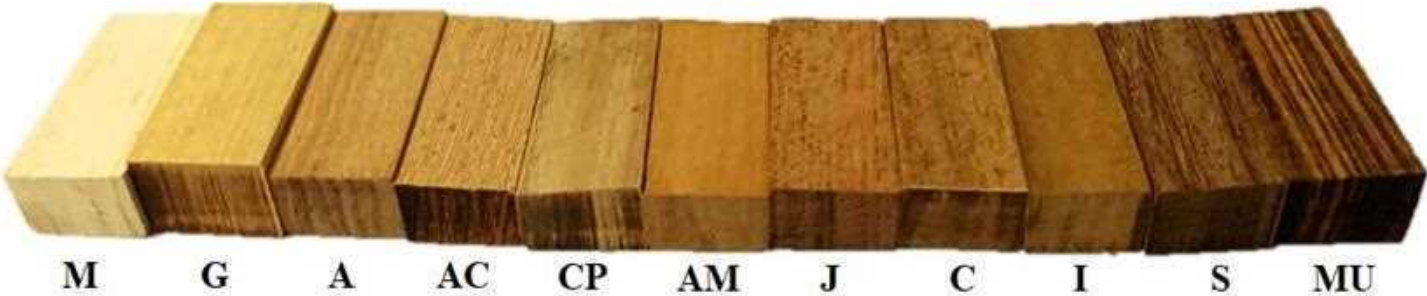


Table 7 – Confusion matrix of the Global PLS-DA models for wood species classification in independent test set

MPA FT-NIR global (model 2, Table 6)													n	n Hits	% Hits
Test set	A	AC	AM	C	CP	G	I	J	M	MU	S	n			
A	10											10	10	100	
AC	3	4				3						10	4	40	
AM			9		1							10	9	90	
C				10								10	10	100	
CP					4			2	4			10	4	40	
G						10						10	10	100	
I				1		1	8					10	8	80	
J								10				10	10	100	
M									10			10	10	100	
MU										10		10	10	100	
S							1				9	10	9	90	
Total												110	94	85	

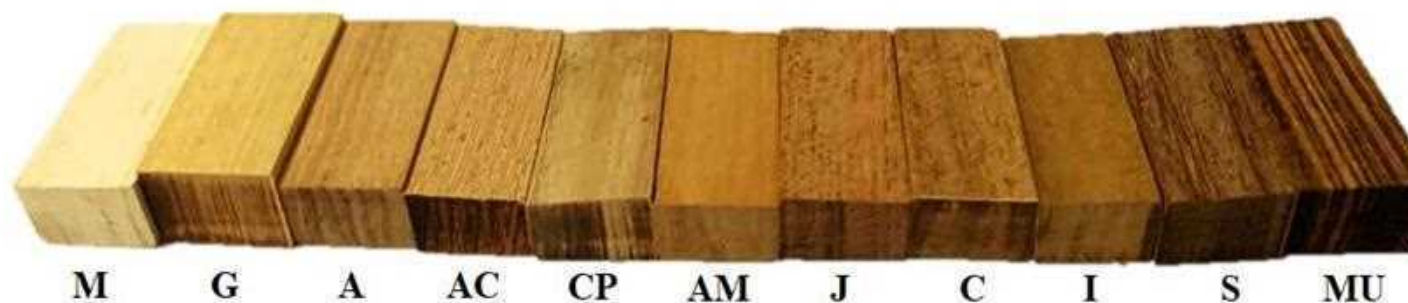


Table 1. Amazonian species used.

Code.	Popular name in Brazil
A	Aroeira
AC	Angelim
AM	Garapeira amarela
C	Cumaru
CP	Castanheira
G	Guajará - curupixá
I	Itaúba
J	Jatobá
M	Marupá
MU	Muracatiara
S	Sucupira

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AC	3	4				3						10	4	40
AM			9		1							10	9	90
C				10								10	10	100
CP					4			2	4			10	4	40
G						10						10	10	100
I				1		1	8					10	8	80
J								10				10	10	100
M									10			10	10	100
MU										10		10	10	100
S							1				9	10	9	90
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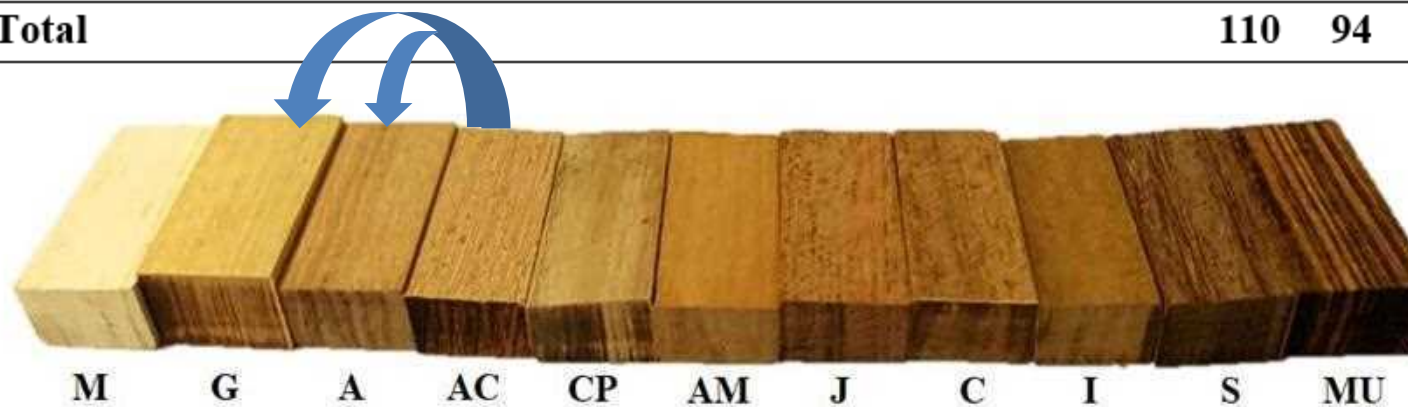


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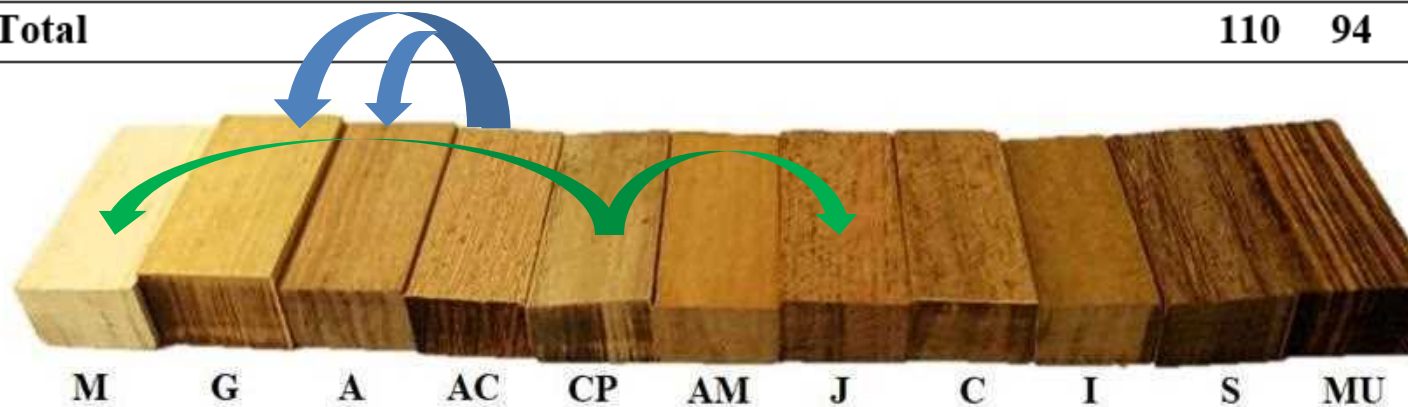


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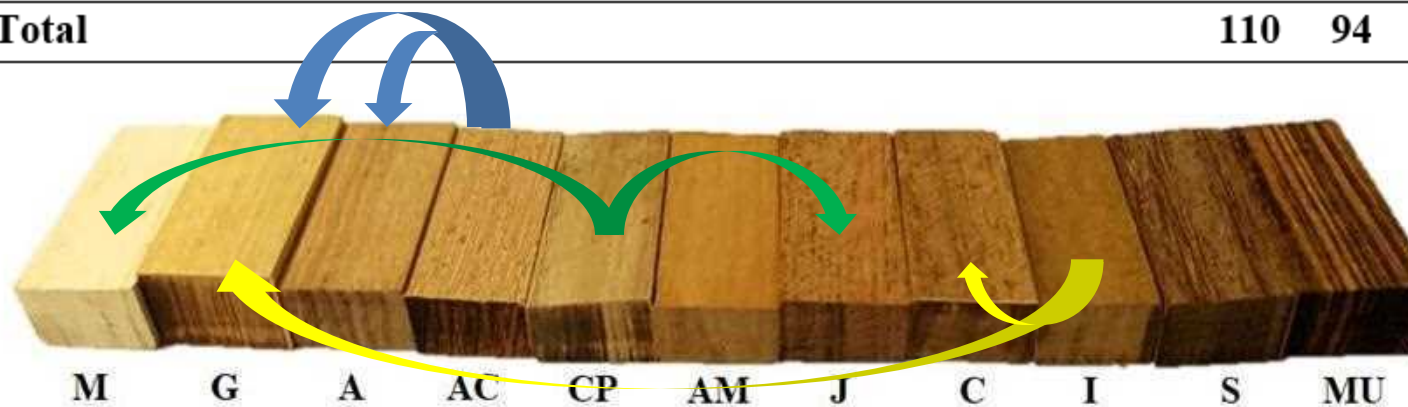


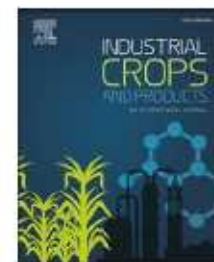
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Water desorption monitoring of cellulose pulps by NIR spectroscopy

Dayane Targino de Medeiros^{a,1}, Fernanda Maria Guedes Ramalho^{a,2}, Felipe Gomes Batista^{a,3},
Adriano Reis Prazeres Mascarenhas^{b,4}, Gilles Chaix^{c,d,e,5}, Paulo Ricardo Gherardi Hein^{a,*,6}

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^e ChemHouse Research Group, Montpellier, France

ARTICLE INFO

Keywords:

Machine learning
Online monitoring
Quality control
Hygroscopicity
Remote sensing

ABSTRACT

Near infrared (NIR) spectroscopy can be implemented in the evaluation of cellulose. The potential of NIR spectroscopy combined with multivariate analysis to evaluate moisture variation in pulp was studied. Samples of four pulp types were conditioned to different moisture levels. The samples were air dried in a controlled environment, at each 10 % moisture reduction the material was weighed and analyzed with the NIR spectrometer. Principal Component Analysis (PCA) and Partial Least Squares Regression (PLS-R) were applied to the spectral signatures and moisture values obtained during drying. Combining NIR spectroscopy with PLS-R, the moisture of the pulps under different conditions was estimated with R^2_p ranging from 0.89 to 0.98 for independent validation and root mean square error (RMSEP) ranging from 5.1 % to 18.3 %. The PLS-R models were applied to NIR spectra taken from other pulps and the estimates were consistent. The models showed robustness for monitoring pulps subjected to moisture variations.

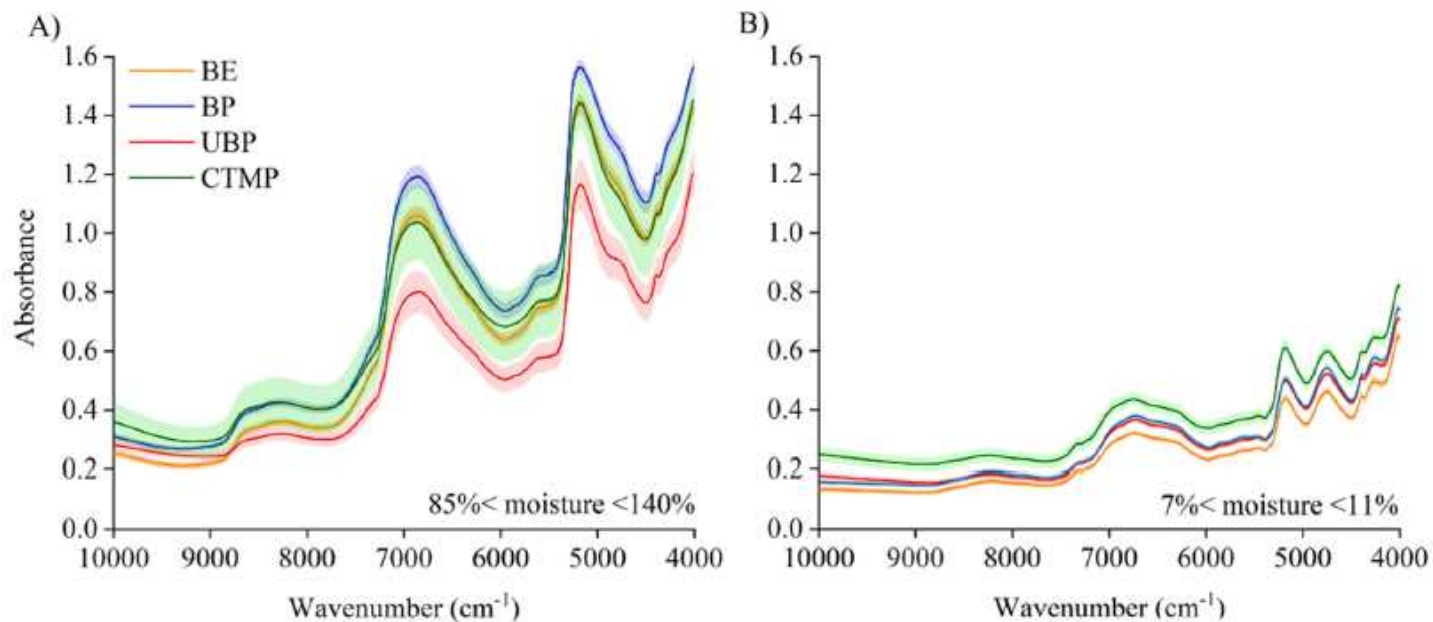


Fig. 3. Original (untreated) NIR spectral signatures by cellulose pulp type at maximum moisture (A) and equilibrium moisture (B).

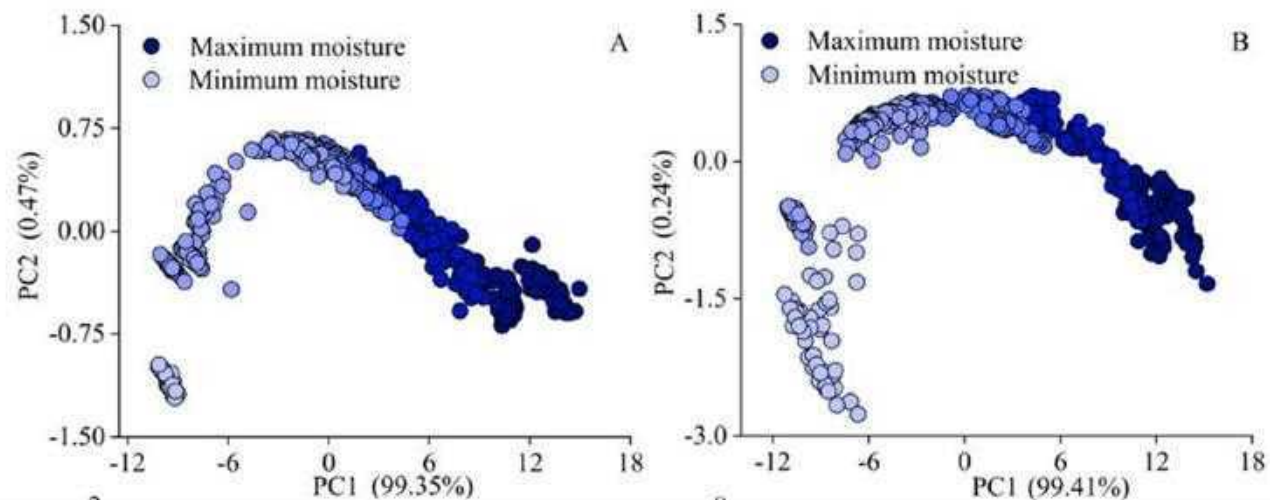


Fig. 6. PCA of the NIR spectra acquired from cellulose pulps of BE (A), BP (B), UBP (C) and CTMP per drying step.

Table 1

Parameters of the PLS-R models for determining the moisture content of commercial cellulose pulps with and without the application of mathematical pretreatments.

Treatment	Type	BE	BP	UBP	CTMP
untreated	R ² cv	0.988	0.976	0.976	0.934
	RMSEcv (%)	5.17	7.67	5.52	13.83
	N cv	520	598	456	384
	RPDcv	9.29	6.53	6.54	3.91
	R ² p (40 %)	0.987	0.977	0.976	0.936
	RMSEP (%)	5.57	7.59	5.6	14.06
	N p	208	239	182	154
1D	RPDp	8.75	6.66	6.53	3.96
	R ² cv	0.988	0.976	0.976	0.934
	RMSEcv	5.16	7.67	5.52	13.84
	R ² p (40 %)	0.988	0.977	0.975	0.941
	RMSEP	5.17	7.62	5.96	13.96
2D	R ² cv	0.989	0.978	0.972	0.898
	RMSEcv	5.00	7.40	6.03	17.28
	R ² p (40 %)	0.988	0.970	0.969	0.898
	RMSEP	5.16	8.65	6.44	18.35
	RMSEP	7.21	8.49	5.61	13.27
SNV	R ² cv	0.976	0.964	0.968	0.929
	RMSEcv	7.34	9.45	6.42	14.44
	R ² p (40 %)	0.977	0.972	0.976	0.946
	RMSEP	7.21	8.49	5.61	13.27
MSC	R ² cv	0.977	0.964	0.958	0.945
	RMSEcv	7.15	9.44	7.32	12.67
	R ² p (40 %)	0.978	0.966	0.957	0.946
	RMSEP	7.13	9.00	7.45	13.30

R²cv - coefficient of determination for cross-validation; RMSEcv - root mean square error for cross-validation; N cv - number of samples for cross-validation; RPDcv - ratio of performance to deviation for cross-validation; R²p - coefficient of determination for prediction; RMSEP - root mean square error for prediction; N p - number of samples for prediction; RPDp - ratio of performance to deviation for prediction. 1D - first derivative; 2D - second derivative; SNV - standard normal variate; MSC - multiplicative scatter correction.

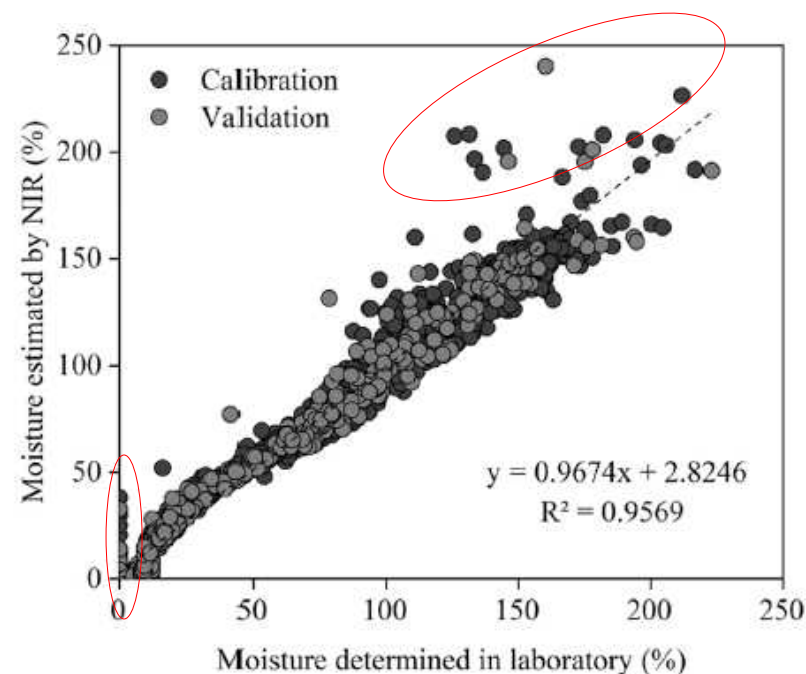
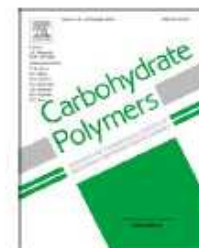


Fig. 7. Plot of global PLS-R with independent validation for estimating the moisture content of commercial cellulose pulps from untreated NIR spectra.



Artificial neural network and partial least square regressions for rapid estimation of cellulose pulp dryness based on near infrared spectroscopic data



Lívia Ribeiro Costa^a, Gustavo Henrique Denzin Tonoli^a, Flaviana Reis Milagres^b, Paulo Ricardo Gherardi Hein^{a,*}

^a Department Forest Science, Universidade Federal de Lavras, 37200-000 Lavras, Minas Gerais, Brazil

^b KLABIN S.A., Fazenda Monte Alegre, CEP: 84275-000, Telêmaco Borba, PR, Brazil

ARTICLE INFO

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Cellulose fibers
Content of solids
NIR
ANN

ABSTRACT

The content of water in fiber suspension and affects pulp refining, bleaching and draining operations. Cellulose pulp dryness estimate through near infrared (NIR) spectroscopy coupled with multivariate regressions or artificial neural network (ANN) techniques are not well explored yet. In this study models were developed to estimate cellulose pulp dryness in pads based on the NIR spectra. Thus, the cellulose pulp pads (4 mm thick) were weighed and their NIR spectra were obtained in several stages during desorption from 13.1 to 98.3% of content of solids. Partial least square regression (PLS-R) was developed from whole NIR spectra (1300 Absorbance values) and six spectral variables (from 1300) were selected for developing the PLS-R (6) and the ANN model. Both trained neural network and regression can predict pulp dryness of unknown cellulose pulp pads from their NIR data with an error of 2.5%. PLS-R models based on whole NIR spectra showed accurate predictions (the R^2 of lab-determined and estimated values plot was 0.99) while the ANN showed the same predictive performance from only six NIR variables. Predictive models developed from full NIR spectra and those based on only 6 variables were compared. Our findings indicate that NIR spectroscopy coupled with multivariate analysis and Artificial neural networks are a promising tool for monitoring the weight variation due to dewatering of the cellulose pulps in real time.

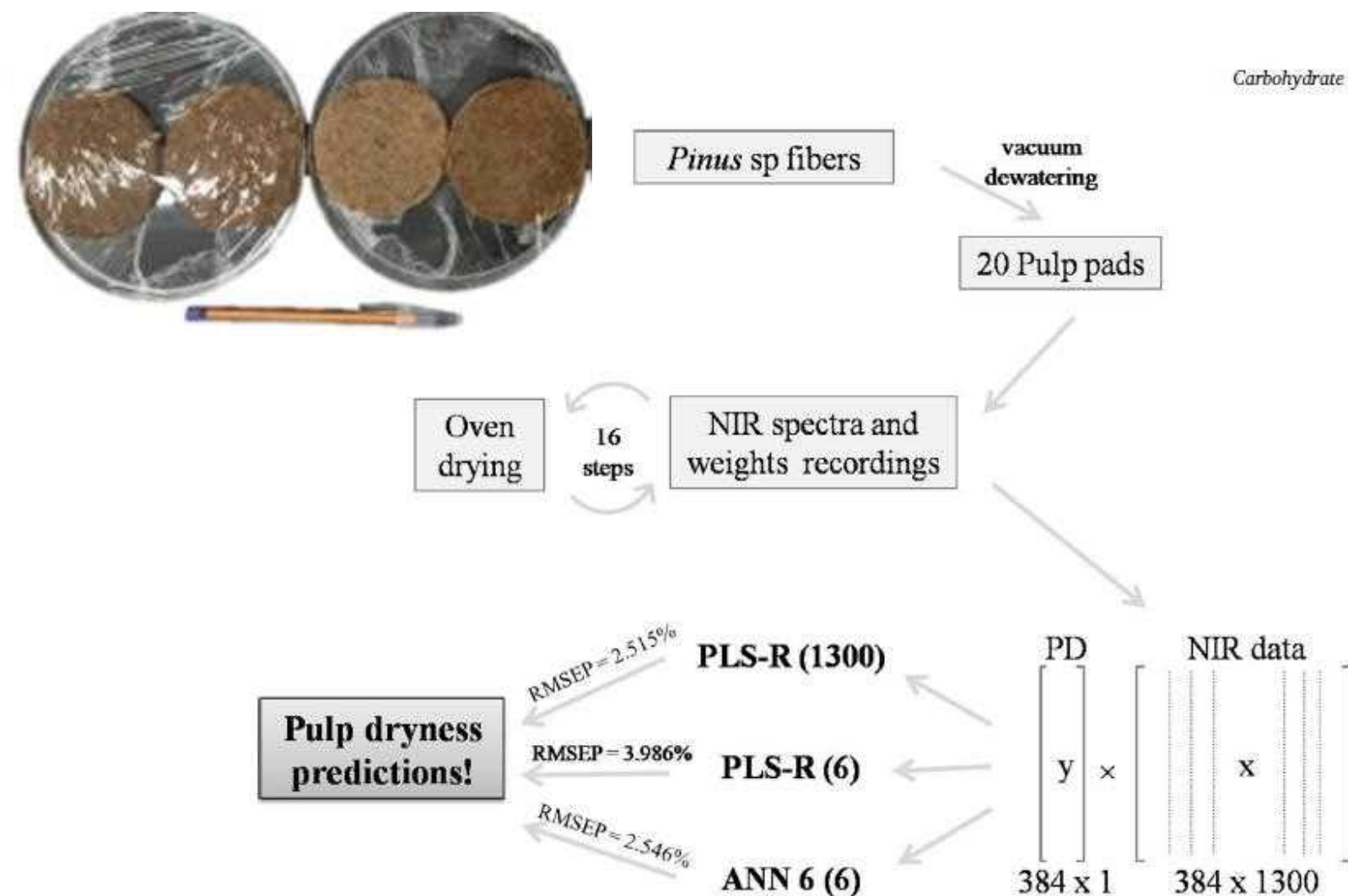


Fig. 1. Strategy of pulp pads production, weight and NIR data recordings for matrix building and PLS-R and ANN modeling for estimating pulp dryness (PD) values from NIR information.

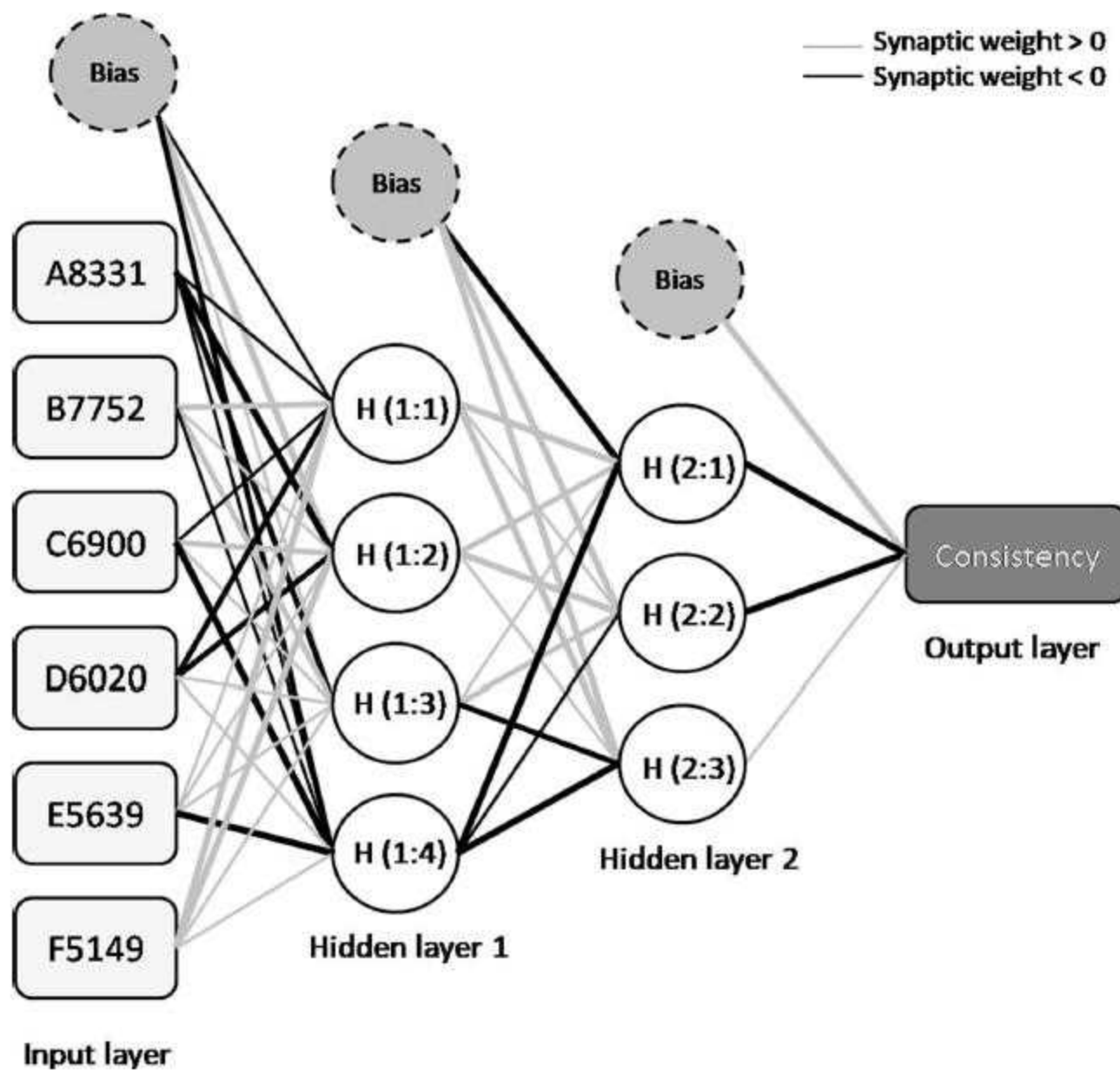


Fig. 2. Network Diagram for estimating pulp dryness values from NIR spectra.

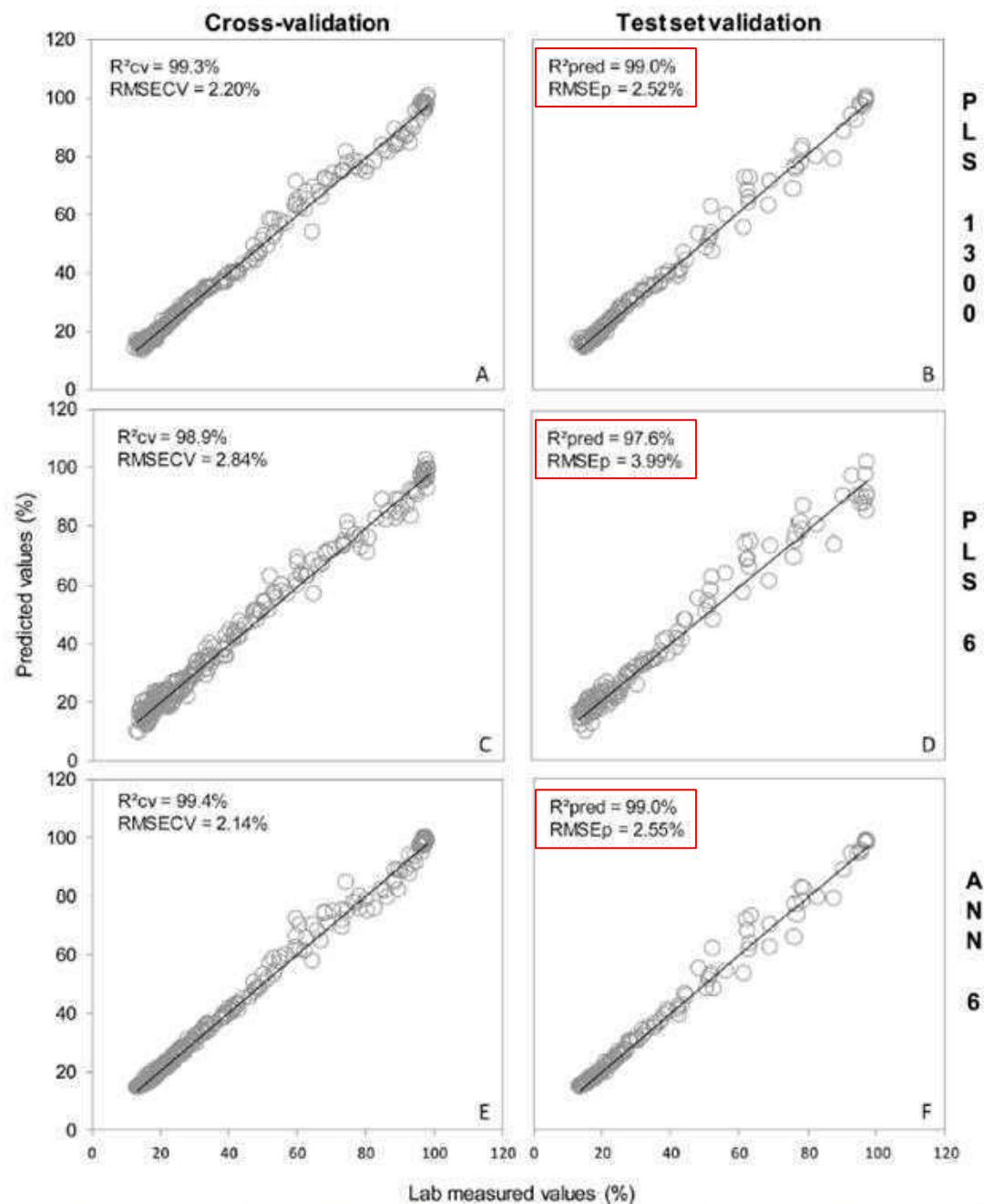


Fig. 4. Pulp dryness values determined in laboratory by gravimetry and estimated based on NIR for the three models generated (PLS1300, PLS6 and ANN6) by cross-validation and test set validation.



CAIO PALMEIRA GOULART

**ESTIMATIVA DA UMIDADE DE TORAS DE *Eucalyptus* sp. EM CAMPO A PARTIR
DE ESPECTROMETROS NO NIR PORTÁTEIS**



Sampling protocol: obtaining wood powder on site



Analytical protocol: determining wood moisture



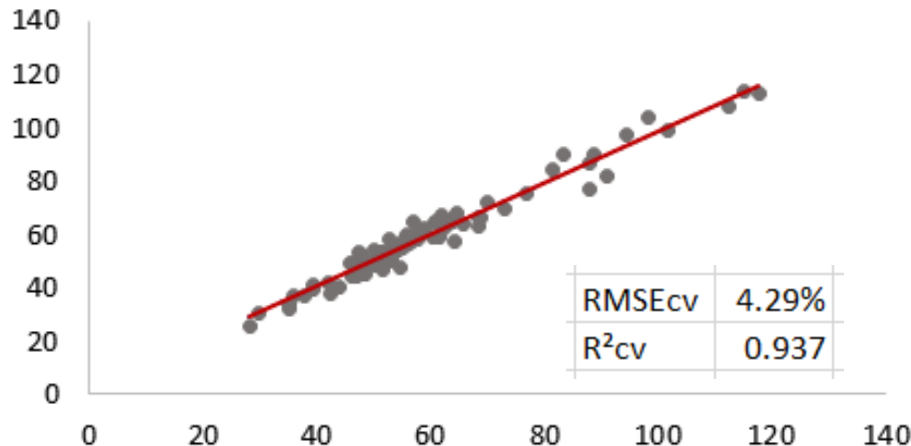
NIR-based models:

estimating wood moisture from powder taken on site



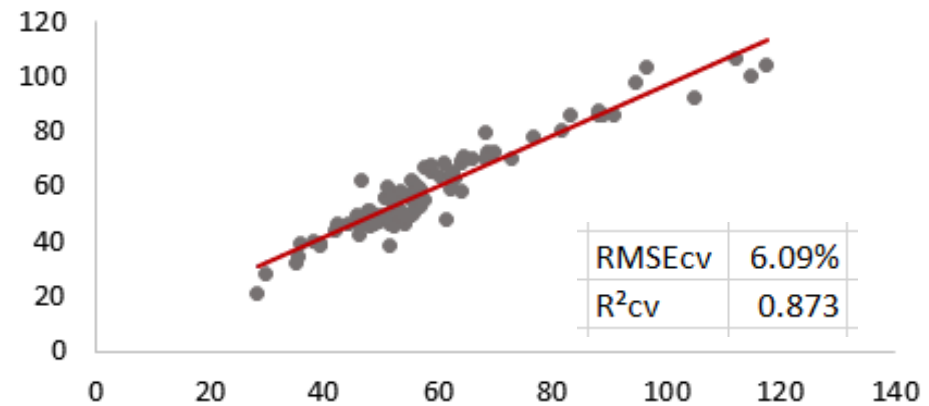
MicroNIR

PSL-R Global brutos



TrinamiX

PSL-R Global brutos



NIR portable applications:

Wood moisture, density, lignin and extractive content, etc.



Criticism and perspectives

Actual Limitations

- ✓ Working with NIR technology in laboratory conditions **is easy!**
- ✓ NIR spectra have been collected with different tools, different protocols and conditions.
- ✓ Using too many NIR models to estimate wood properties makes their practical application unfeasible!



What is missing?

- ✓ Combine several sampling and conditions
- ✓ Establish a standard protocol to perform analysis
- ✓ We need to develop practical solutions that can be applied in real-world situations





From the lab to the field: How much does moisture affect NIR readings in wood?



Thank you!

