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NIRS in the Field: Opportunities and Limitations of On-Farm Analysis

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GraiNit s.r.l. (University of Padua Spin-off)

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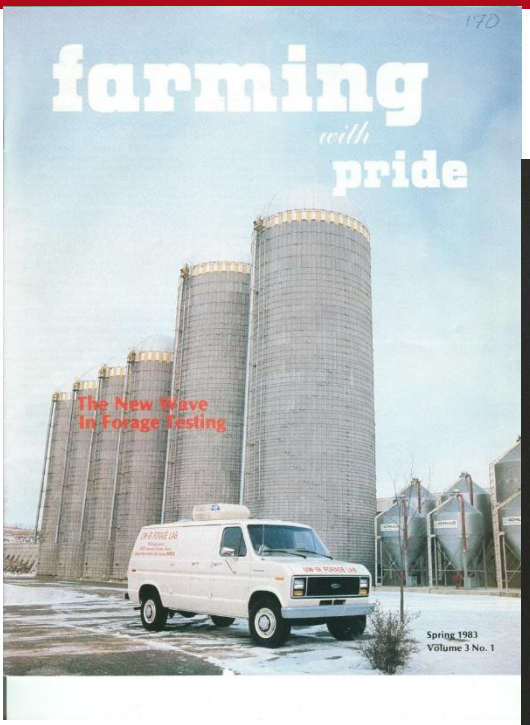
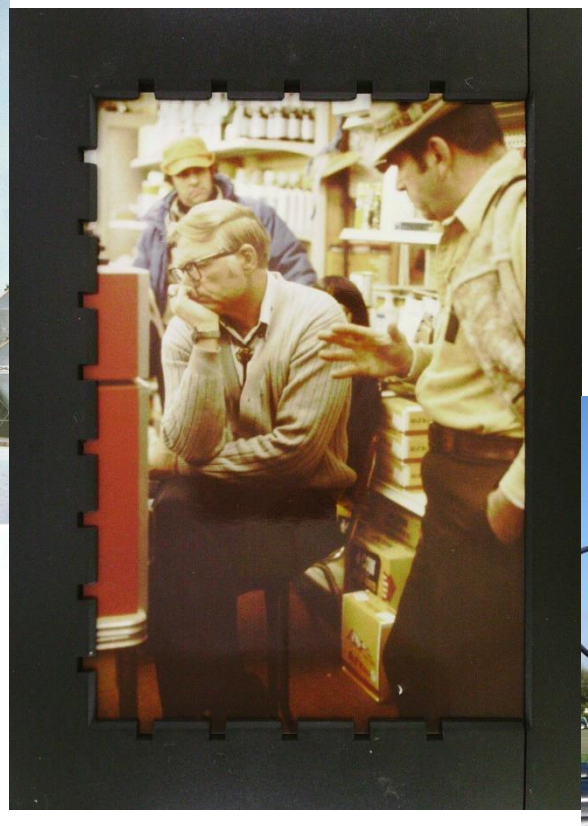
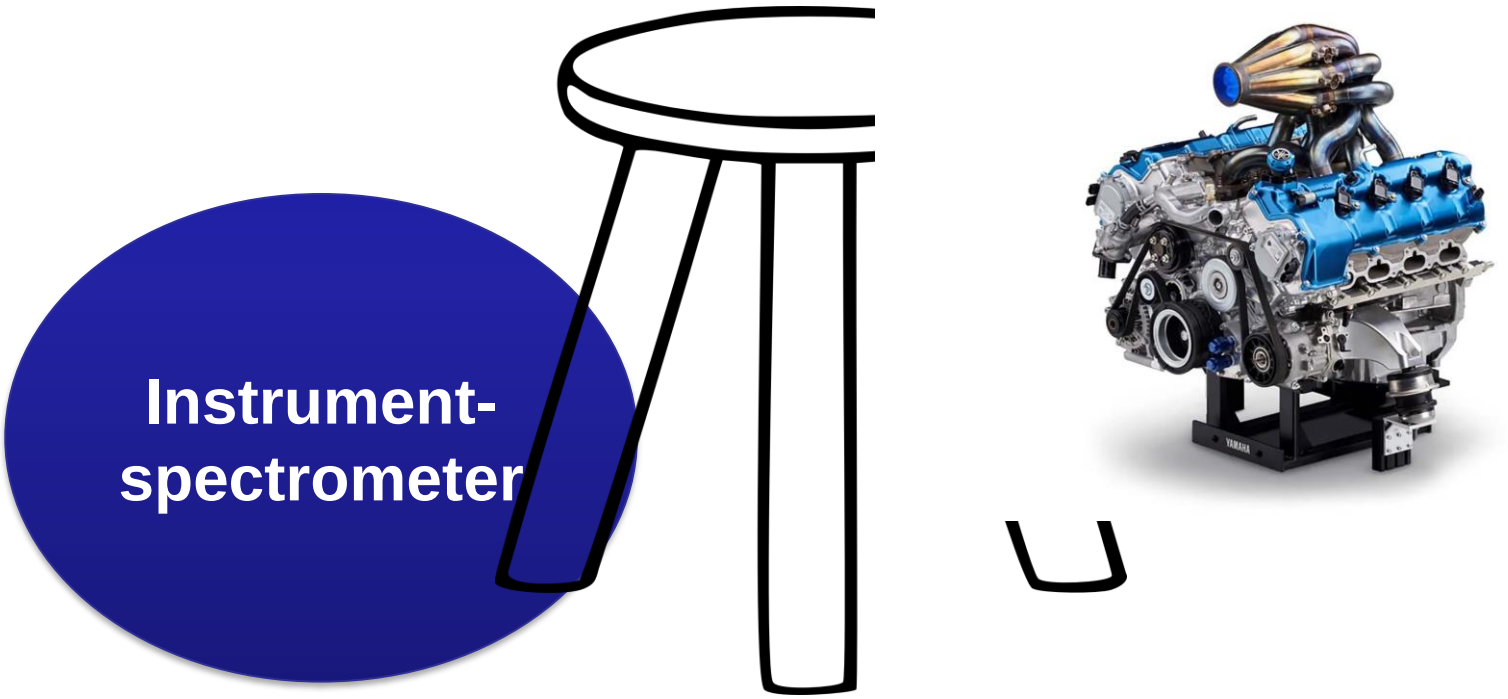
Portable instruments

Started long time ago….



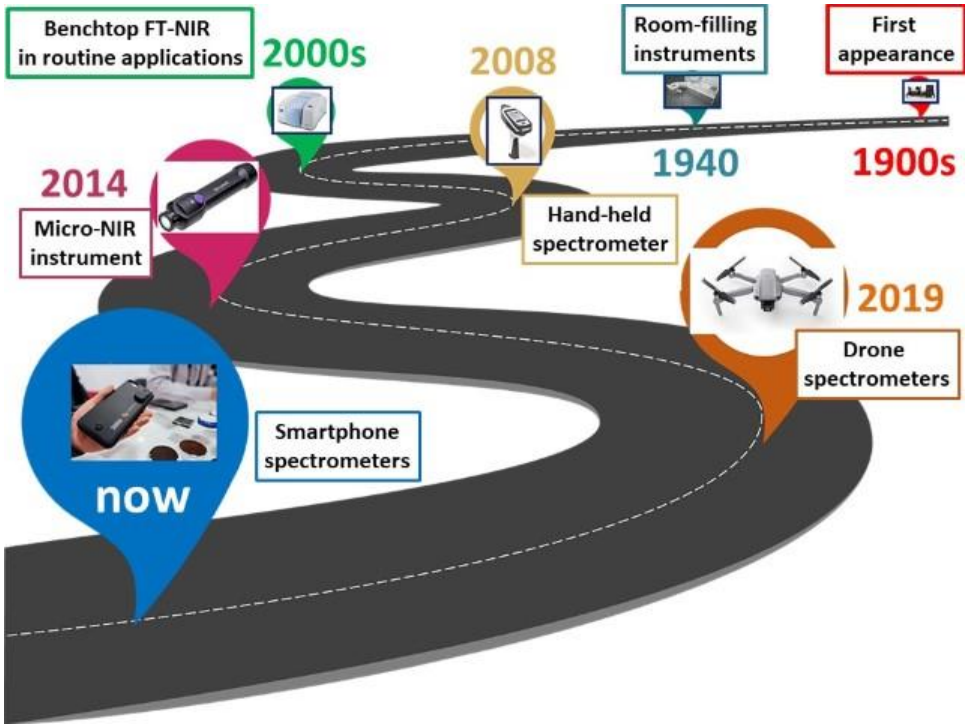


Pillars of NIR applications



Pillars of NIR applications

Instrument-spectrometer



Bec and Huck, 2023

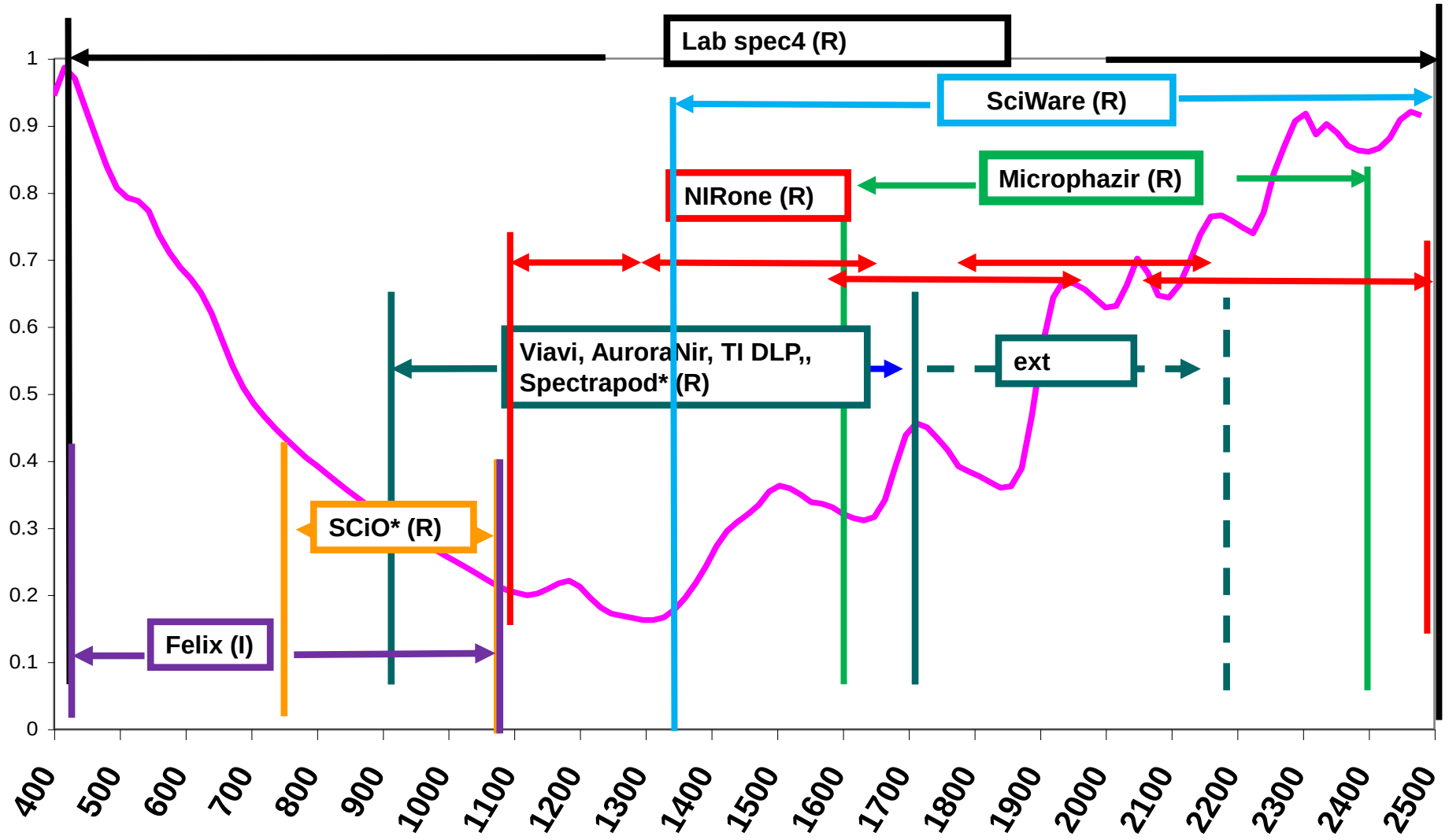
Pillars of applications

Instrument spectrometer

Many reviews

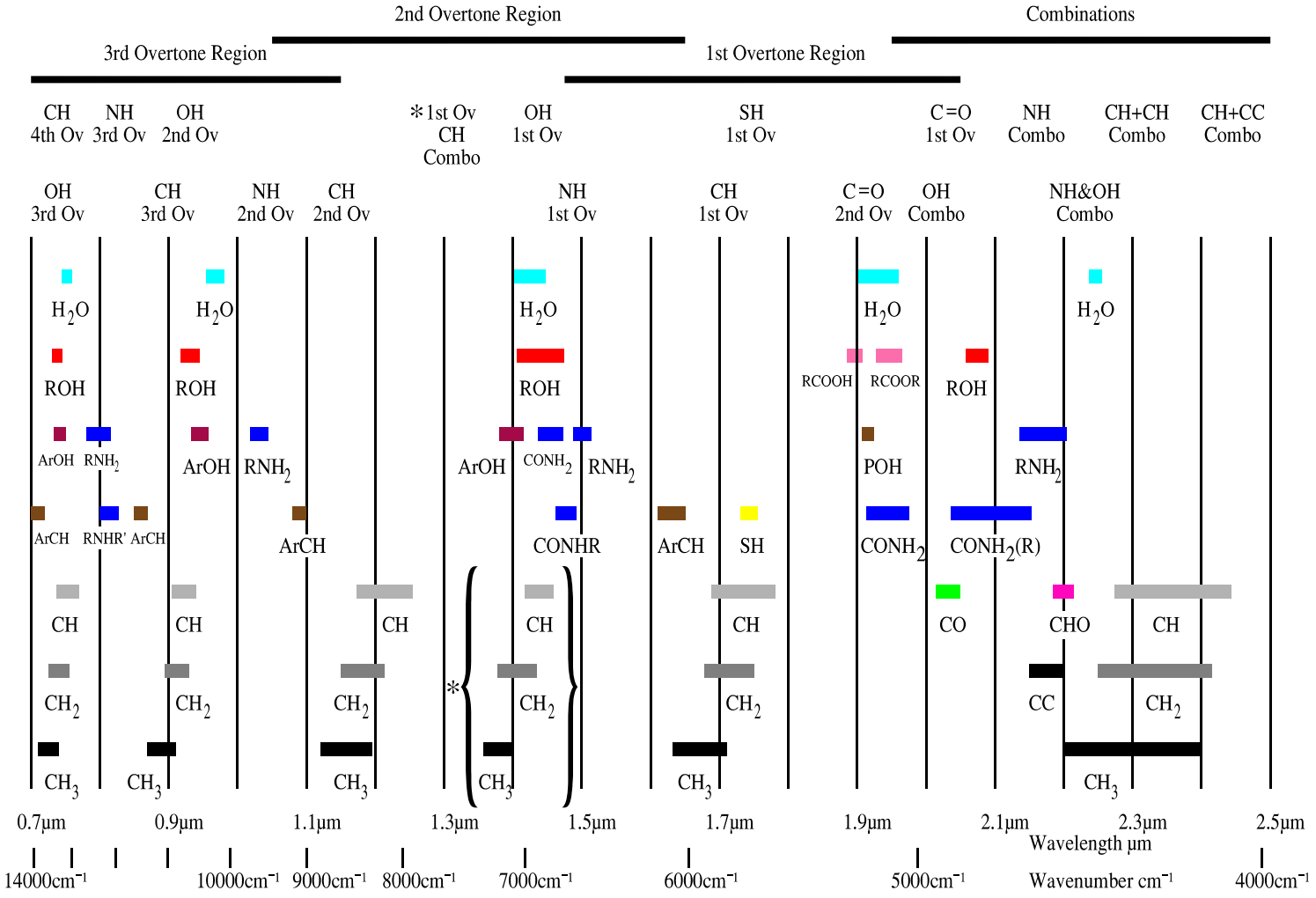
- Bec et all., Miniaturized NIR Spectroscopy in Food Analysis and Quality Control: Promises, Challenges, and Perspectives. Foods 2022, 11, 1465.
- Zhu et all., Review of portable near infrared spectrometers: Current status and new techniques. JNIR 2022 Vol. 30(2) 51 –66
- Yan et all., Handheld Near-Infrared Spectroscopy: State-of-the-Art Instrumentation and Applications in Material Identification, Food Authentication, and Environmental Investigations. Chemosensors 2023, 11, 272.
- Yan and Siezler. Hand-held near-infrared spectrometers: State-of-the-art instrumentation and practical applications. 2018 Vol. 29(7) 8–12
- Bec et all., Miniaturized near-infrared spectroscopy in current analytical chemistry: from natural products to forensics. Molecular and Laser Spectroscopy. https://doi.org/10.1016/B978-0-323-91249-5.00009-0

Spectral Range



* Discrete number of wavelength

Absorption Bands in the Near-Infrared



Computers and Electronics in Agriculture 182 (2021) 106013

Contents lists available at ScienceDirect

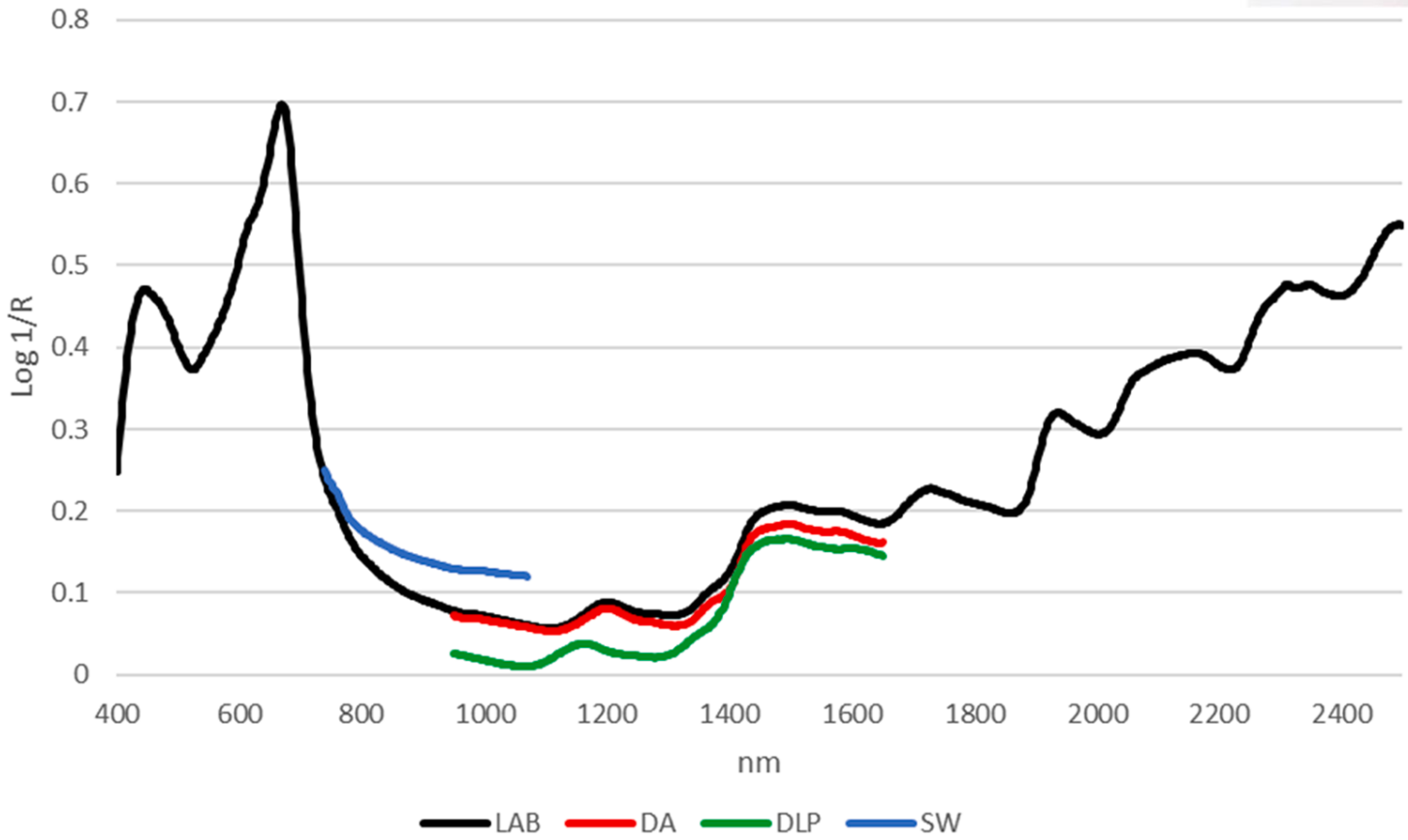
Computers and Electronics in Agriculture

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

Original papers

Prediction performance of portable near infrared reflectance instruments using preprocessed dried, ground forage samples

P. Berzaghi [a,*], J.H. Cherney [b], M.D. Casler [c]



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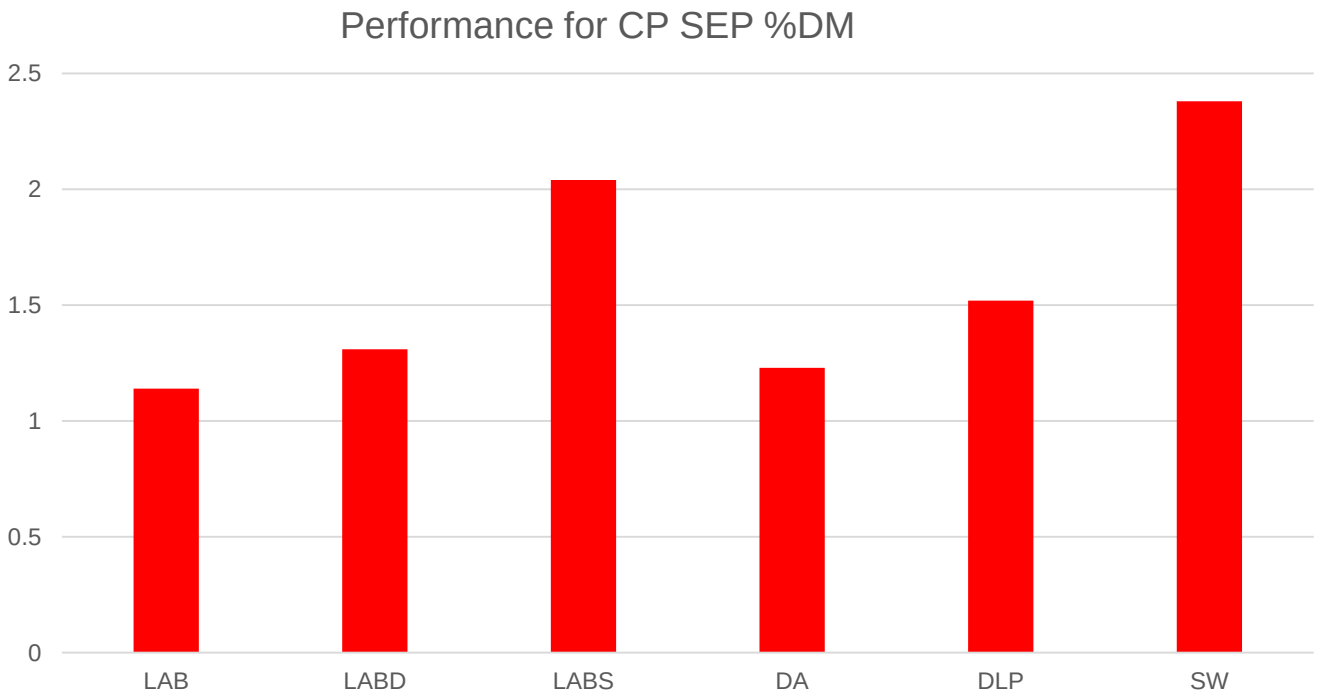

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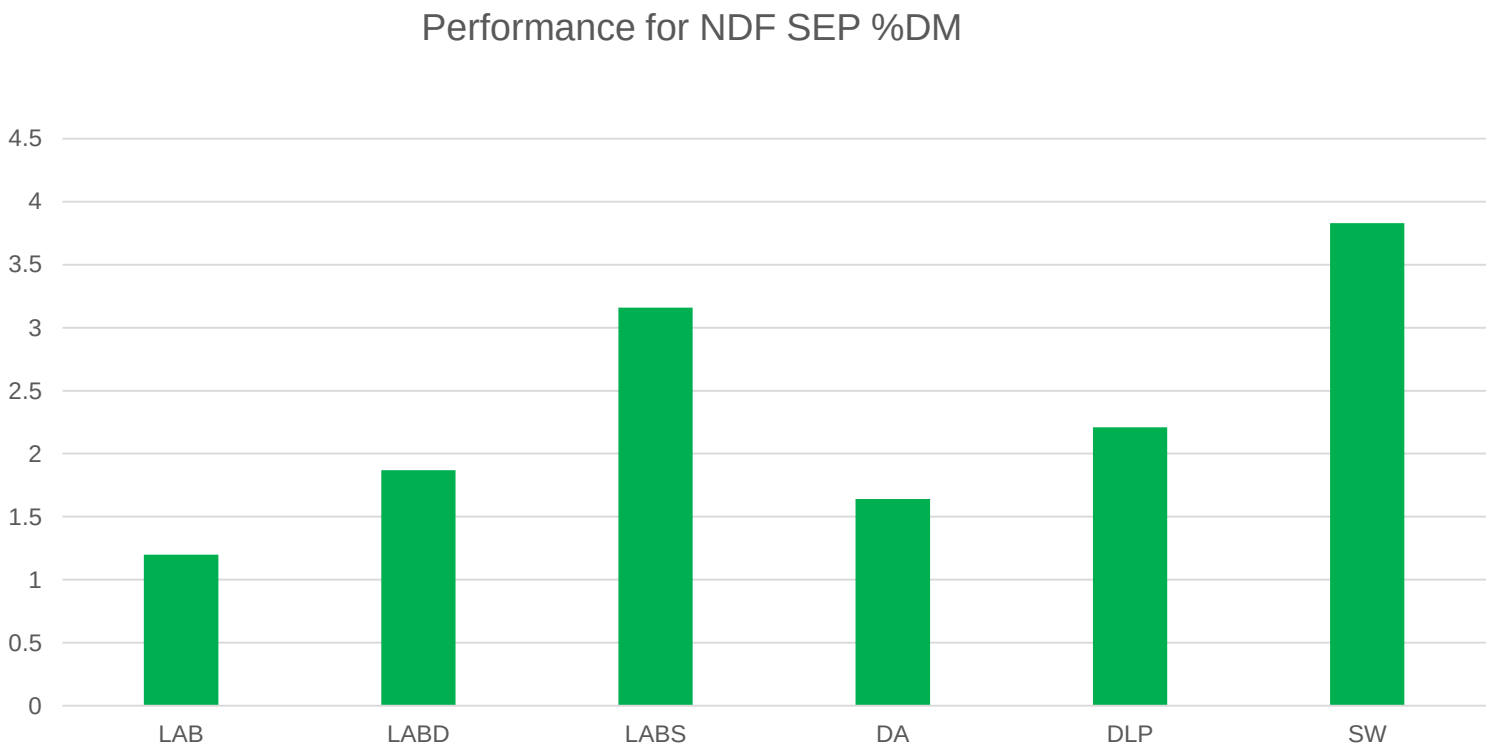
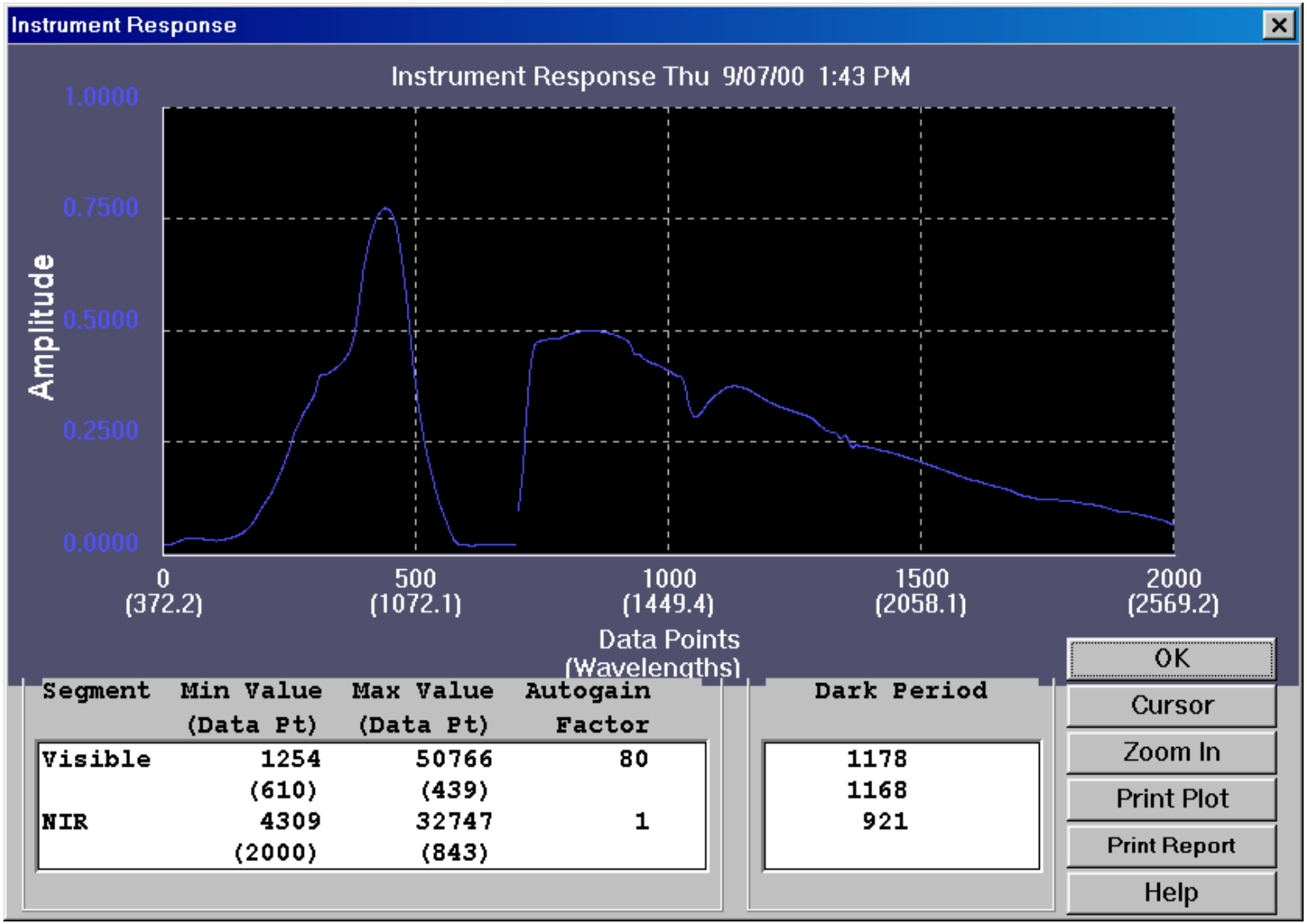
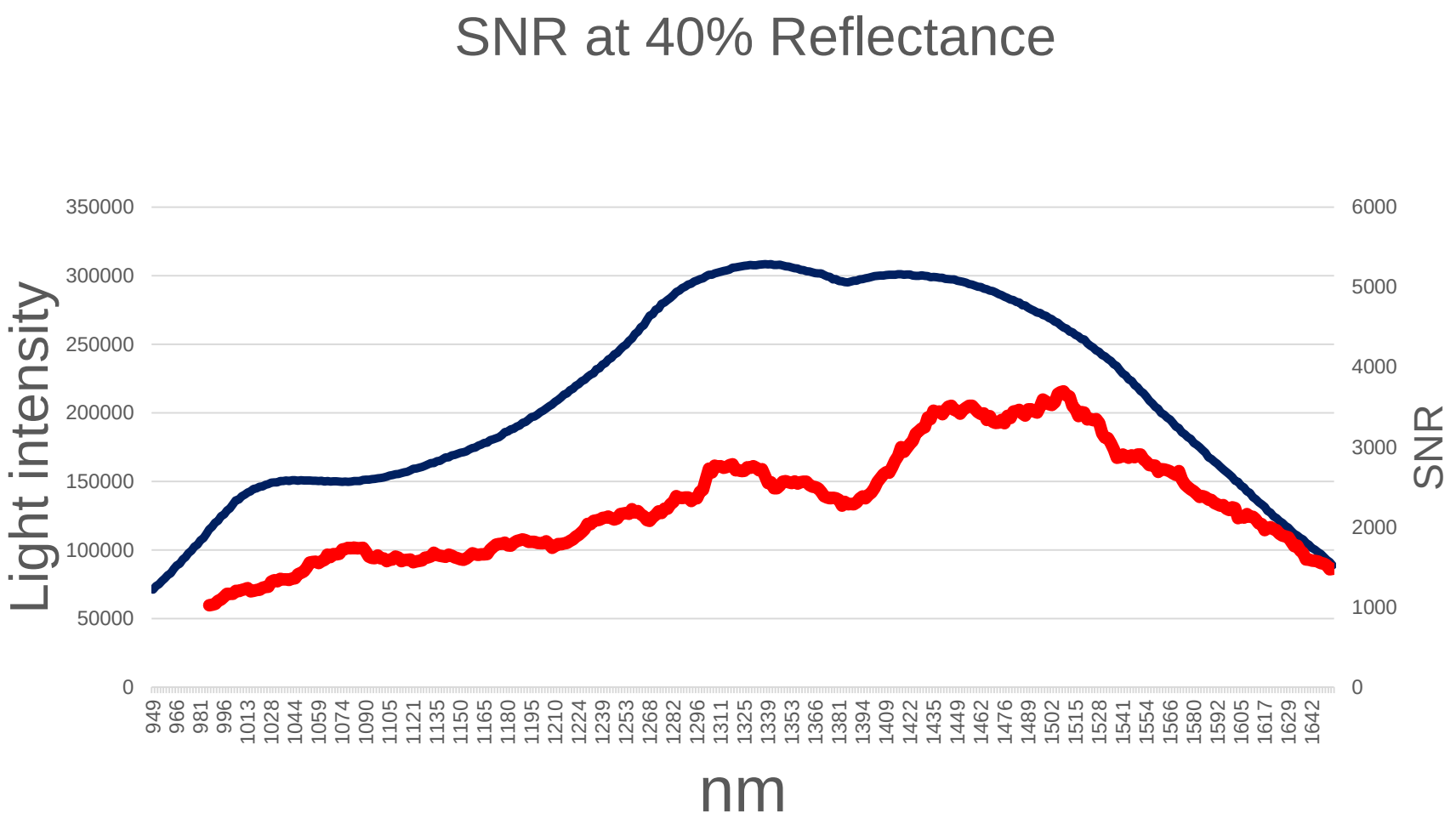


Reference for a Foss



Signal to Noise Ratio



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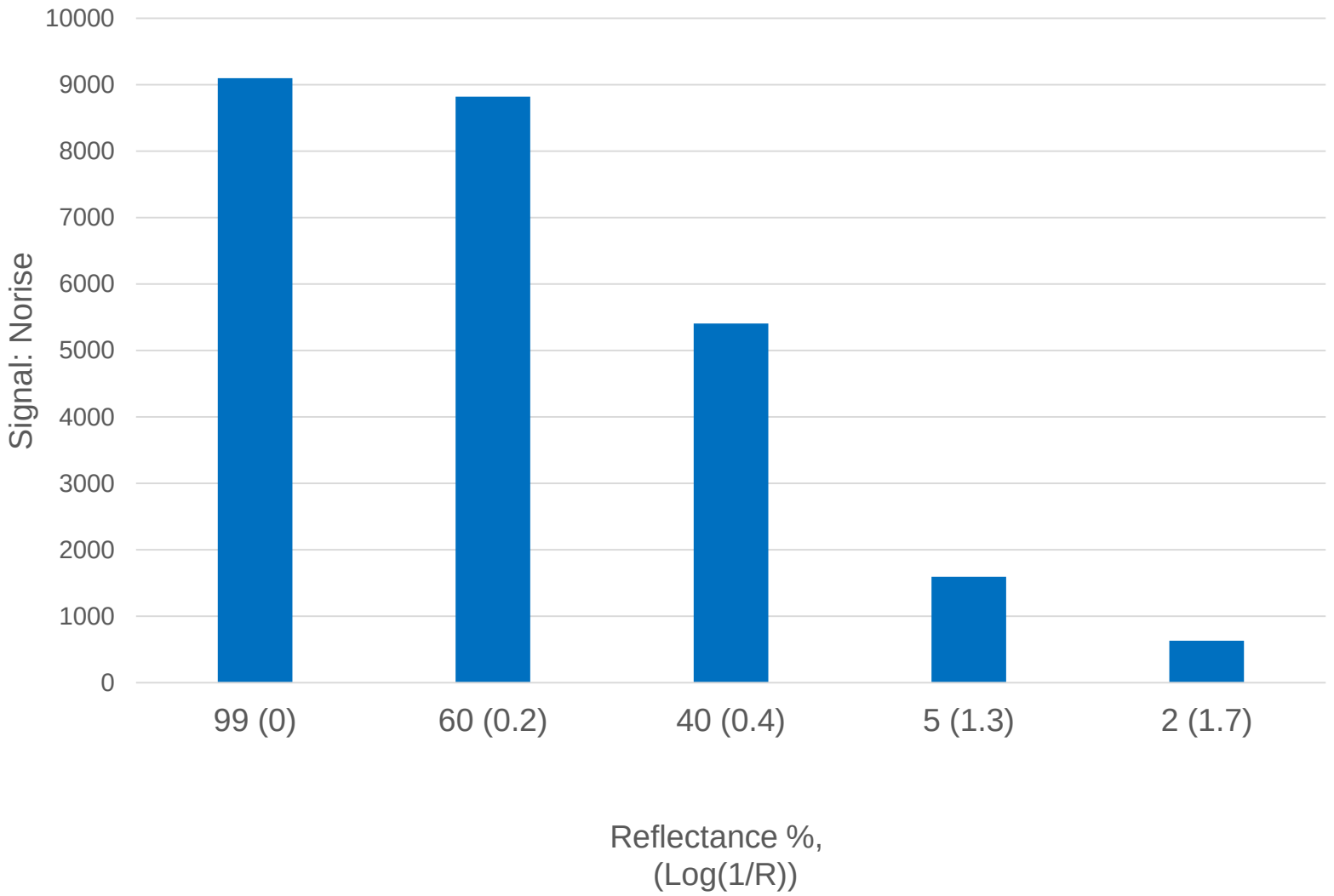

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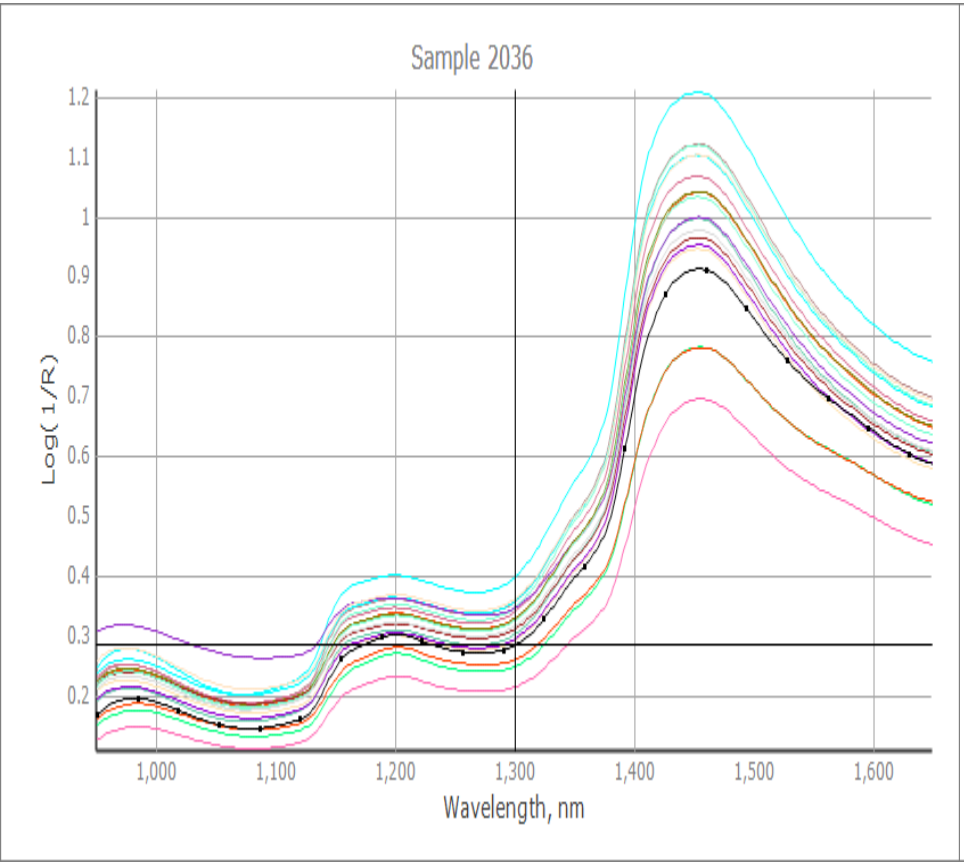
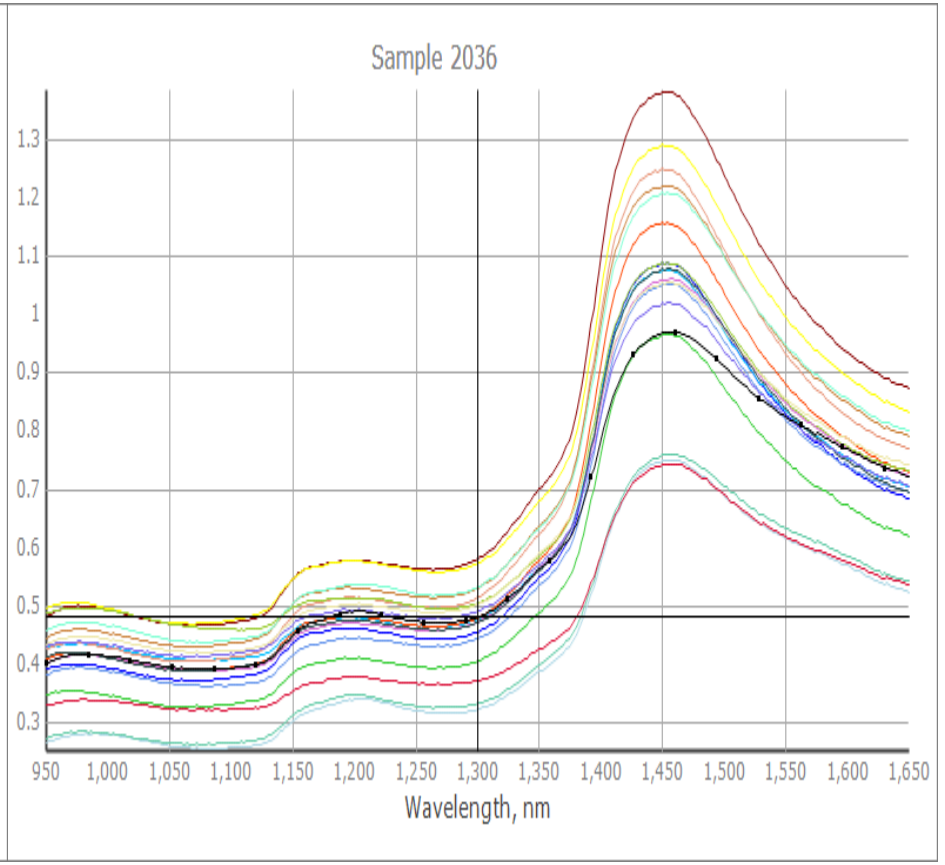
Look at spectra: Corn whole plant (wet)

Sensor A

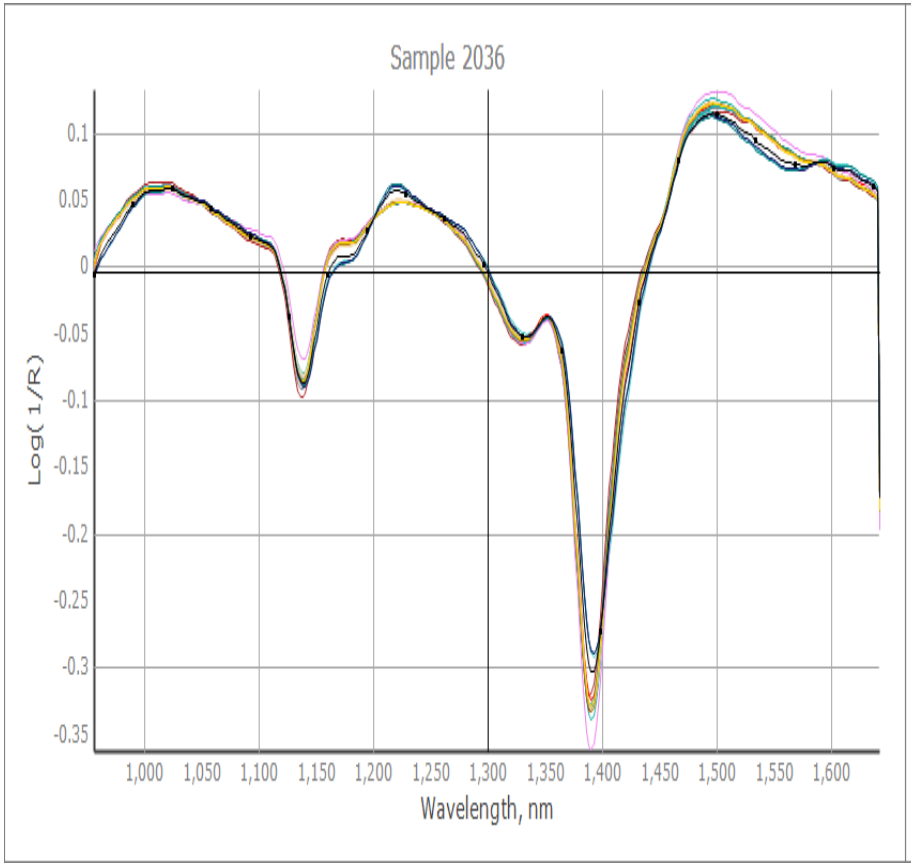


Sensor B

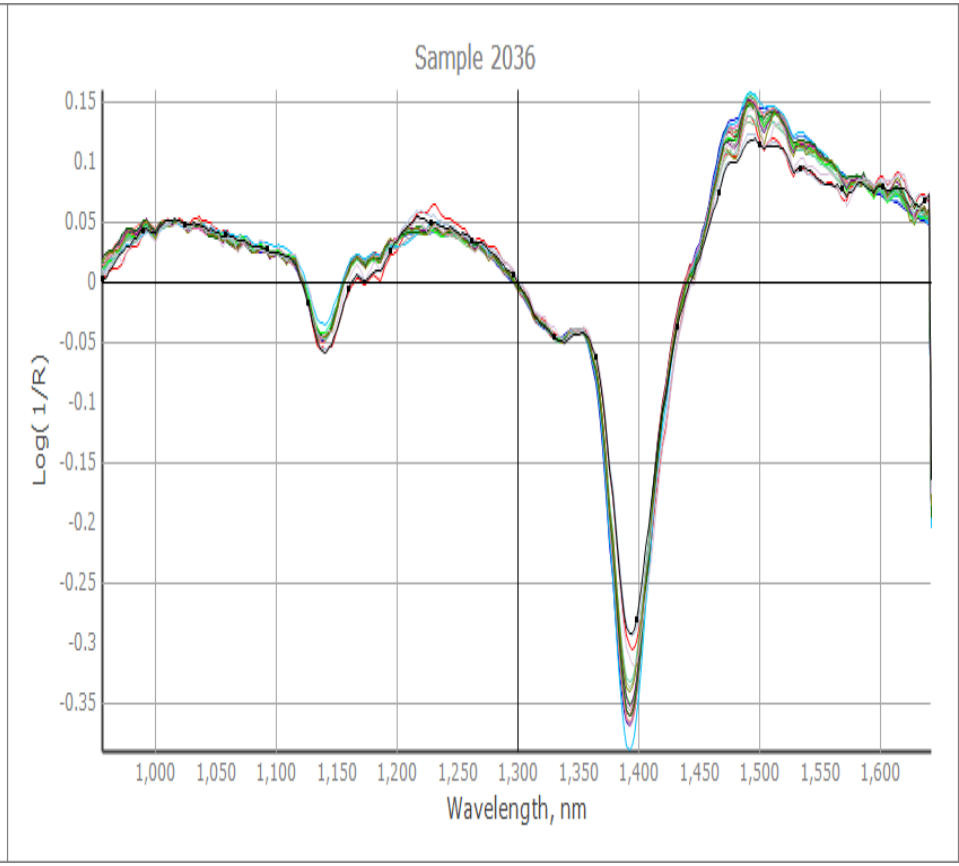


Look at spectra: Corn plant (wet), Der 1

Sensor A



Sensor B



Pillars of applications

- Spectral range
- Signal to noise
- Optical resolution
- Dynamic range
- Stray light
- Reproducibility/Repeatability
- Scanning time
- Size/weight
- *Sample presentation*
- **Cost**
- …

Evaluation of instruments

- Lab instruments have great performances
- Portables will loose in overall accuracy

But…..

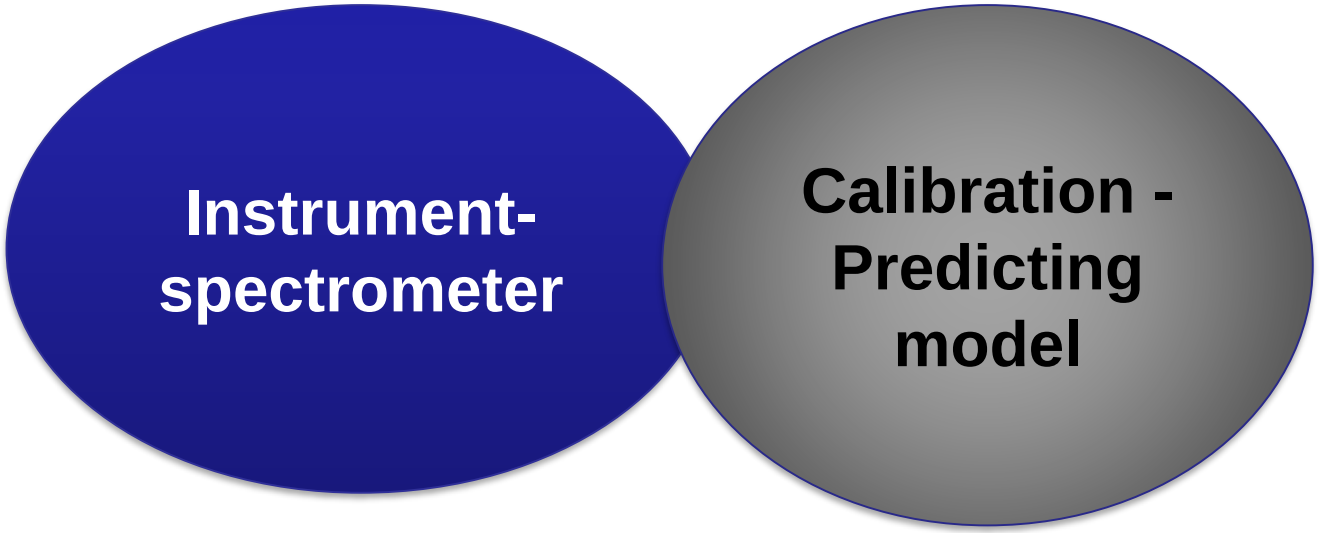
- Under same conditions and used by skilled users, portable can have great performances

Pillars of NIR applications

Calibration - Predicting model

- Transferability
  - Between same instruments
  - Across different instruments

Pillars of NIR applications



Pillars of NIR applications

Sample preparation presentation - Sampling

“Power is nothing without control”

Pirelli

Pillars of NIR applications

Sample preparation presentation - Sampling

What

It (the instrument)

See

Is

What

You

Get

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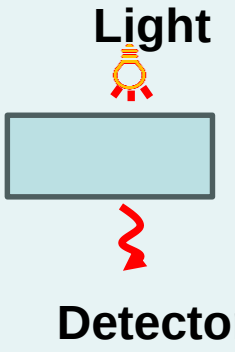
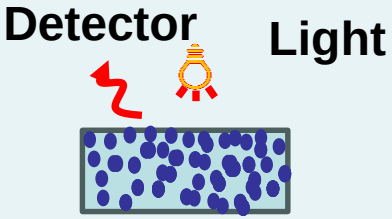
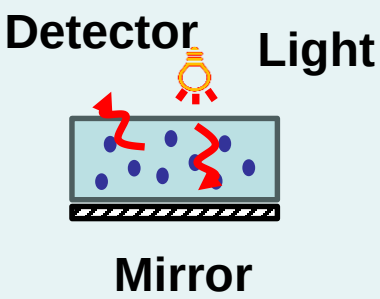
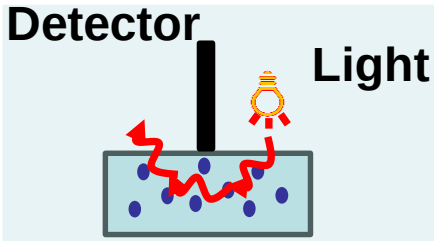
Light interaction sample presentation

Transmittance	Reflectance	Transflectance	Interactance
			

Yang & Berzaghi, 2024
In A. M. Jiménez-Carvelo et al. (eds.), *Non-invasive and Non-destructive Methods for Food Integrity*,
https://doi.org/10.1007/978-3-031-76465-3_3

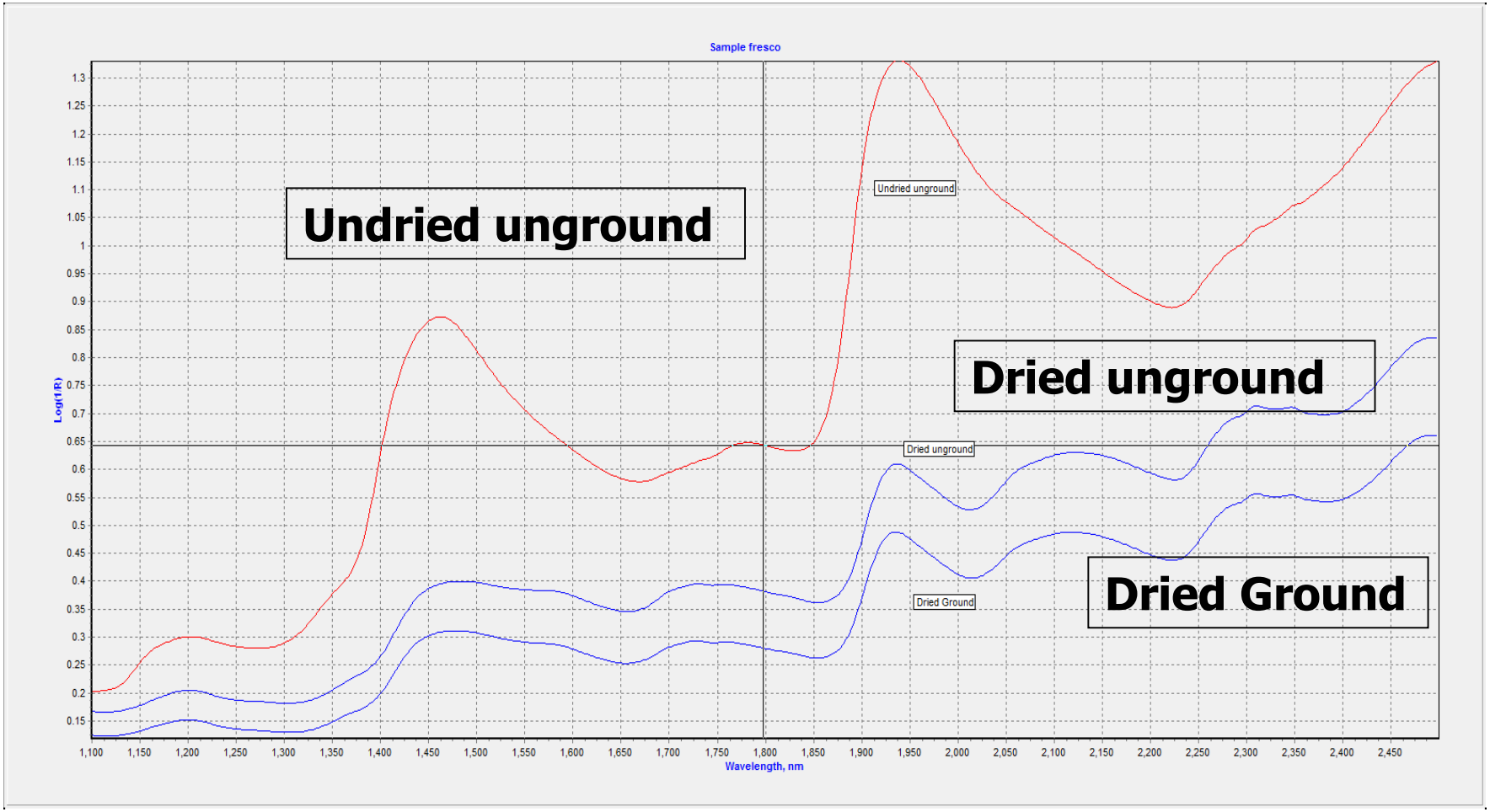
Pillars of NIR applications

Sample preparation presentation - Sampling

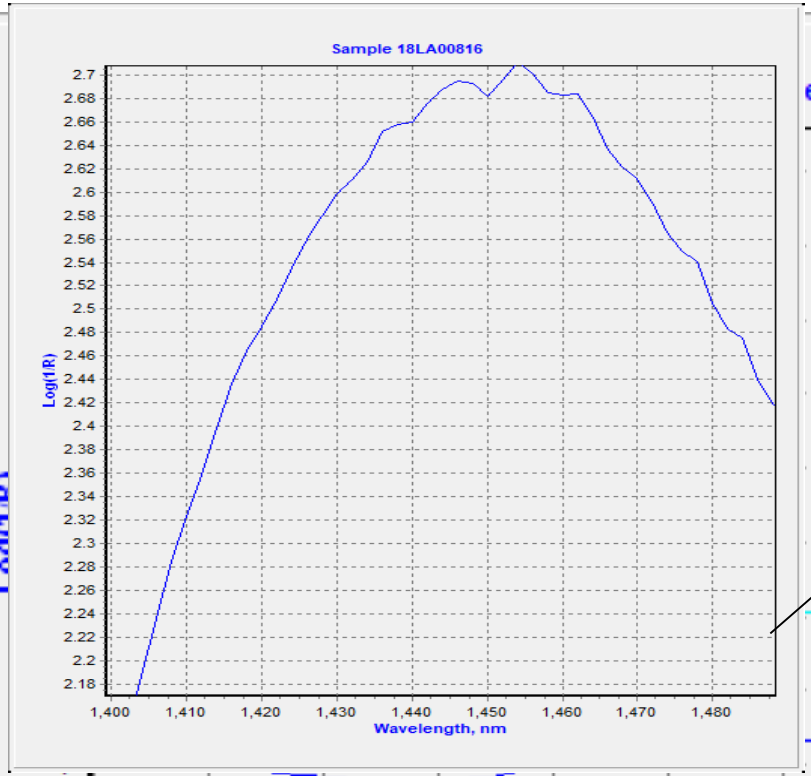
- Liquid/solid
- Wet/dry
- Particle size
- Homogeneity
- Representative scanning
- Sample moving
- .

On-farm NIR analysis…

Moisture covering large portions of spectra



High Moisture, High absorption



Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 316 (2024) 124287

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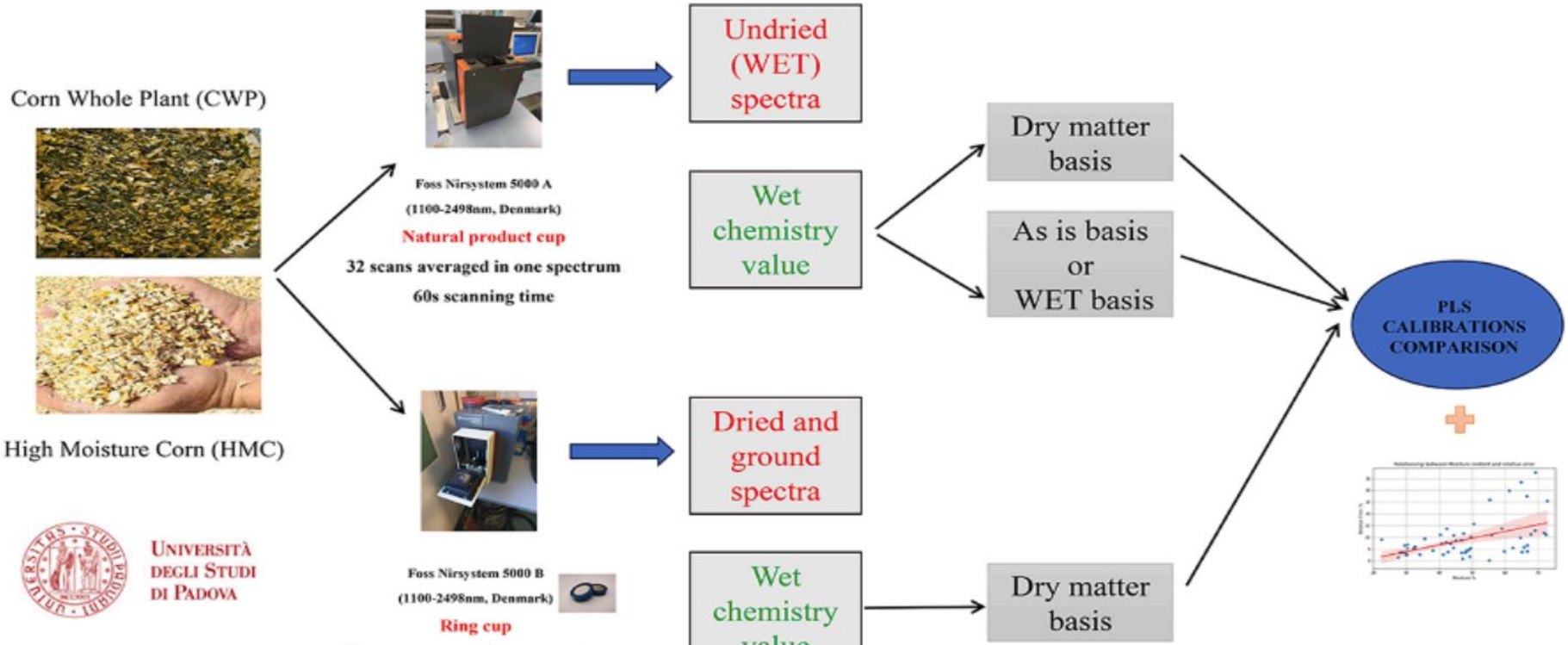
Spectrochimica Acta Part A:
Molecular and Biomolecular Spectroscopy

journal homepage: www.journals.elsevier.com/spectrochimica-acta-part-a-molecular-and-biomolecular-spectroscopy

Comparative near Infrared (NIR) spectroscopy calibrations performance of dried and undried forage on dry and wet matter bases

Xueping Yang [a,b,*,1], Alejandra Arroyo Cerezo [d,1], Paolo Berzaghi [b,c,*], Luisa Magrin [b]



Material and methods

2010-2014

Corn whole plant (CWP) (No.=492)

High moisture corn (HMC) (No.=405)

2010-2013 Calibration PLS (R)

CWP (No.=456)

HMC (No.=364)

2014 Validation

CWP (No.=36)

HMC (No.=41)

Corn Whole Plant

High Moisture Corn

Sample processing

Drying at 60°C
48hrs

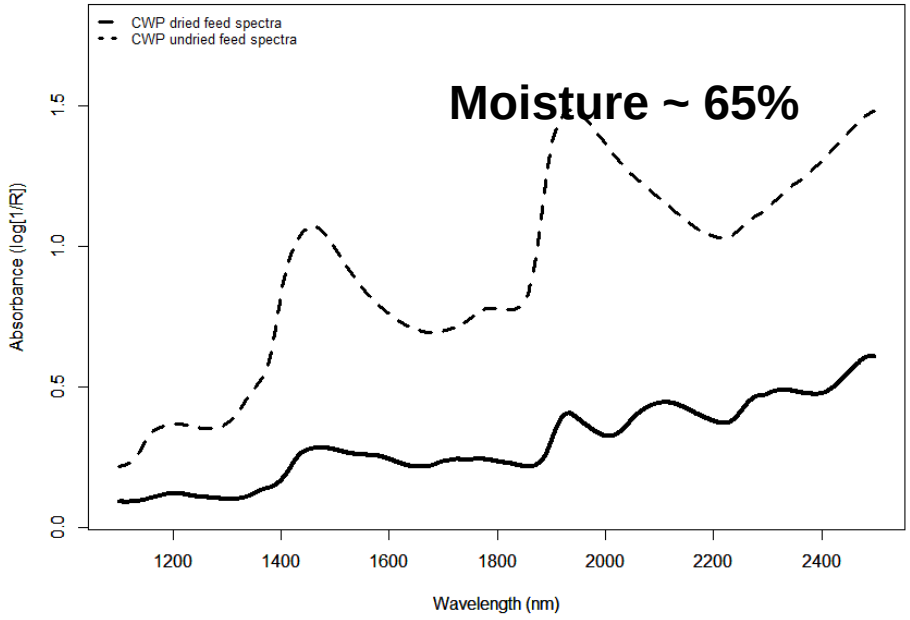
Grinding 1mm
5 min

Wet ~ 70% Moisture

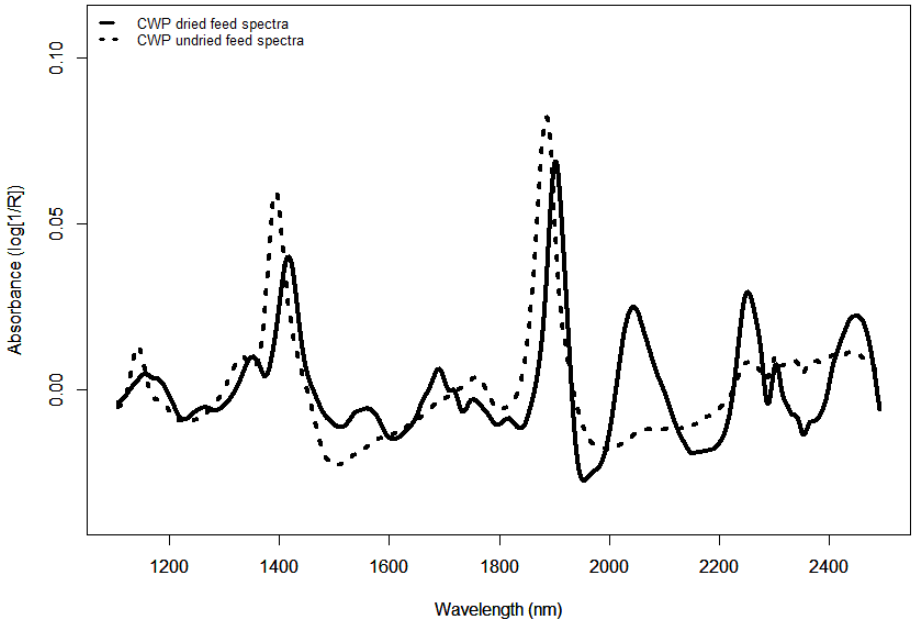
Dried ~ 8% Moisture

Dried & Ground (1mm)

Corn Whole Pplant dried and undried samples average spectrum



(a) Raw spectra



(b) Preprocessed spectra (SNV+Detrend+SavitzkyGolay)

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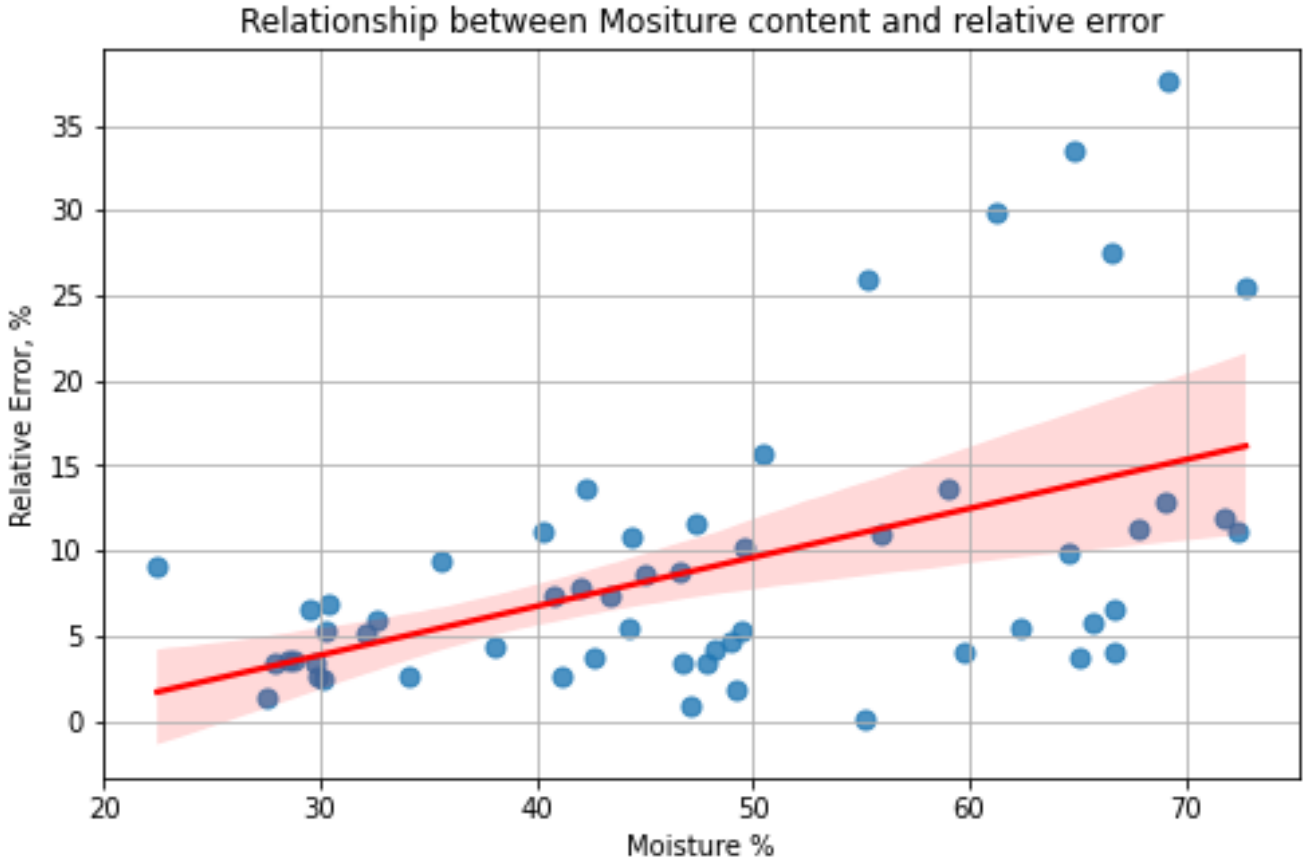
Error tend to increase with greater moisture



Particle size

Effect of particle size on perceived colour of copper sulphate $Cu\ SO_4.\ 5H_2O$ in reflectance

As you grind stuff, it just seems to look paler in colour. As the particles get finer the mean pathlength or depth of penetration, gets shorter so selective wavelength absorption gets less and the specular reflection gets proportionally larger.

Seems you grind the colour out! The early painters knew that!

Murray. 2003

Grinding Alfalfa hay

Alfalfa Hay

Fine 1mm

Constituent	N	PC	Mean	SD	SEC	RSQ	SECV	RSQcv
DM	127	6	89.53	0.71	0.30	0.83	0.32	0.80
Ash	128	6	10.35	1.25	0.58	0.78	0.63	0.75
CP	125	6	15.58	2.94	0.85	0.92	0.91	0.91
NDF	124	6	54.52	6.86	2.00	0.92	2.15	0.90
ADF	128	6	38.09	5.73	2.31	0.84	2.45	0.82

Coarse

Constituent	N	PC	Mean	SD	SEC	RSQ	SECV	RSQcv
DM	127	6	89.53	0.70	0.38	0.71	0.41	0.67
Ash	126	3	10.30	1.20	0.86	0.48	0.94	0.38
CP	126	3	15.73	2.85	1.76	0.62	1.80	0.60
NDF	127	4	54.36	6.81	4.18	0.62	4.31	0.60
ADF	128	5	37.87	5.48	3.83	0.51	4.00	0.47

Berzaghi, unpublished

Bad habits are going to the lab too!

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Sample presentation is also part of sampling

Repeatability of corn silage analysis:

- 10 corn silage samples of about 2 kg each
- Each sample was spread over an area of about 30x40cm
- Calibration: Corn Silage_Dry Matter
- Scanning: each sample was scanned 30 times in different position (one spot = ~1.0 cm^2)
- Predictions by averaging an increased number of «spots»
- Reference DM : 105 °C 24hrs

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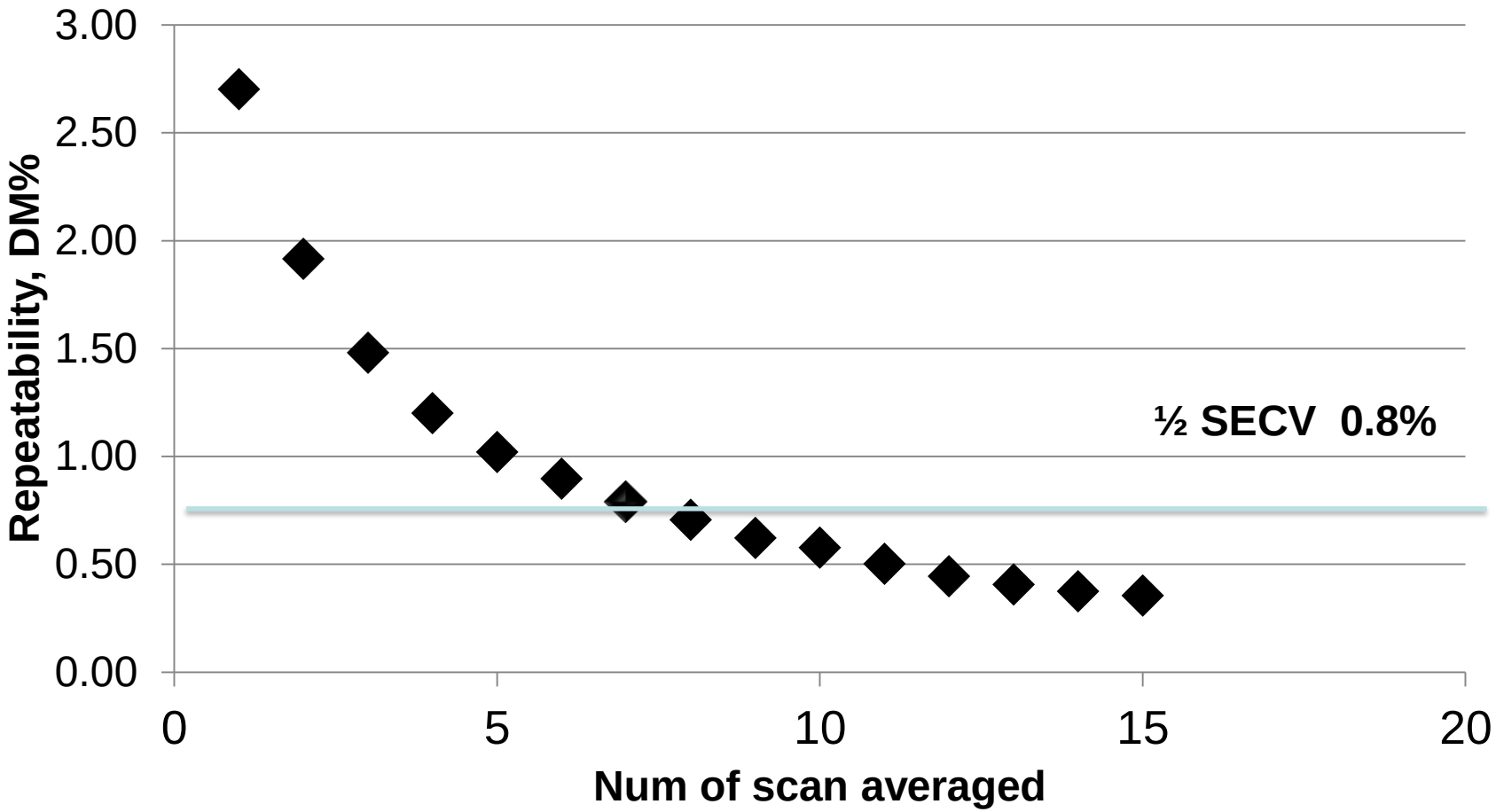
Calibration performances

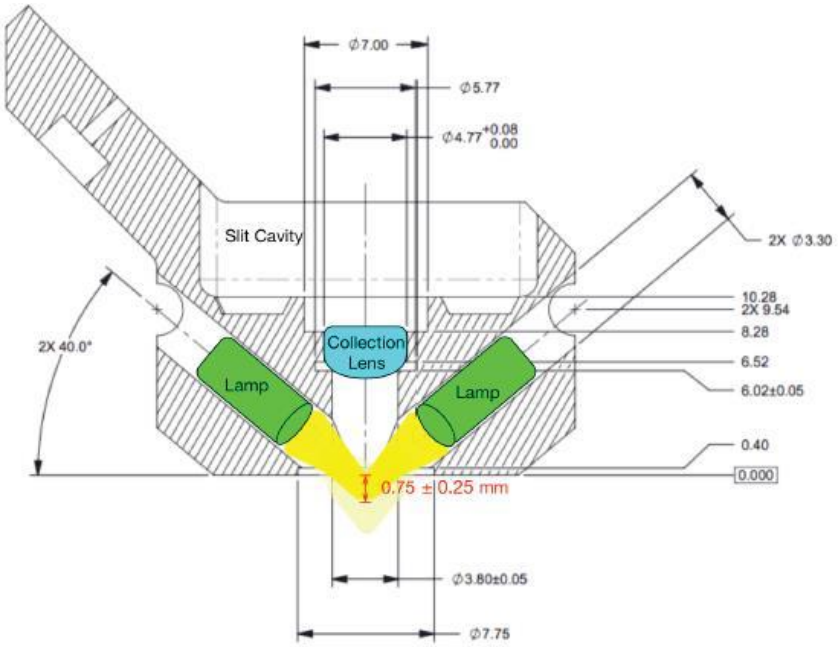
	Calibration	Test set
Num.	256	10
Min, %	19.8	25.6
Max, %	63.1	37.2
Avg,%	34.5	32.1
SD, %	7.1	3.0
RSQ	0.95	0.82
SEL, %	**0.8**	
SECV, %	**1.6**	
SEP, %		**1.2**

Repeatability of DM prediction with increasing number of averaged spots scan

Sufficient repeatability by scanning and averaging 10 spots (about 10 sq cm)



Focal point



Direct Contact

At 3mm

Coarse particles will separate

Repeatability of Total Mixed Ration (TMR)

- 35 samples
- Scanned in a dual face sample holder (35x9x9cm)
- Scan mode for 5s over the surface of the sample in the holder
- Duplicate scans on top and bottom of the chamber.

Coarse particles will separate (TMR)

TOP portion of the cup

BOTTOM portion of the cup

NDF -2.7 %DM
CP +1.1 %DM

Berzaghi & Benozzo, 2017

Coarse particles will separate (Alfalfa)

For sample that easily separate (TMRs, dry hay) use the dual side cup (twice top and bottom= 4 times).

Dual side cup

- The cup has two lids
- First scan the top, flip it and then scan the bottom

Practical Considerations for Using the NeoSpectra-Scanner Handheld Near-Infrared Reflectance Spectrometer to Predict the Nutritive Value of Undried Ensiled Forage

Xiaoyu Feng [1], Jerry H. Cherney [2], Debbie J. R. Cherney [3] and Matthew F. Digman [4,*]

- Three units of the same portable
- Forage (Alfalfa, grass, alfalfa-grass mix ,corn plant) quality including NDFD

- Better to include multiple units in the calibration
- Better when scanning larger surface
- Good prediction for DM, but not for quality parameters

B A S E *Biotechnol. Agron. Soc. Environ.* 2022 **26**(S), 309-318 OPEN ACCESS

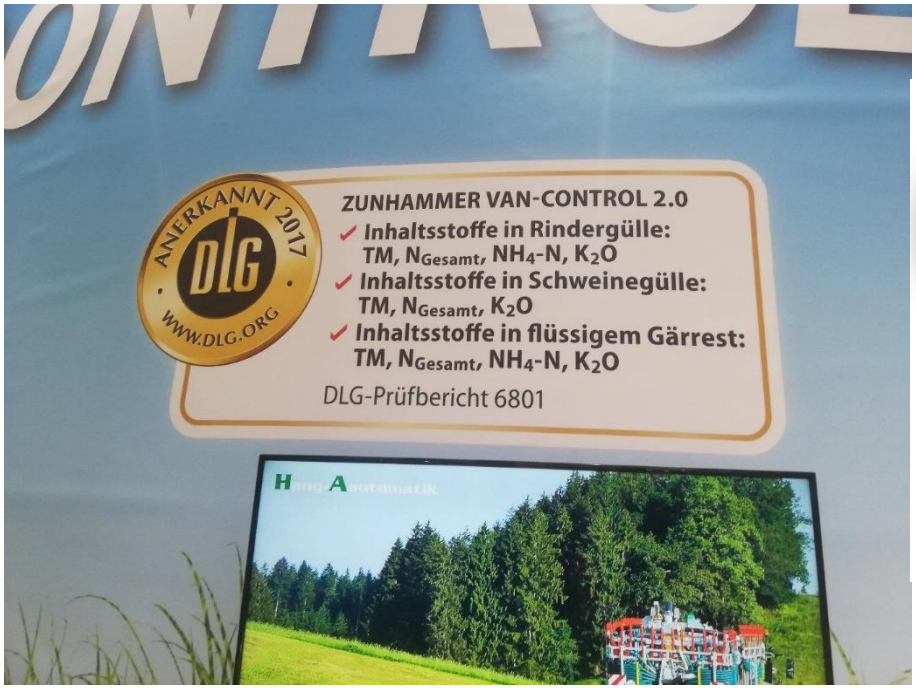
Performance of three handheld NIR spectrometers for predicting grass silage quality

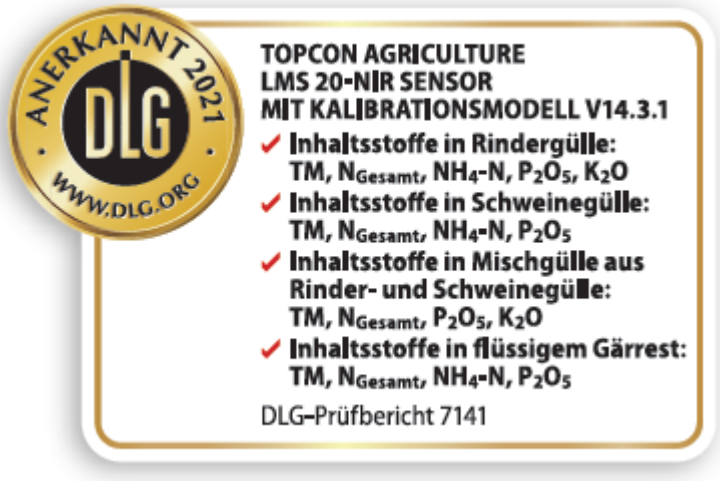
Juan Antonio Fernández Pierna [(1)], Philippe Vermeulen [(1)], Nicolas Chamberland [(1)], Virginie Decruyenaere [(2)], Eric Froidmont [(3)], Olivier Minet [(1)], Bernard Lecler [(1)], Vincent Baeten [(1)]

	Parameter	SEL	XDS SECV dry	ratio SEP fresh actual/XDS SECV dry			
				XDS	MicroNIR	FlameNIR	FieldSpec 4
PLS							
	DM (%)	1.05					
	CP (%)	0.2	0.87	1.4	2.1	2.4	1.3
	CEL (%)	0.95	1.50	0.7	1.0	1.6	1.6
	Ash (%)	0.15	1.34	1.0	1.4	0.7	0.8
	NDF (%)	0.4	1.76	1.4	2.5	2.0	2.4
	ADF (%)	0.3	1.17	1.5	1.4	2.9	2.7
Local PLS							
	DM (%)	1.05					
	CP (%)	0.2	0.87	0.4	1.9	1.6	0.9
	CEL (%)	0.95	1.50	0.4	1.3	0.6	1.5
	Ash (%)	0.15	1.34	0.3	1.4	0.8	1.0
	NDF (%)	0.4	1.76	0.7	1.6	1.5	1.5
	ADF (%)	0.3	1.17	0.2	1.4	1.7	2.3

NIRS and slurry

NIRS and slurry





NIRS and slurry

DLG test

- 5 samples

Liquid digestate from cattle or pig manure with renewable raw materials	DM in % by weight	○
	N_{Total} in kg/m³	○
	P_2O_5 in kg/m³	++
	K_2O in kg/m³	++

*** DLG-assesment scheme:**

++ = passed, very good (4/5 value pairs within a manure type ≤ 10 % and no > 20 % rel. deviation)
\+ = passed, good (4/5 value pairs within a manure type ≤ 15 % and no > 25 % rel. deviation)
○ = passed (3/5 value pairs within a manure type ≤ 25 % and no > 35 % rel. deviation))
– = failed

On-farm NIR analysis…

Challenges

- Complex analytical system in the hands of unskilled professionals (for analytical work)
- Samples preparation…. May not be an option (coarse and wet samples)
- Calibration maintenance….expensive for just one instrument, must be transferable

Farm-SOP

Farm - **S**tandard **O**perating **P**rocedure:

- Feed and forage sampling
- Sample handling
- Scanning procedure
- Spectral quality evaluation

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At best, analytical results will be as accurate as sampling accuracy

WISIWYG!!!!!!!

(What It See Is What You Get)

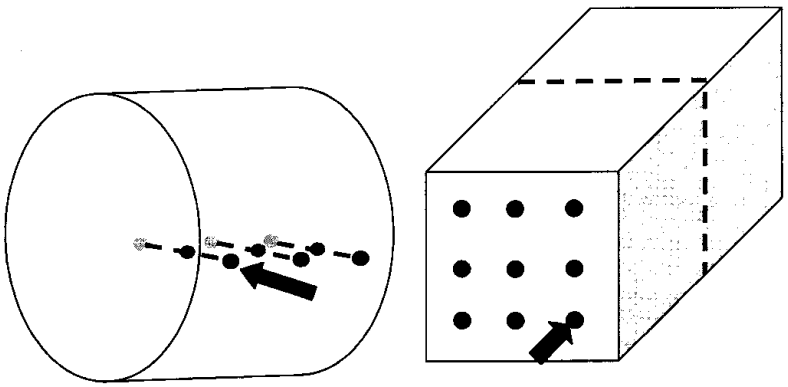

Figure 1. Sampling patterns of round and rectangular bales.

What concerns me

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Take Home Message

- **Instrument:**
  - Signal/noise; Spectral range; time of scanning; Internal referencing
- **Calibration:**
  - Who is in control?; Updates; Transferability; quality control (e.g. GD, ND…) , LOCAL, AI will help?
- **Sample and sample presentation:**
  - Can you scan a large surface? Modify scanning procedures for non homogeneous samples. Particle size?

Take Home Message

- On-farm portables will **not** replace lab analysis
- Major physical limitation are sample (wet and coarse particles) and sample presentation

BUT portables……

- work well for DM tracking (greatest source of farm variability)
- are good tools within farm, to monitoring forage changes and decide for lab analysis
- Are great resources for places/countries with limited analitical resources