NC STATE UNIVERSITY

Uso de Espectroscopía de Infrarrojo Cercano (NIRS) para Medición de Calidad en Materia Prima Agroindustrial

Miguel S. Castillo, Ph.D.
Forage & Grassland Program, Crop & Soil Sciences Department
www.forages.ncsu.edu
mscastil@ncsu.edu

XX Conferencia Internacional en Palma de Aceite
Cartagena, Colombia (26 – 30 Septiembre 2022)

Enfoque para Uso y Desarrollo de NIRS

Utilizar sensores NIRS para determinar parámetros de calidad

- Método rápido
- Bajo costo
- Precision comparable con métodos tradicionales
- Oportunidad para análisis *in situ*

Agenda

- Tecnología NIRS
- Aplicaciones en Agro-industria
- Oportunidades y Retos

Esquema Básico de un Espectrofotómetro

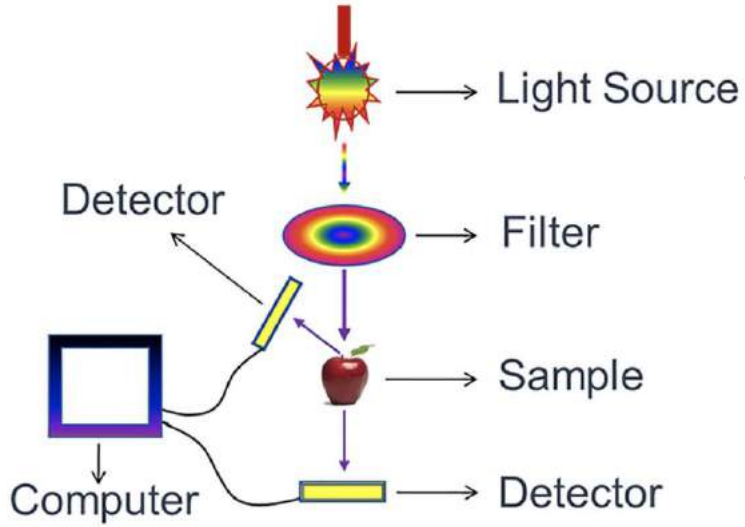
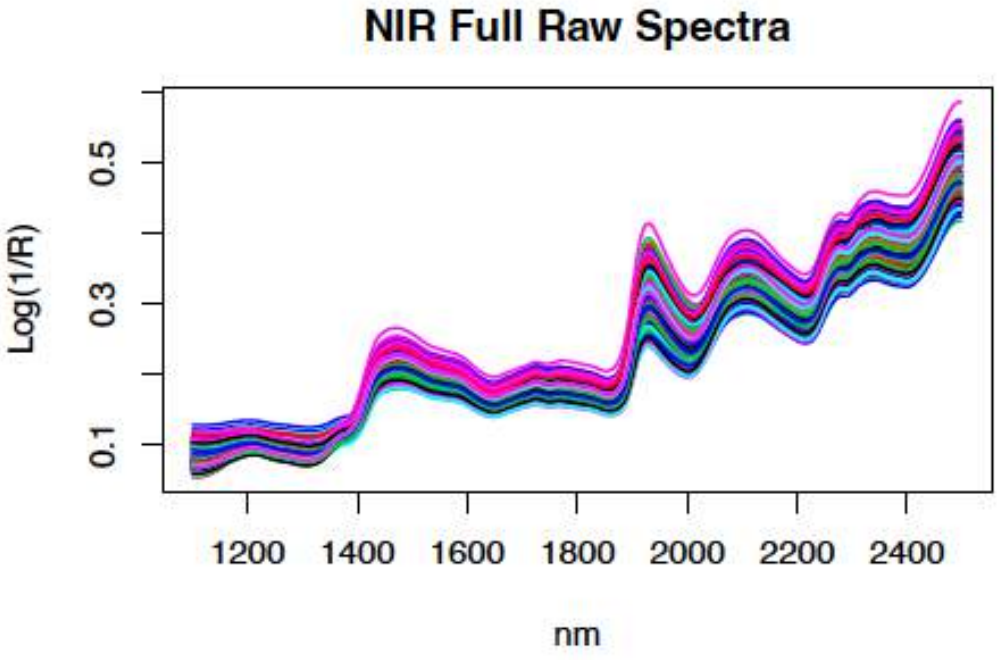


Fig. 1 Schematic of the near-infrared spectrophotometer

- Infrarrojo Cercano (NIRS: 700 – 2500 nm)

Food Anal. Methods (2019) 12:2438–2458

Los Sensores Proveen Firma Espectral



Relación NIRS-Biología

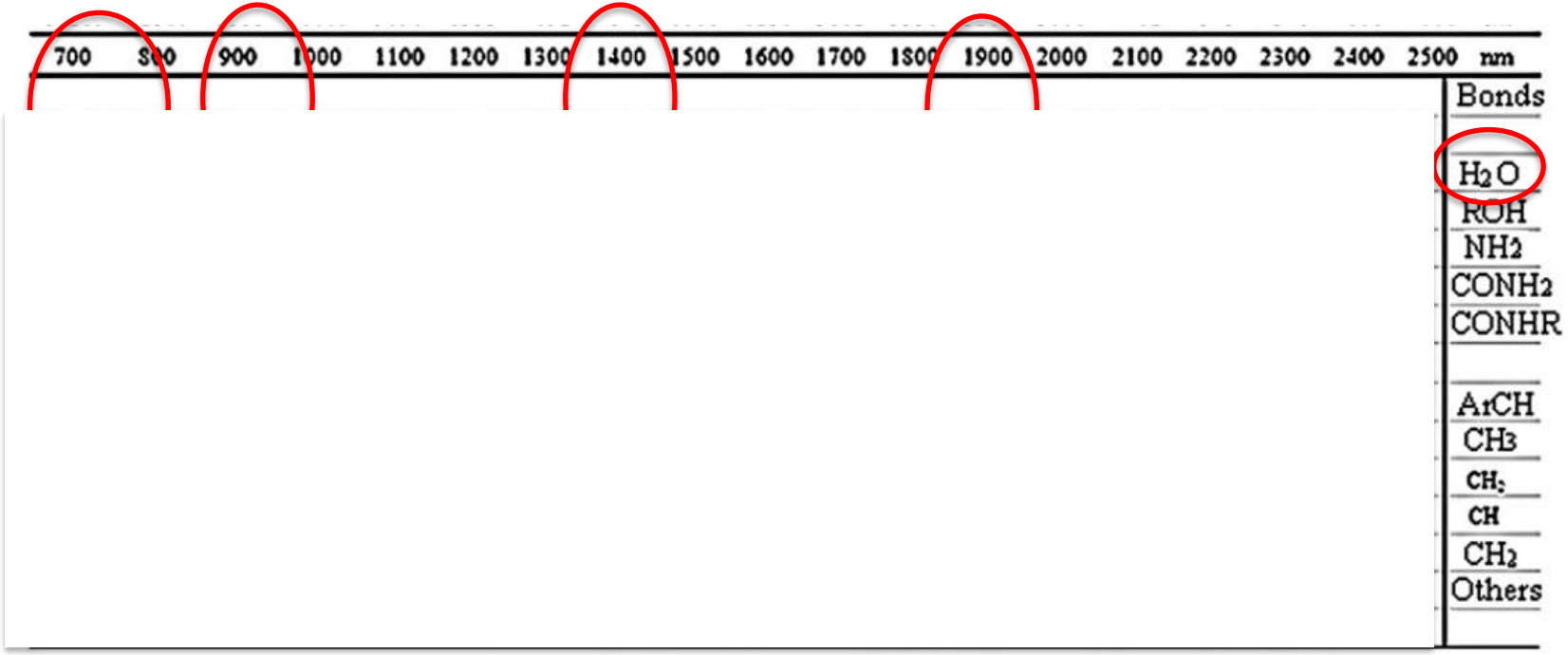
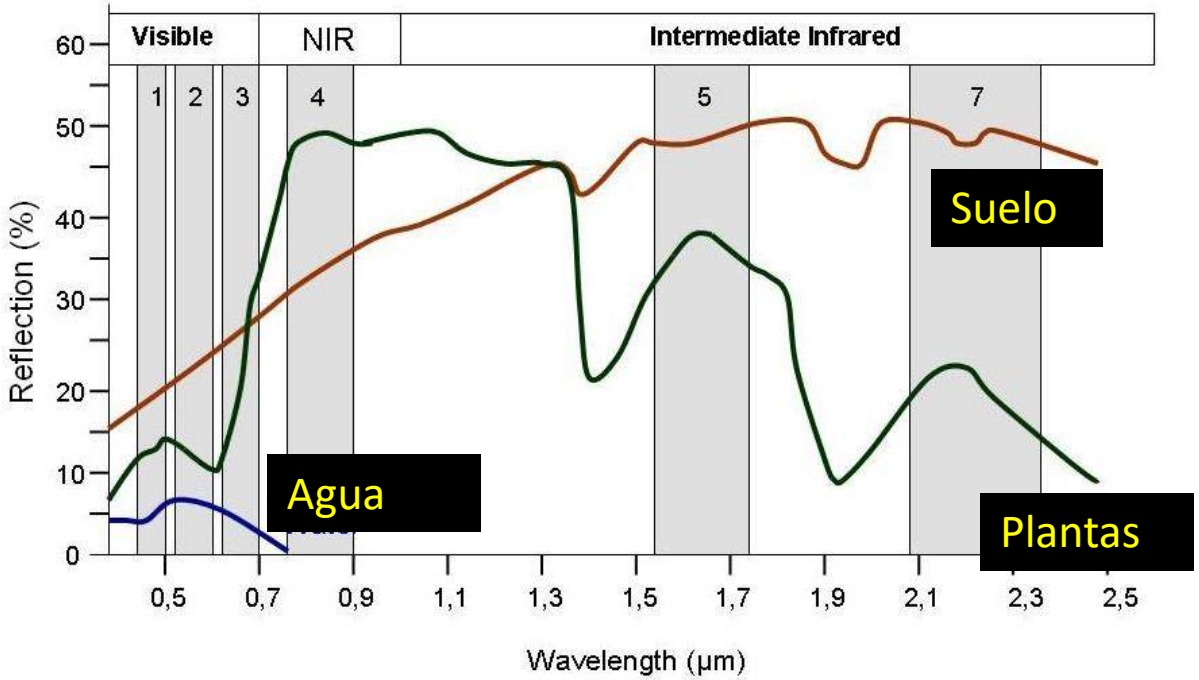
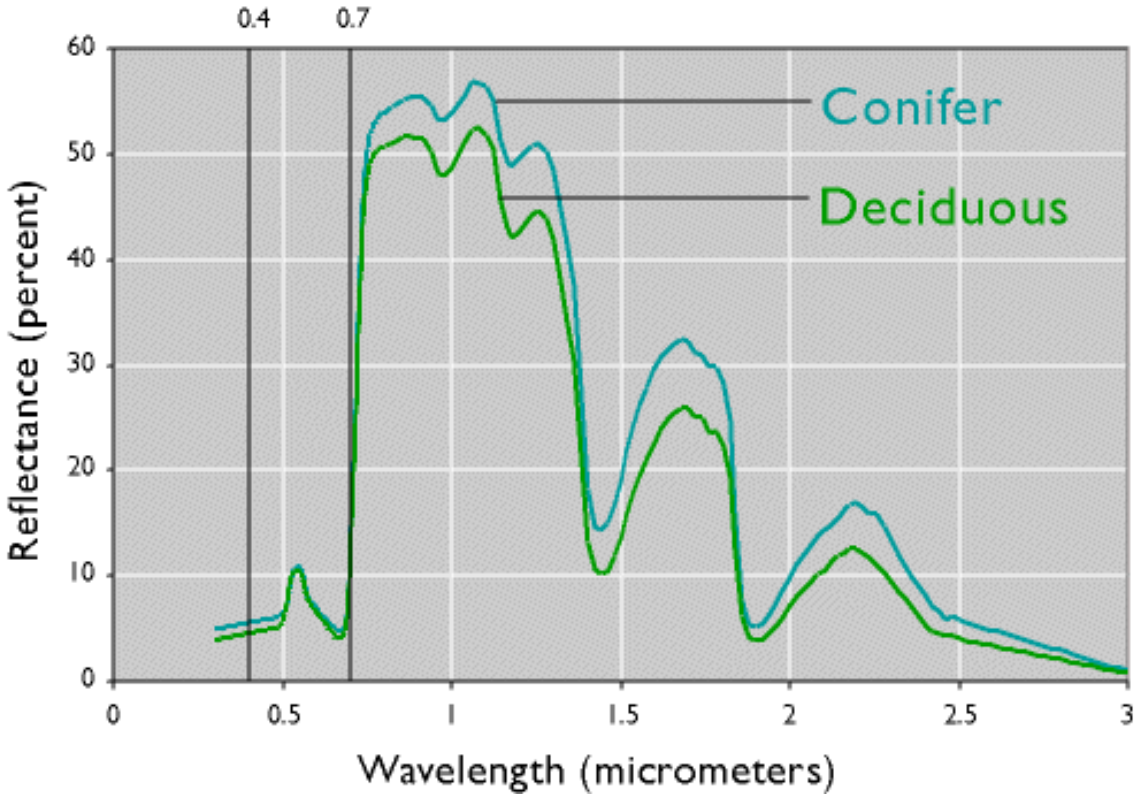


Fig. 1. The distribution of overtone and overtone combination of main organic bonds in electromagnetic wave. "=": absorption position of bonds, "C": tone combination, "2C": overtone combination, "ArCH": bond CH on the aromatic groups, "2, 3, 4, 5": first, second, third and fourth overtone. Food Science & Technology 18 (2007) 72e83

Patrones Espectrales Diferentes por Tipo de Material

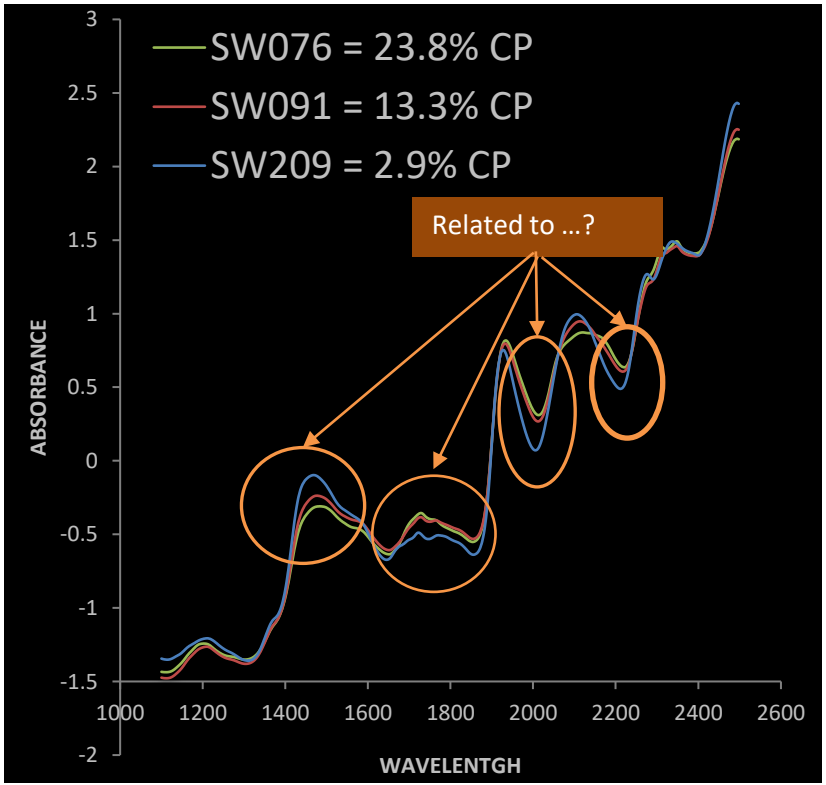


Patrones Espectrales Diferentes por Material Vegetativo



Patrones Espectrales Diferentes por Composición del Material

- Muestras del mismo cultivar de forraje con diferente concentración de proteína cruda



Desarrollo y Uso de Tecnología NIRS

Desarrollo de modelos

Firma espectral

+

Química humeda

Modelo NIRS

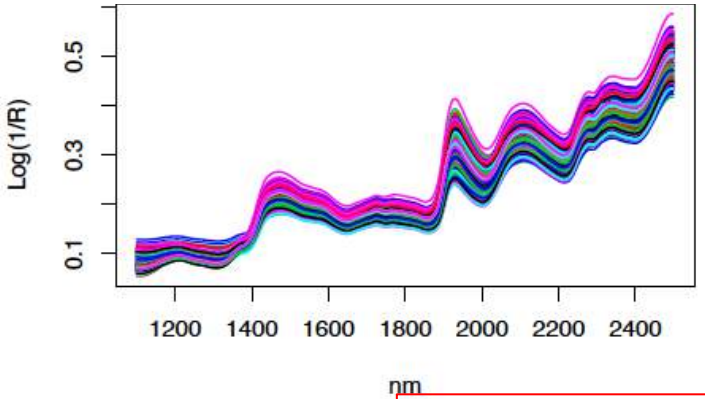
(calidad de modelos es crítico)

Uso de modelos

Valores de calidad de materia prima de nuevas muestras es determinada a partir de firmas espectrales

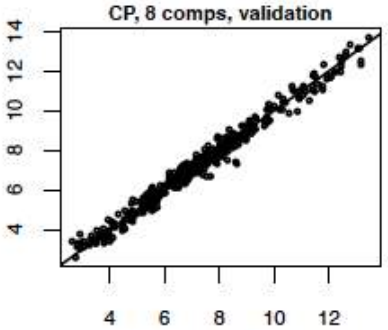
(reducir/eliminar química húmeda)

Desarrollo de Modelos NIRS

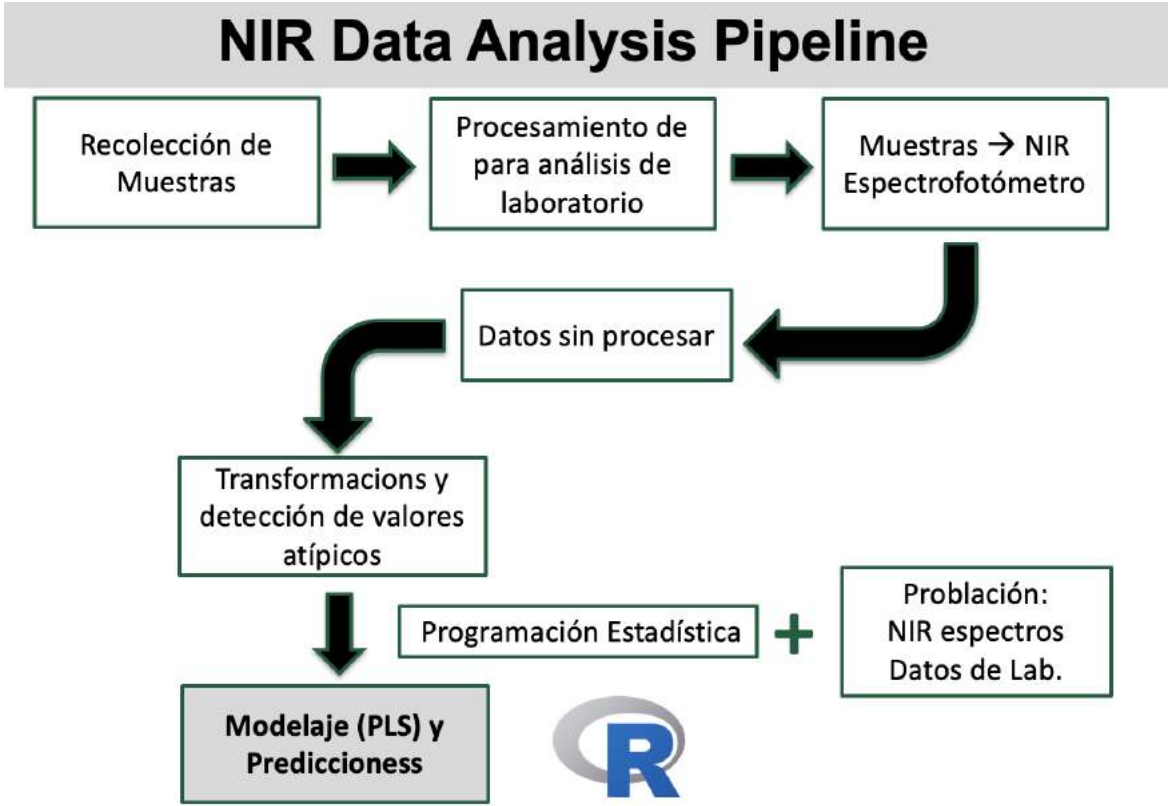


Response Variables
(Ag., Environ., Food Sci.)

Modeling (development, calibration, validation)

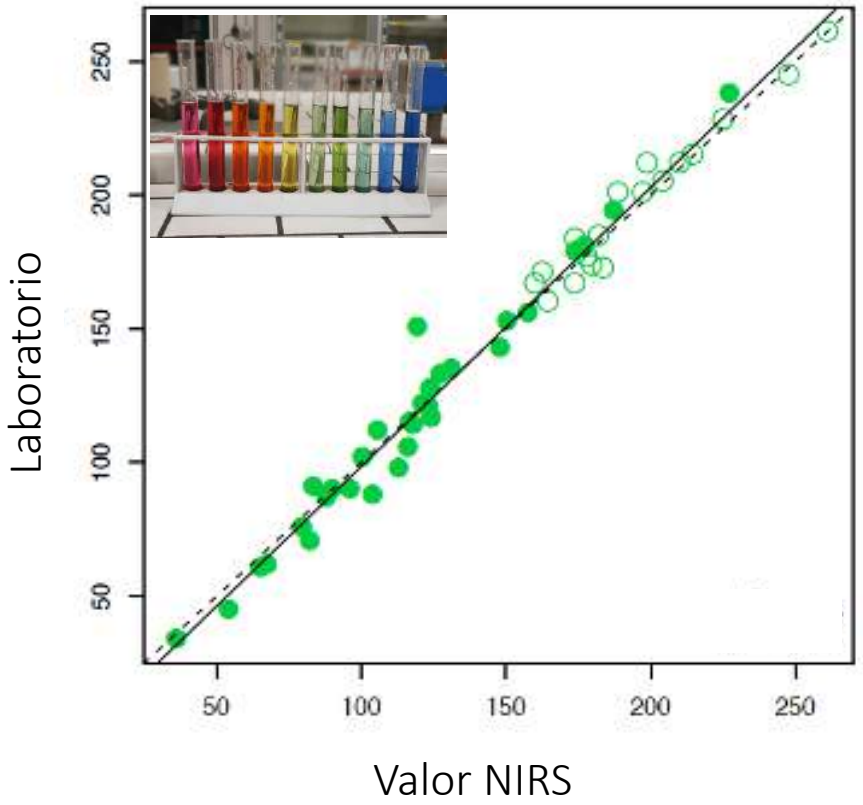


Desarrollo de Modelo



Modelo NIRS Adecuado

- Coeficiente de determinación alto (r^2 cercano a 1)
- Errores de prediccion bajos (cercano a 0)
- Pendiente de regresión cercana a 1



Diversidad de Equipos NIRS

(precio, tamaño, resolución)

Foss 6500

- Spectra: 1100-2500 nm
- Interval: 2 nm
- 700 wavelengths
- Cost (USD $): +100,000

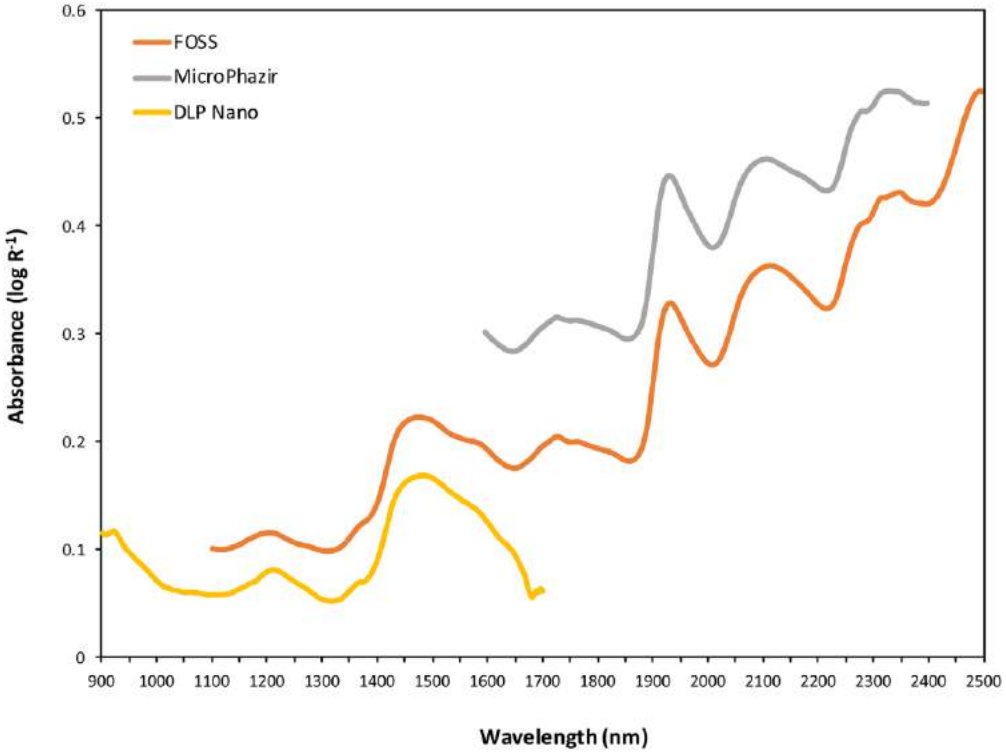
microPHAZIR (Thermo Fisher)

- Spectra: 1600-2400 um
- Interval: 8 um
- 100 wavelengths
- Cost (USD $): ~30,000

DLP NIRscan Nano (TI)

- Spectra: 900-1700 nm
- Interval: 5 nm
- 160 wavelengths
- Cost (USD $): ~1,000

Firma Espectral Varía por Equipo NIRS



Acosta, Castillo, & Hodge. Crop Sci. (2020)

Agenda

- Tecnología NIRS
- Aplicaciones en la Agroindustria
- Oportunidades y Retos

Aplicaciones NIRS en Agro-industria

Calidad de Biomasa

- Calidad:
  - Proteína, energía, digestibilidad (nutrición animal)
  - Fibra, ceniza (bioenergía)

- Materias primas:
  - Forrajes, residuos o byproductos (e.j. bagazo)

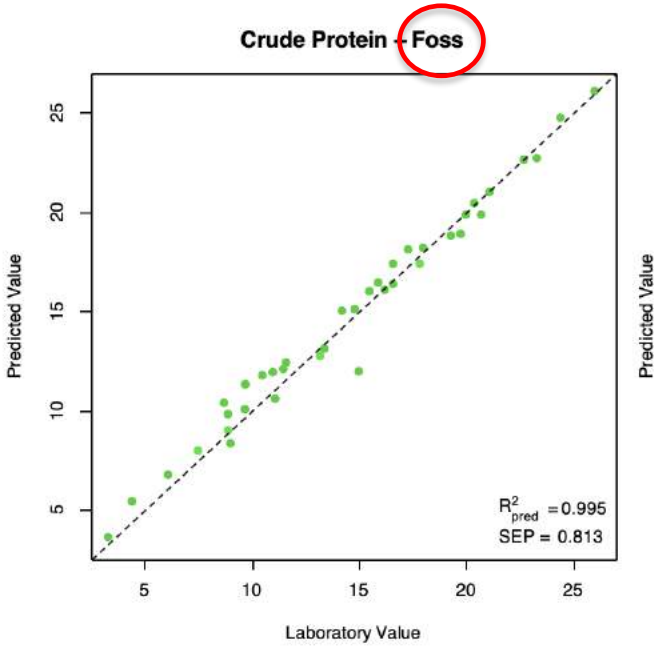
Crop Science Journal, 2020.

Acosta, J.J., Castillo, M.S., & Hodge, G.R. . Comparison of bencthop and handheld near infrared spectroscopy devices to determine forage nutritive value. Crop Sci. doi.org/10.1002/csc2.20264.

Proteína


Crude Protein – Foss
Crude Protein – MicroPhazir
Crude Protein – DLP Nano

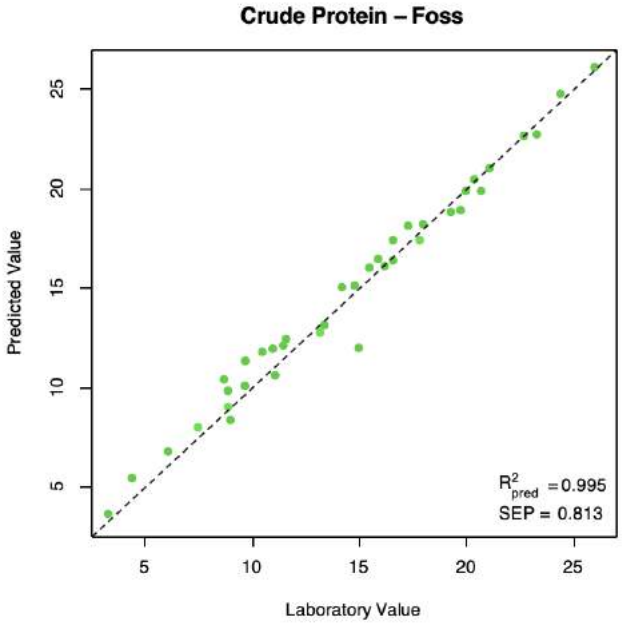
Proteína

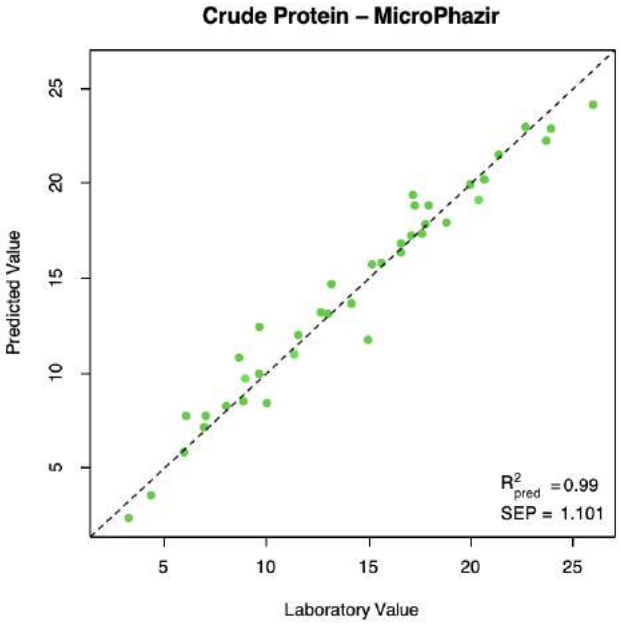


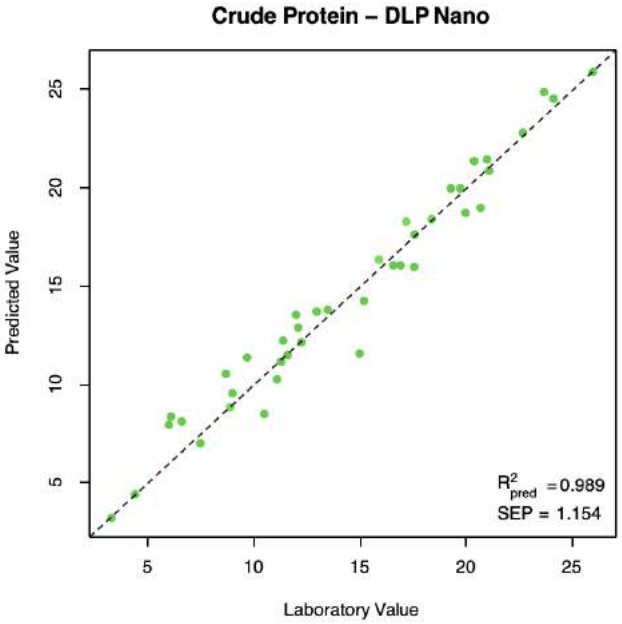
Crude Protein – MicroPhazir

Crude Protein – DLP Nano

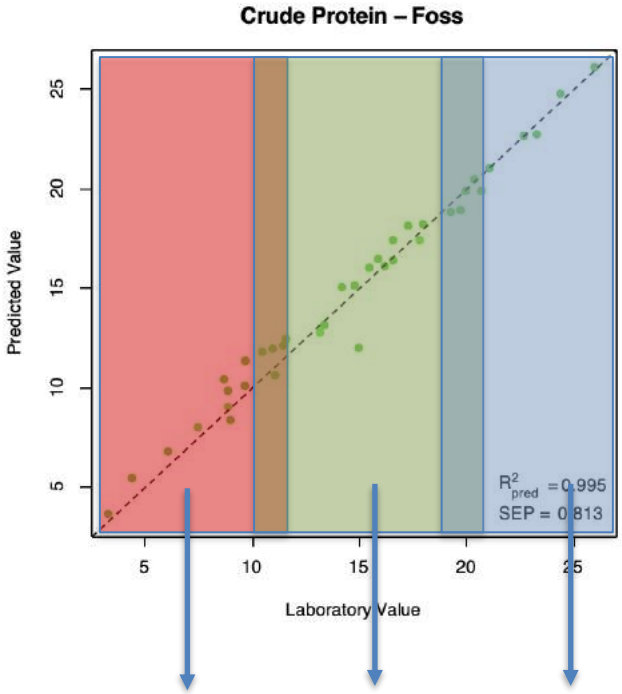
Proteína

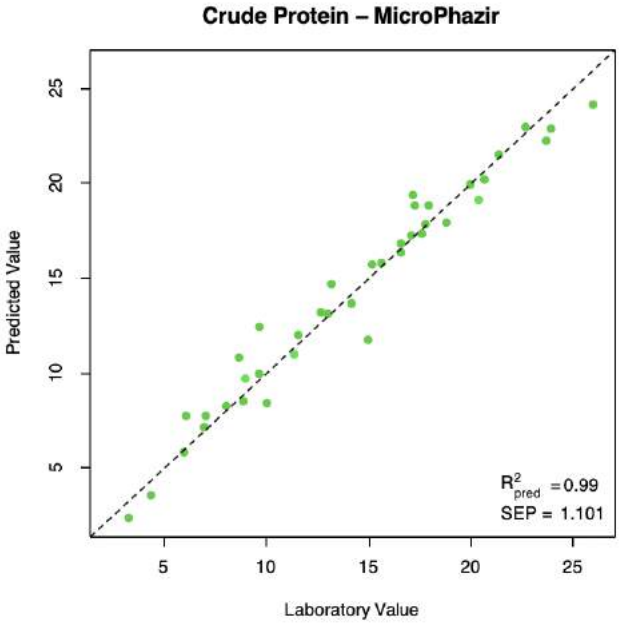

Crude Protein – Foss
Predicted Value
Laboratory Value
R^2_{pred} = 0.995
SEP = 0.813

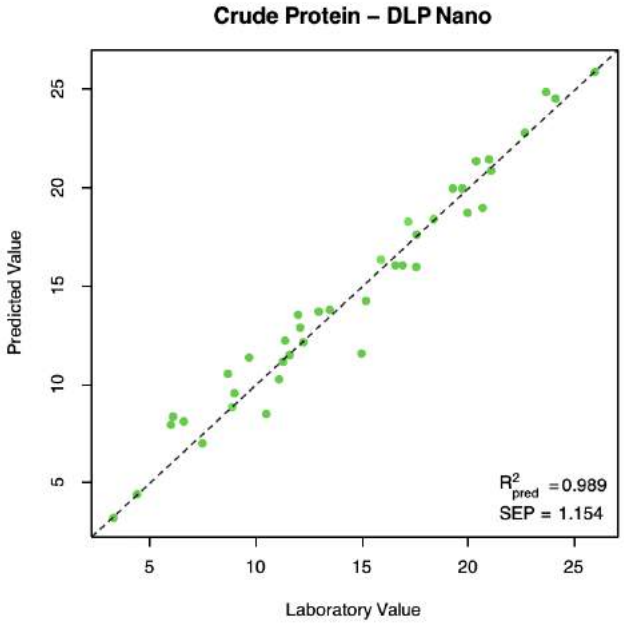

Crude Protein – MicroPhazir
Predicted Value
Laboratory Value
R^2_{pred} = 0.99
SEP = 1.101


Crude Protein – DLP Nano
Predicted Value
Laboratory Value
R^2_{pred} = 0.989
SEP = 1.154

Proteína

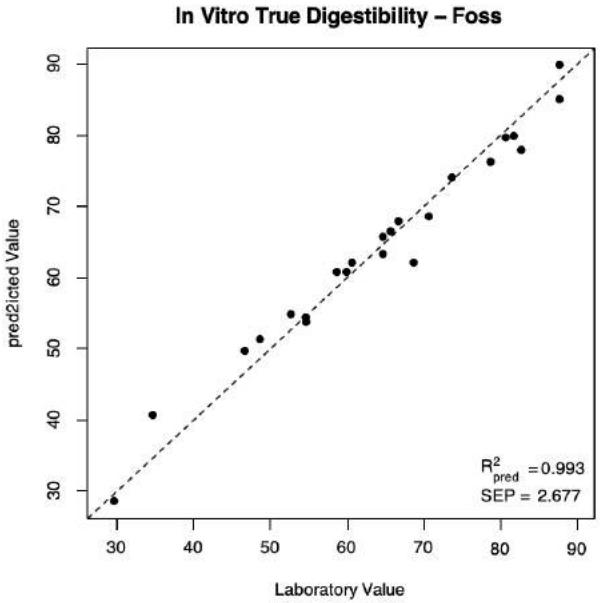


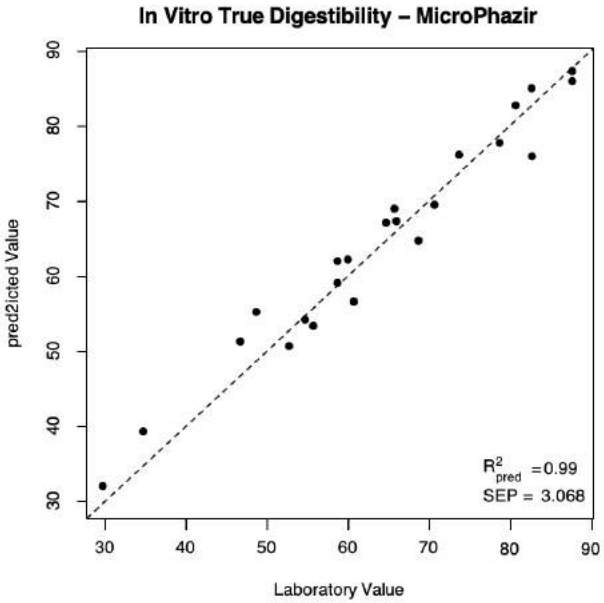


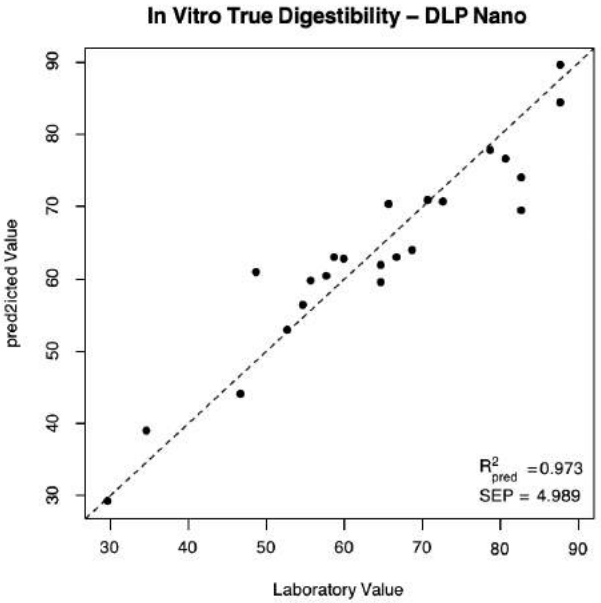


Bajo Optimo En exceso

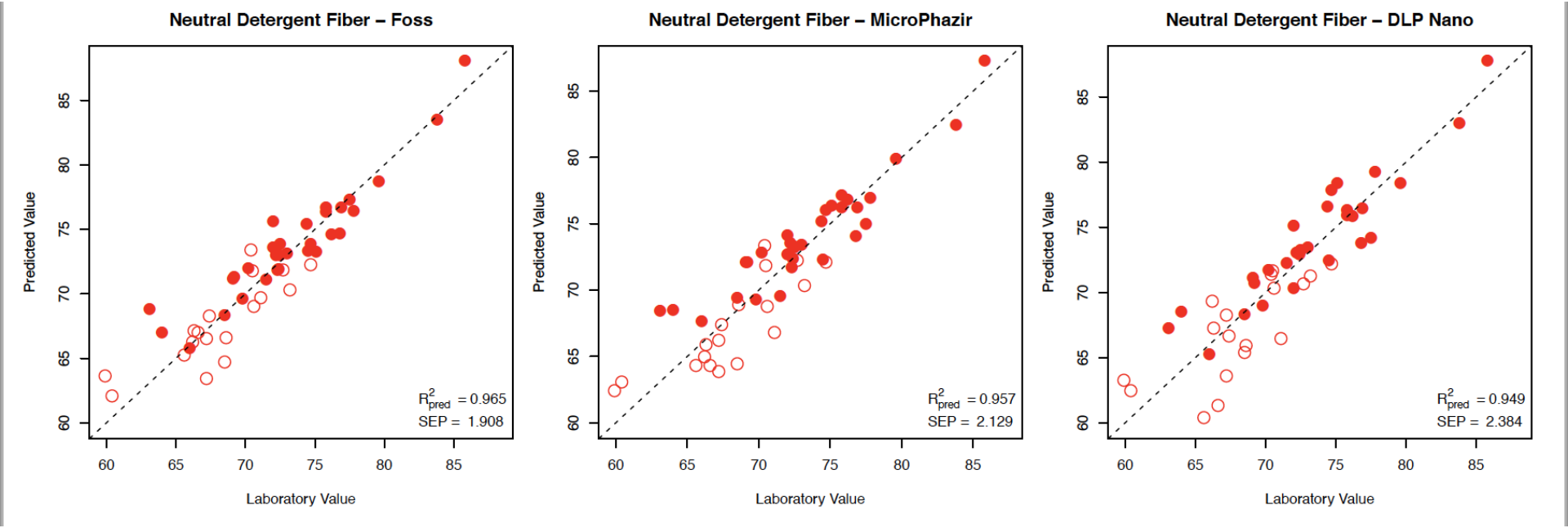
Digestibilidad (Energía)



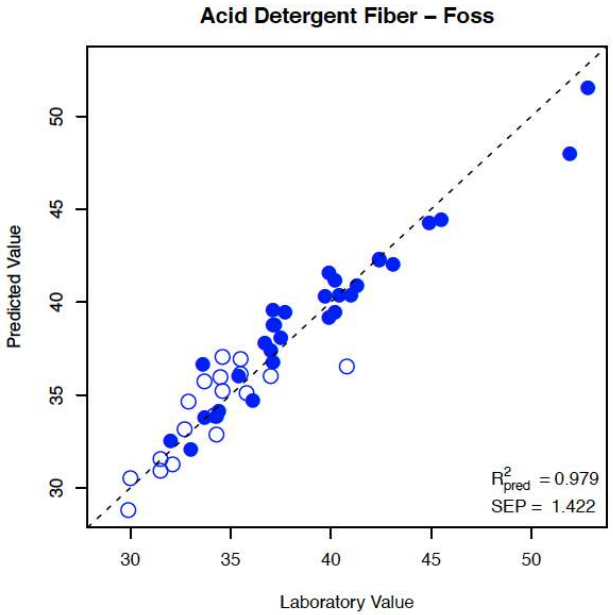


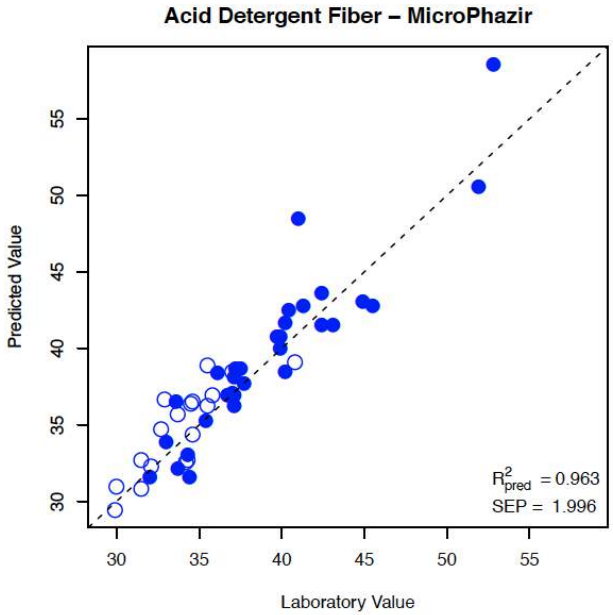


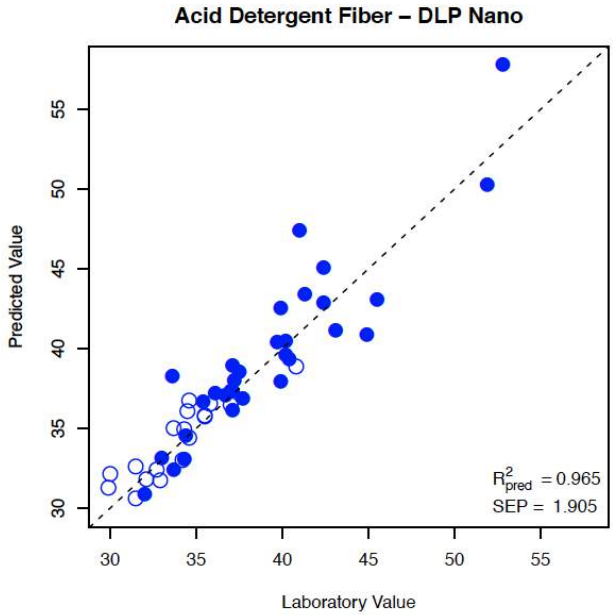
Fibra Neutro Detergente



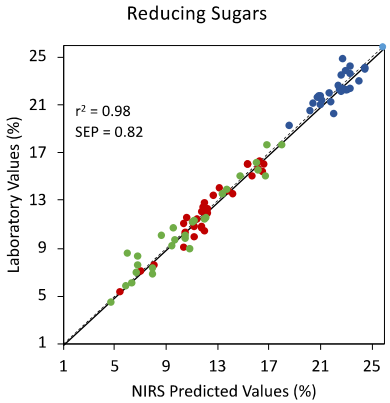
Fibra Acido Detergente

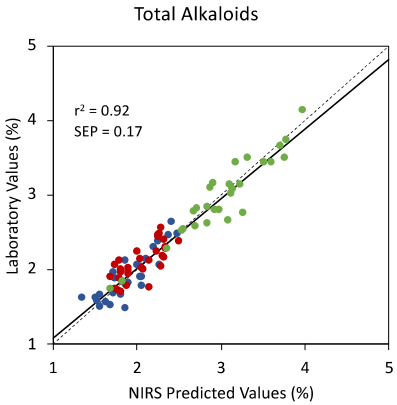


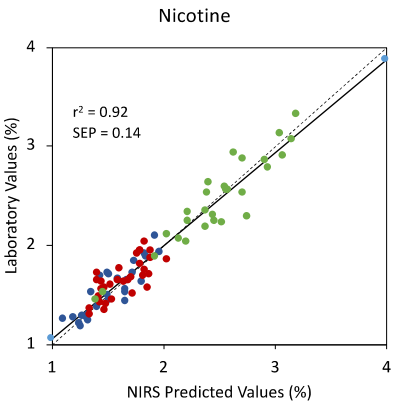




Tabaco

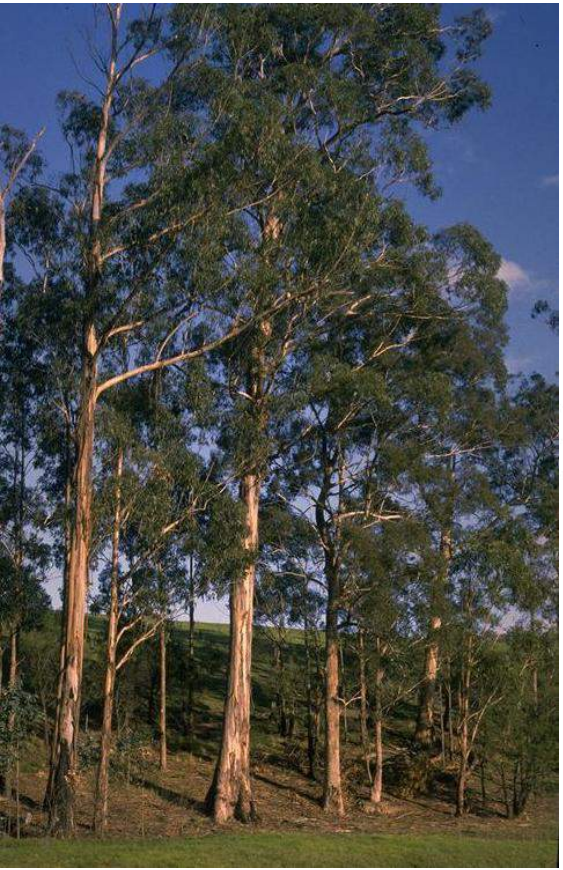


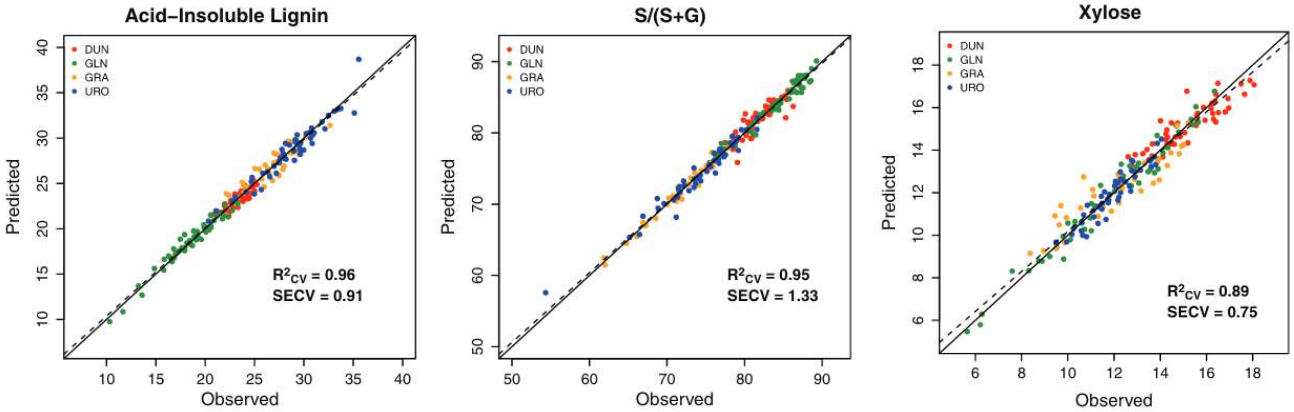




Castillo, Acosta, et al. (2022). JNIRS (in review)

Trees - Eucalyptus





Hodge, Acosta, et al. (2018). JNIRS.

The use of near infrared spectroscopy to predict foliar nutrient levels of hydroponically grown teak seedlings

William Andrew Whittier[1], Gary R Hodge[1], Juan Lopez[1], Carole Saravitz[2] and Juan Jose Acosta[1]

Table 6. Fit statistics for foliar nutrient level NIR calibration models for FOSS 6500.

	Wetlab			FOSS 6500 NIR Model						
Trait	Mean	StDev	Range	Transformation	Factors	R^2	SEC	r^2_{cv}	SECV	RPD_{cv}
Nitrogen (%)	3.3	0.9	1.2–6.0	SNV	10	0.96	0.15	0.96	0.18	5.00
Phosphorus (%)	0.5	0.2	0.2–1.4	NIR	15	0.94	0.069	0.90	0.092	2.17
Potassium (%)	3.2	0.7	1.4–5.0	DT_SG7	9	0.94	0.19	0.83	0.30	2.33

JNIRS JOURNAL OF NEAR INFRARED SPECTROSCOPY

Near infrared spectroscopy: a rapid and non-destructive technique to assess the ripeness of oil palm (*Elaeis guineensis* Jacq.) fresh fruit

Divo Dharma Silalahi,[a]* Consorcia E. Reaño,[b] Felino P. Lansigan,[b] Rolando G. Panopio,[c] Nathaniel C. Bantayan,[d] Fabrice Davrieux,[e] J.P. Caliman,[a] Yong Yit Yuan[a] and Sudarno[a]

Figure 2. Oil palm fresh fruit bunch: unripe and ripe.

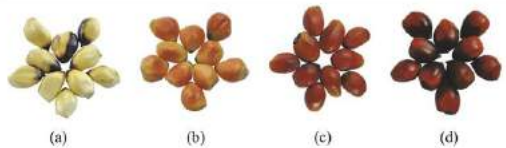


Figure 3. Individual fruit appearance based on ripeness grades: (a) unripe; (b) under-ripe; (c) ripe; (d) over-ripe.

Table 2. Ripeness grades based on oil to dry mesocarp and moisture content.

Oil to dry mesocarp (%)	Moisture content (%)	Grade
<30	⩾80	Unripe
30–75	45–80	Under-ripe
75–85	35–45	Ripe
⩾85	<35	Over-ripe

NIRS: Análisis de Plantas

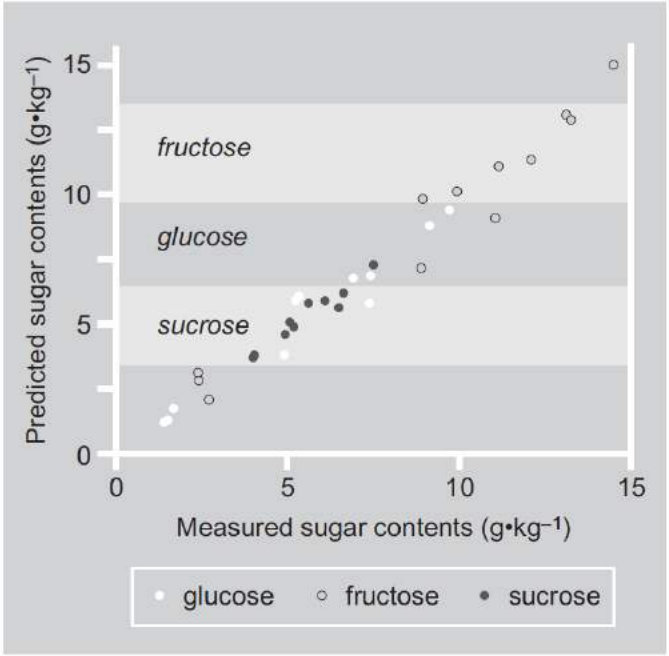


Figure 6.
Correlation of banana sugar contents measured chemically as well as non-destructively by means of NIR spectroscopy.

Fruits, 2003, vol. 58, p. 135–142. 2003 Cirad/EDP Sciences
DOI: 10.1051/fruits:2003001

NIRS: Análisis de Plantas

Analytical Methods

ROYAL SOCIETY OF CHEMISTRY

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Cite this: *Anal. Methods*, 2022, **14**, 114

Non-destructive prediction of the hotness of fresh pepper with a single scan using portable near infrared spectroscopy and a variable selection strategy†

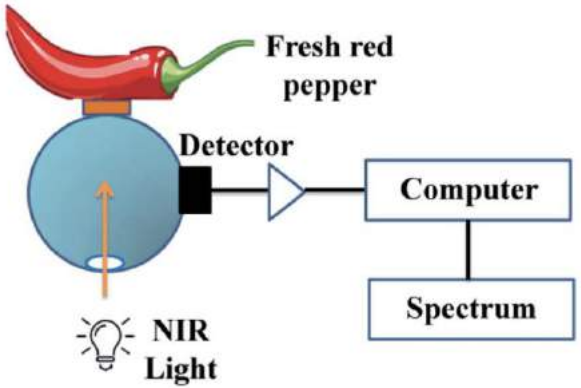


Fig. 1 Structure of the portable NIRS device.

NIRS: Análisis de Plantas

Food Analytical Methods (2018) 11:1510–1517
https://doi.org/10.1007/s12161-017-1137-2

Quality Control of Commercial Cocoa Beans (*Theobroma cacao* L.) by Near-infrared Spectroscopy

Food Analytical Methods (2020) 13:50–60
https://doi.org/10.1007/s12161-019-01503-w

Quality Control Parameters in the Roasted Coffee Industry: a Proposal by Using MicroNIR Spectroscopy and Multivariate Calibration

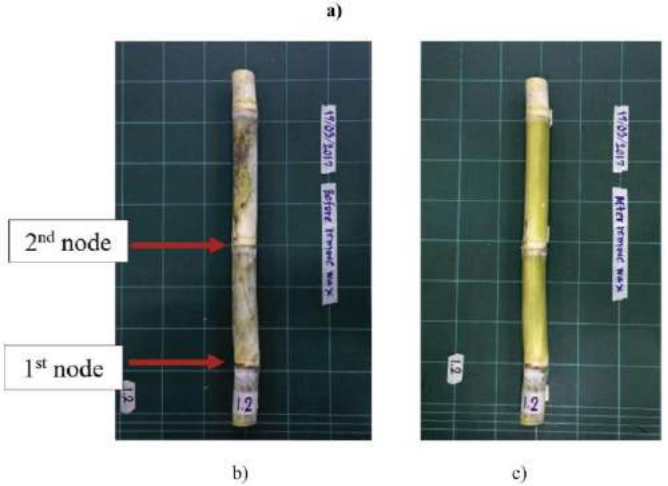
NIRS: Análisis de Plantas

Contents lists available at ScienceDirect

Sensing and Bio-Sensing Research

journal homepage: www.elsevier.com/locate/sbsr

A portable near infrared spectrometer as a non-destructive tool for rapid screening of solid density stalk in a sugarcane breeding program



NIRS: Análisis de Plantas

Azúcares totales (r^2 = 0.94; medido en jugo)

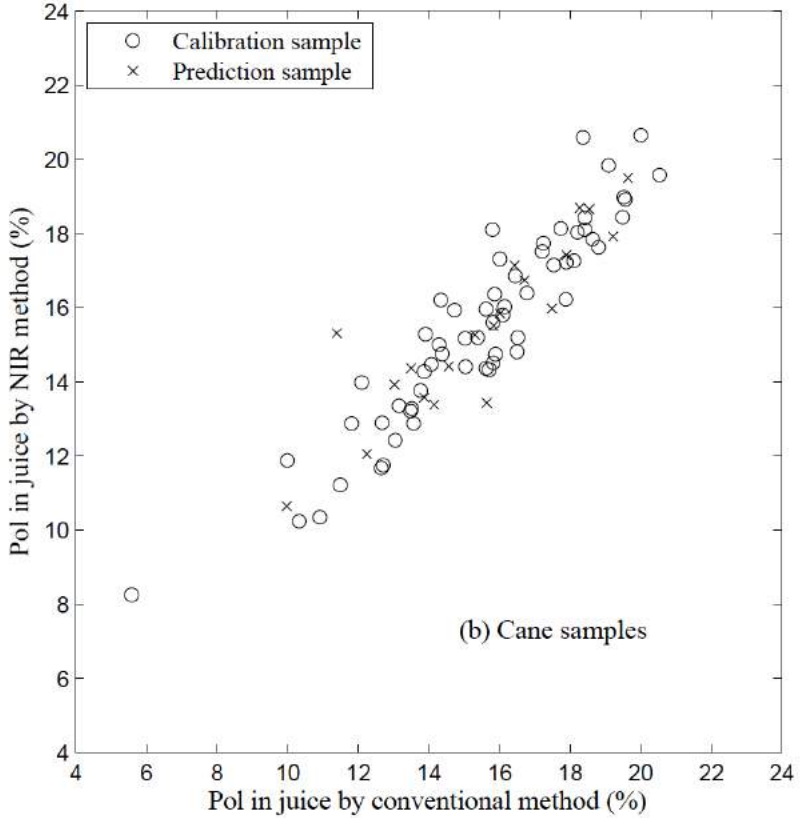
Glucosa y fructosa en jugo

Brix

Fibra (celulosa, hemicelulosa, lignina)

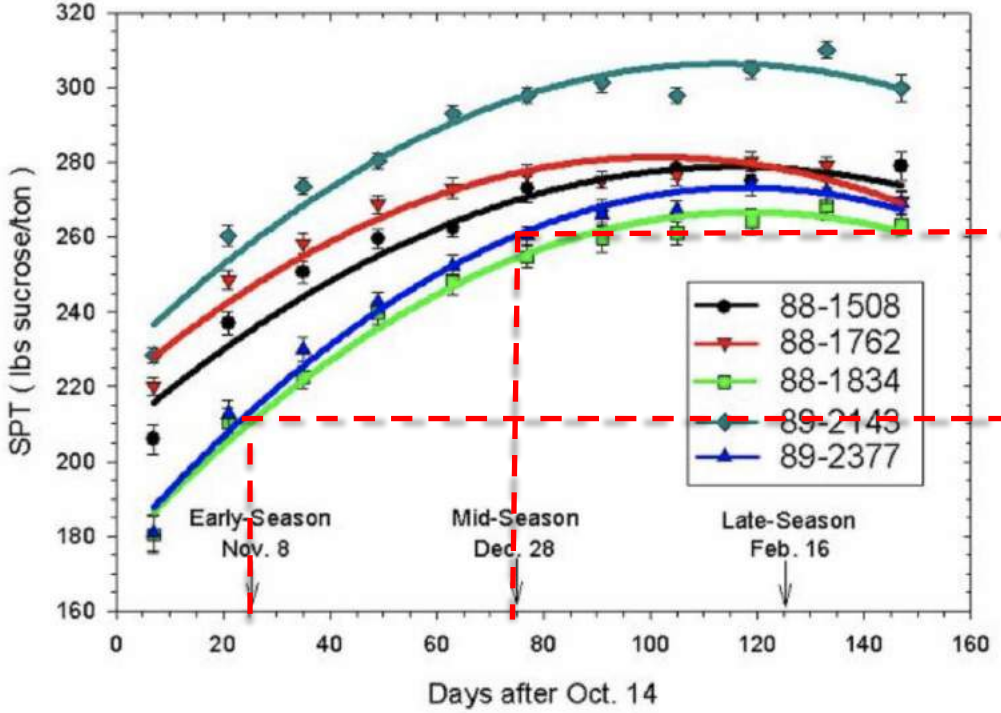
Humedad

Figure 1. Non-destructive cane measurement using a portable NIR (near infrared) spectrophotometer in transmittance mode.



J. Near Infrared Spectrosc. 21, 281–287 (2013)

NIRS: Análisis de Plantas



~25 - 30%

Figure 4. Sugar per ton (Y) versus harvest date (X) for CP clones 88-1508, 88-1762, 88-1834, 89-2143, and 89-2377.

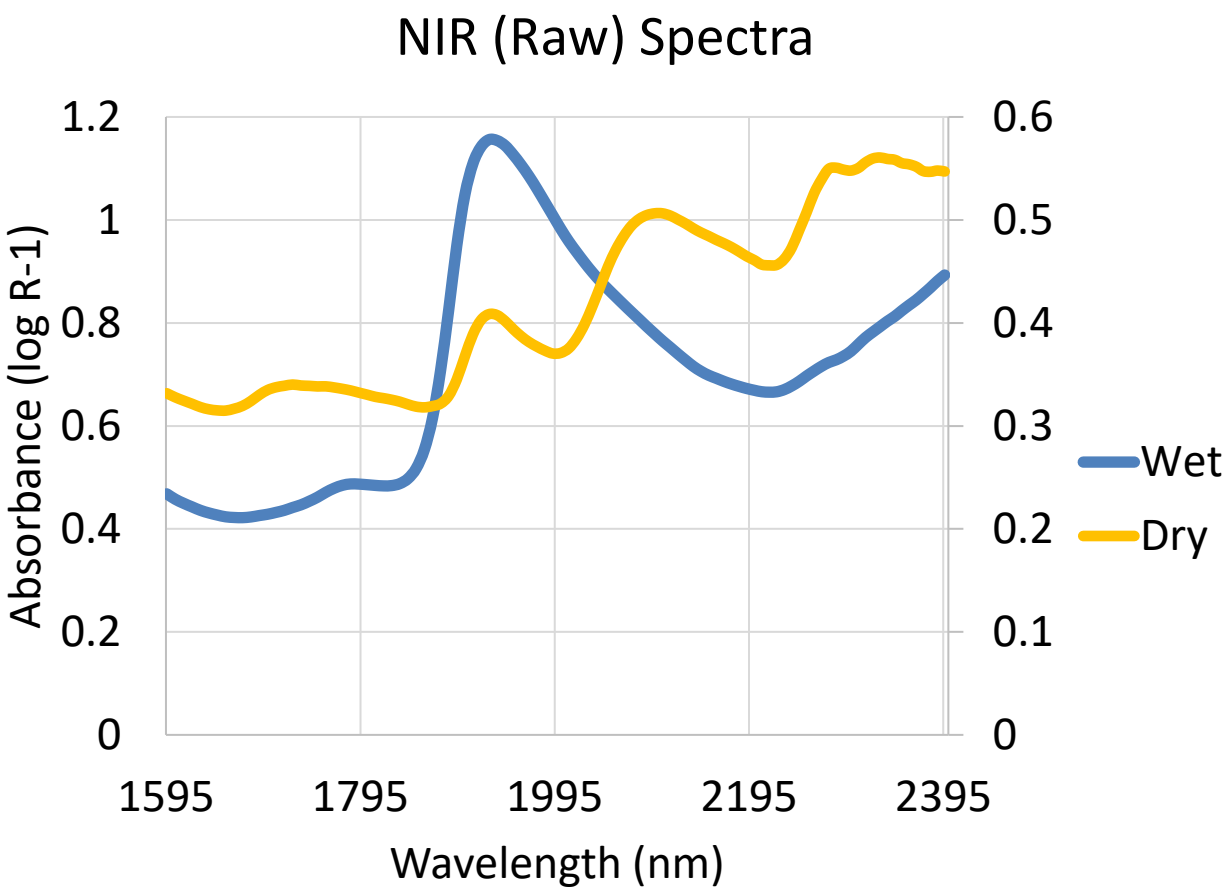
Agenda

- Tecnología NIRS
- Aplicaciones en la Agroindustria
- Oportunidades y Retos

Oportunidades y Retos

- “Llevar el laboratorio al campo, y no la muestra al laboratorio”

Retos: humedad, tamaño de muestra, muestreo representaivo


NIR (Raw) Spectra
Absorbance (log R-1)
1.2
1
0.8
0.6
0.4
0.2
0
0.6
0.5
0.4
0.3
0.2
0.1
0
1595
1795
1995
2195
2395
Wavelength (nm)
Wet
Dry

Area effective de muestreo del dispositivo de mano

Oportunidades y Retos

- “Llevar el laboratorio al campo, y no la muestra al laboratorio”
- Desarrollar protocolos estándarrs de muestreo

Adaptar (no adoptar) Tecnología a Procesos Establecidos

Toma de muestra:

- Cuando…?
- Cómo…?
- Representativo…?

Oportunidades y Retos

- “Llevar el laboratorio al campo, y no la muestra al laboratorio”
- Desarrollar protocolos estándarrs de muestreo
- Resultados en tiempo real


trinamiX
Textiles
Coffee
Plastics
Data Collection

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“Technology should improve your life, not be your life” B.C.

Gracias.

Miguel S. Castillo
Crop & Soil Sciences
mscastil@ncsu.edu