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Evaluation of a combination of NIR micro-spectrometers to predict chemical properties of sugarcane forage using a multi-block approach

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Abstract

Forage quality is essential in livestock farming and has an important role
in the functioning of agricultural farms.

Access to biochemical variables provides an estimation of the feed value of
crop for animal feed at harvest. Near infrared (NIR) spectroscopy provides
measurements indirectly related to biochemical variables. In recent years,
several micro-spectrometers have been developed that offer the opportunity
to predict such biochemical variables at low cost. In this study, the poten-
tial of a combination of micro-spectrometers is evaluated to predict crude
protein (CP) and total sugar content (TS) of sugarcane. First, each micro-
spectrometer with optimal pretreatments was individually compared to a ref-
erence laboratory spectrometer. Then, a combination of micro-spectrometers
is proposed and prediction models were established by a multi-block method
from data fusion called Sequential and Orthogonalised - Partial Least Squares

(SO-PLS). For CP, the combination of micro-spectrometers provides model (sep=0.69%; bias=0.15%; R^2_{test} =0.910) close to those obtained with the reference spectrometer (sep=0.56%; bias=-0.13%; R^2_{test} =0.935). For TS, the results obtained with this combination of micro-spectrometers (sep=2.38%; bias=-0.52%; R^2_{test} =0.983) are better than those obtained with the reference spectrometer (sep=2.59%; bias=0.41%; R^2_{test} =0.978). For both chemical variables, the combination of the micro-spectrometers significantly increases the performance of the predictive models compared to the models obtained with the micro-spectrometers independently. Using several low-cost micro-spectrometers, combined with a multi-block method would give results as good as a single laboratory spectrometer with a lower cost.

Keywords: Food control, Micro-spectrometer, Spectroscopy, Data fusion, Forage, multi-block regression, Multivariate Data Analysis

1. Introduction

Forage quality is essential in livestock farming and has an important role in agricultural farm management (Ball et al., 2001; Collins and Fritz, 2003). Forage must respond to a set of constraints related to farms, production costs, animal requirements and environment (Wilkins, 2000). Forage feed value, including energy value or protein and mineral contents, ensures a nutritional quality for a good metabolic development of animals. Information such as protein or sugar content represents a major interest to estimate feed value of crops at harvest time. Accessing these parameters is possible by direct destructive laboratory measurements (Ball et al., 2001). However, these measurements have time and cost constraints.

50 In laboratory, near-infrared (NIR) spectroscopy is an alternative to ac-
51 cess these parameters in an indirect and non-destructive manner ([Stuth et al.,](#)
52 [2003](#); [Deaville and Flinn, 2000](#); [Barton II and Windham, 1988](#)). In the NIR
53 range, spectral bands are related to harmonics and combinations of fun-
54 damental molecular vibrations, in particular stretching, bending and some
55 deformations ([Siesler et al., 2008](#); [Workman and Springsteen, 1998](#)).

56 In recent years, several micro-spectrometers have been developed ([Yang](#)
57 [et al., 2021](#)). These micro-spectrometers provide fast and non-destructive
58 measurements with a very low cost compared to laboratory spectrometers.
59 With this technology, the increased use of NIR spectroscopy is expected to
60 lead to new applications ([Yan and Siesler, 2018](#); [Wiesner et al., 2014](#); [Siesler](#)
61 [et al., 2008](#)) directly accessible to crop producers.

62 To this end, micro-spectrometers are expected to be widely used. Hence,
63 appropriate multivariate data analysis methods must be proposed to exploit
64 spectral data from NIR spectroscopy ([Wiesner et al., 2014](#)). The reference
65 method is Partial Least Squares Regression (PLS-R)([Wold et al., 2001](#)) which
66 is a bilinear regression method that allows to predict biochemical variables
67 from spectral data.

68 Generally, prediction quality of regression models can be improved by
69 choosing the best pretreatment according to variables to be predicted, spec-
70 tral region considered and undesired spectra to be corrected ([Engel et al.,](#)
71 [2013](#); [Rinnan et al., 2009](#)). Another way to increase predictive capabilities
72 is to predict a response variable from several complementary data sources
73 (blocks), using so-called multi-block methods ([Mishra et al., 2021](#)). Re-
74 cently, Sequential and Orthogonalised - Partial Least Squares (SO-PLS) was

75 proposed as an extension of PLSR (Naes et al., 2011) involving an orthog-
76 onalisation procedure to sequentially capture additional information from
77 different blocks. This category of methods offers the possibility to predict
78 a response variable from a combination of several blocks such as NIR mea-
79 surements combining with physicochemical parameters for the monitoring of
80 anaerobic digestion (Awhangbo et al., 2020).

81 In this study, the potential of a combination of micro-spectrometers is
82 evaluated to predict chemical variables of sugarcane for forage application.
83 The main objective is to study the contribution of a multi-block method to
84 exploit spectra resulting from a combination of a set of micro-spectrometers.
85 In a first step, PLS models are established for each micro-spectrometer with
86 optimal pretreatments. These models are compared to a model from a ref-
87 erence laboratory spectrometer. In a second step, a combination of micro-
88 spectrometers is proposed and SO-PLS is used to build a prediction model.

89 2. Materials and methods

90 2.1. Sample preparation and reference analysis

91 A set of sixty sugarcane samples from different plant parts (leaf, stem
92 or whole aerial part) were collected in the French West Indies (Guadeloupe)
93 (Zgouz et al., 2020). Before chemical analysis, the samples were dried for 72h
94 at 85°C, milled with a Retsch SM100 mill (Retsch GmbH, Germany) with a
95 1 mm exit sieve and analysed in the Cirad Selmet feed laboratory (Mont-
96 pellier, France) to determine total sugar content (TS) and Crude Protein
97 content (CP). CP content was estimated from the total nitrogen content (N)
98 measured by Kjeldahl method, with the relationship $CP = N * 6.25$ and TS

99 content was determined by adapted Luff-Schoorl method (noa, 1997). CP
 100 and TS are expressed as a percentage (%) of Dry Matter (DM).

101 2.2. Spectral measurement protocols

102 All samples were measured by a laboratory spectrometer used as refer-
 103 ence: LabSpec 4 (ASD, Boulder, CO, USA).

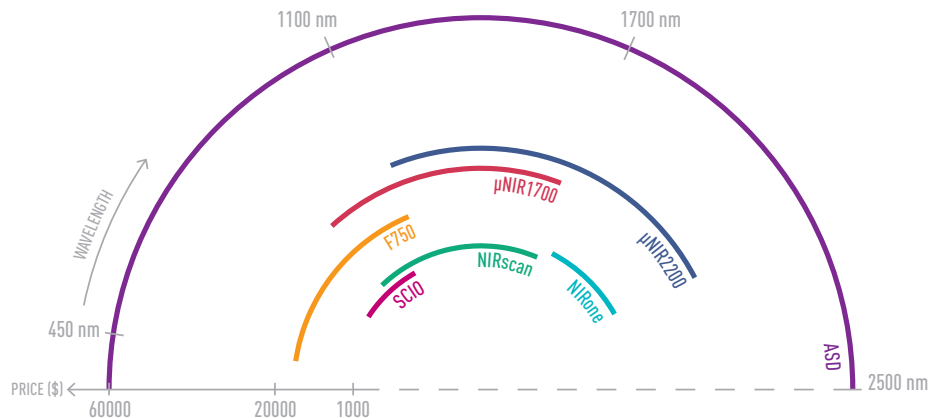


Figure 1: Spectral range according to approximate price for all spectrometers

104 Spectral acquisitions were also performed on the same samples (in a same
 105 FOSS cup) using different micro-spectrometers: SCIO (Consumer Physics,
 106 Israel), F750 (Felix Instrument, Camas, USA), μ NIR1700 (Viavi, Solution-
 107 Milpitas, USA), DLP NIRscan Nano (Texas Instrument s Inc., Texas, USA),
 108 μ NIR2200 (Viavi, Solution-Milpitas, USA) and NIRONE 2.2 (Spectral En-
 109 gines, Finland). Fifty spectra were averaged for each spectrometer acqui-
 110 sition.

111 These micro-spectrometers, covering different visible and near-infrared
 112 spectral ranges (see Table 1), were used to establish predictive models and

were compared with the ASD Labspec 4 which covers a much larger spectral range. Approximate price values of all spectrometers are displayed for comparison purposes (see Fig. 1). The lowest priced micro-spectrometers were the NIRone, NIRscan and SCIO with values close to 1000\$. The reference spectrometer (ASD) was about 60x more expensive compared to these micro-spectrometers. μ NIR1700 and μ NIR2200 have intermediate values corresponding to 20x more expensive than NIRone, NIRscan and SCIO. The F750 is a compromise (8000\$) between the micro-spectrometers in terms of price.

Table 1: Detail for each spectrometer/micro-spectrometers: acronym used on the document, spectral range and spectral resolution of the NIR spectrometers

Acronym	Manufacturer	Device model	Spectral range (nm)	Spectral resolution (at λ) (nm)
ASD	ASD Inc.	LabSpec 4	350 - 2500	3 (at 700 nm) - 10 (at 1300/2100 nm)
SCIO	Consumer Physics	SCIO	740 - 1070	not communicated
F750	Felix Instrument	F750	450 - 1140	8
μNIR1700	JDSU/VIAVI	MicroNIR1700	908 - 1676	10
μNIR2200	JDSU/VIAVI	MicroNIR2200	1150 - 2150	20
NIRscan	Texas Instrument	DLP NIRscan Nano	901 - 1701	10
NIRone	Spectral Engines	NIRone 2.2	1750 - 2150	20-26

2.3. Data analysis

2.3.1. Regression models

In the first section, Partial Least Squares Regression (PLSR) (Wold et al., 2001) was used to build models to predict chemical variables, from spectra, represented by a matrix \mathbf{X} . Each chemical variable is represented by a vector \mathbf{y} . A model was established for each micro-spectrometer where the final PLS equation can be established as follows:

$$\mathbf{y} = \mathbf{X}\mathbf{b} + \mathbf{r}_X \quad (1)$$

where \mathbf{b} is a vector containing regression coefficients and \mathbf{r}_X is corresponding to residuals of the model.

In the second section, Sequential and Orthogonalized Partial Least Squares (SO-PLS) (Naes et al., 2011) was used as a multi-block method to predict variables from multiple blocks. This method was used to evaluate a combination of micro-spectrometers, i.e. blocks corresponding to the spectra measured by these micro-spectrometers.

This method extracts the information sequentially from each data block. First, the SO-PLS algorithm started as PLS method with the first block containing spectral data, as previously described (eq. 1).

Then, an orthogonalisation procedure was performed to remove information (from the first regression) on the second block, defined by the matrix \mathbf{Z} . This orthogonalisation, providing \mathbf{Z}_\perp , can be written as follows:

$$\mathbf{Z}_\perp = \mathbf{Z} - \mathbf{T}(\mathbf{T}^t\mathbf{T})\mathbf{T}^t\mathbf{Z} \quad (2)$$

where \mathbf{T} corresponds to the score matrix of \mathbf{X} in a PLS procedure.

Then, a second PLS model is established between the residual vector, corresponding to the vector \mathbf{r}_X (eq. 1) and the matrix \mathbf{Z}_\perp . This regression is established by following the same procedure as previously for the regression between \mathbf{X} and \mathbf{y} (eq. 1). At the end of this procedure, a vector \mathbf{c} containing the regression coefficients is obtained. The final equation of the SO-PLS multi-block method can be written as follows:

$$\mathbf{y} = \mathbf{X}\mathbf{b} + \mathbf{Z}_{\perp}\mathbf{c} + \mathbf{r}_{X,Z} \quad (3)$$

149 With $\mathbf{r}_{X,Z}$, the residual vector of the SO-PLS model.

150 2.3.2. Model evaluation

151 To evaluate model performances, a calibration set and a test set from
 152 available samples were defined by random selection. The calibration set was
 153 constituted by using two thirds of the samples, i.e. forty samples. Spectra
 154 corresponding to these 40 samples were used to build the prediction model.
 155 This step was performed in k-fold cross validation (five blocks) to select the
 156 relevant number of latent variables (LV).

157 Spectra from the 20 remaining samples, corresponding to the remaining
 158 third of the whole available samples, were used as an internal test set. Each
 159 model obtained in cross-validation procedures was applied to the test set.

160 To evaluate SO-PLS models, the order of the blocks was defined in the
 161 order of the spectral ranges (i.e. the lowest spectral range corresponds to the
 162 first block).

163 2.3.3. Pretreatments

164 Pretreatments commonly used in chemometrics were tested to establish
 165 the best prediction models: Standard Normal Variate (SNV) ([Barnes et al.,](#)
 166 [1989](#)), Variable Sorting for Normalization (VSN) ([Rabatel et al., 2020](#)) and
 167 Multiple Scatter Correction (MSC). These corrections were also combined
 168 with a Savitzky-Golay type smoothing ([Savitzky and Golay, 1964](#)) by varying
 169 the window size with common values corresponding to 20 nm to 400 nm as

well as varying the polynomial order from 1 to 3. In addition, the first and second derivatives were also studied to these Savitzky-Golay smoothings.

A choice on the best pretreatment (including no pretreatment) was made for each spectrometer according to several criteria from cross-validation procedure. More especially, this choice was motivated by minimizing validation errors while selecting a low number of latent variables.

3. Results and discussion

3.1. Data overview

3.1.1. Y values

For each variable describing the chemical properties, value distributions for the calibration set and the test set are displayed in figure 2.

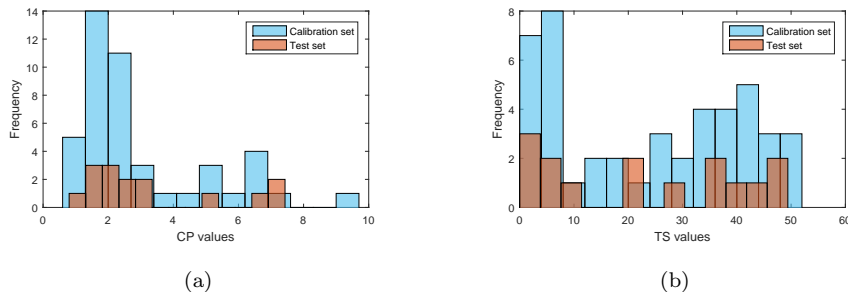


Figure 2: Histograms of calibration and test sets for each biochemical variable: (a) Crude protein content (CP, %DM), (b) Sugar content (TS, % DM)

For the calibration set, CP content (Fig. 2a) has values ranging from 1% to 10% of total dry matter with a distribution mainly between 1% and 4% and very few values above 4%. The calibration set value distribution of TS

184 content (Fig. 2b) ranges from 0% to 50% with many observations having
185 either low values between 0% and 5% or values around 40%.

186 For both chemical variables, test sets have similar value distributions
187 than those of the corresponding calibration set. The visualization of value
188 distributions confirms that the test set covers the whole value range.

189 3.1.2. Spectra analysis

190 Pseudo-absorbance spectra defined by $\log(1/R)$ (where R is the reflectance
191 spectrum measured by a spectrometer) of all calibration and test sets are
192 shown for each spectrometer (Fig. 3).

193 Spectra from ASD have a spectral range from 350 nm to 2500 nm (Fig.
194 3a). These spectra have shapes consistent with what is generally found in
195 NIR spectroscopy of fruits and vegetables (Nicolai et al., 2014): NIR spectra
196 are dominated by water contribution. Two water-related absorption bands
197 can be identified: 1436 nm, 1938 nm. A small peak at 1200nm can be ob-
198 served. The same observations are made for the spectra measured in the
199 near infrared range with the other spectrometers (Fig. 3d, 3e, 3f and 3g).
200 A visible base line shift effect was observed in absorbance raw spectra, for
201 all spectrometers. The increase in the optical path length traveled by the
202 photons in a scattering medium reflects a multiplicative effect on the spectra
203 (Osborne et al., 1993; Ryckewaert et al., 2020) resulting in baseline drifts of
204 the ideal absorbance spectra. In the spectral range between 350 and 1000 nm,
205 these scattering effects are much more dominant (Fig. 3a) and 3b) and re-
206 sult in a decreasing slope (Ishimaru, 1978). Weaker absorption peaks are
207 present at 670 nm (Fig. 3a and 3b) and 1200 nm (Fig. 3a, 3d, 3e and 3f). In
208 vegetable products, the absorption bands at 670 nm and 1200 nm have been

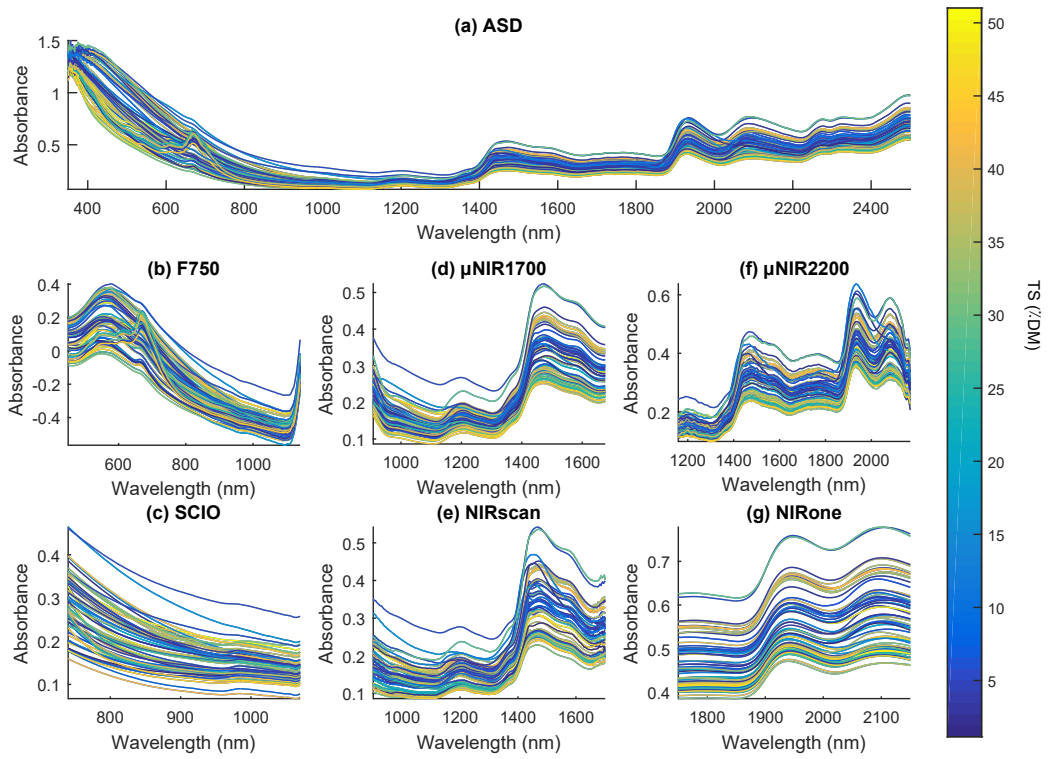


Figure 3: Absorbance spectra for each spectrometer: (a) ASD, (b) F750, (c) SCIO, (d) μ NIR1700, (e) NIRscan, (f) μ NIR2200, (g) NIRone

209 respectively associated with chlorophyll and sucrose (Osborne et al., 1993).

210 3.2. Regression model by spectrometer

211 3.2.1. Pretreatment and calibration model

212 The best models obtained by cross-validation to predict CP and TS vari-
 213 ables by micro-spectrometers/spectrometer are presented in Table 2. For
 214 each variable (CP and TS), results are classified according to the error val-
 215 ues obtained in cross-validation (*i.e.* secv).

Table 2: Calibration results for prediction of the two variables: CP and TS. The spec-
 trometers are ranked in order of best to worst model based on SECV values. ; savgol
 (width (in nm) /deriv/order)

Y	Spectrometer	pretreatment	LV	sec (%DM)	secv (%DM)	R_{cv}^2
CP	μ NIR2200	savgol(245/2/2) - SNV	9	0.29	0.51	0.942
	NIRone	SNV	9	0.45	0.55	0.929
	ASD	savgol(41/0/0)	10	0.40	0.57	0.926
	μ NIR1700	savgol(185/1/2) - SNV	12	0.49	0.64	0.930
	F750	savgol(75/2/2)	3	0.65	0.73	0.87
	SCIO	savgol(90/1/1)	5	0.64	0.75	0.87
	NIRscan	savgol(53/2/2) - SNV	8	0.51	0.99	0.77
TS	ASD	savgol(41/0/0) - SNV	8	1.15	1.83	0.989
	μ NIR2200	savgol(203/0/0) - SNV	9	1.48	2.46	0.981
	μ NIR1700	savgol(155/1/1) - SNV	8	2.37	3.40	0.960
	NIRscan	savgol(88/2/2)	13	1.84	4.24	0.939
	NIRone	savgol(30/2/2) - SNV	9	3.00	6.31	0.87
	F750	savgol(105/1/1) - SNV	13	4.17	6.42	0.87
	SCIO	savgol(45/1/1)	4	7.79	8.33	0.76

216 For the CP variable, best models from cross-validation procedure are
 217 obtained with the μ NIR2200 micro-spectrometers (secv=0.51%; R_{cv}^2 =0.942),
 218 the NIRone (secv=0.55%; R_{cv}^2 =0.929), the ASD (secv=0.57%; R_{cv}^2 =0.926)

219 and the $\mu\text{NIR1700}$ ($\text{secv}=0.64\%$; $R_{cv}^2=0.930$). The models obtained with
 220 the NIRscan ($\text{secv}=0.99\%$; $R_{cv}^2=0.77$), the SCIO ($\text{secv}=0.75\%$; $R_{cv}^2=0.87$)
 221 and the F750 ($\text{secv}=0.73\%$; $R_{cv}^2=0.87$) have higher errors and a lower R_{cv}^2 .

222 For the TS variable, the best model from the cross-validation is obtained
 223 with the ASD ($\text{secv}=1.83\%$; $R_{cv}^2=0.989$). The best models using micro-
 224 spectrometers are obtained with the $\mu\text{NIR2200}$ ($\text{secv}=2.46\%$; $R_{cv}^2=0.981$)
 225 and the $\mu\text{NIR1700}$ ($\text{secv}=3.40\%$; $R_{cv}^2=0.960$). The worst models are ob-
 226 tained with the SCIO ($\text{secv}=8.33\%$; $R_{cv}^2=0.76$), the F750 ($\text{secv}=6.42\%$; R_{cv}^2
 227 $=0.87$) and the NIRone ($\text{secv}=6.31\%$; $R_{cv}^2=0.87$) The NIRscan ($\text{secv}=4.24\%$;
 228 $R_{cv}^2=0.939$) shows intermediate results.

229 In most cases, best models are obtained with savgol smoothing of differ-
 230 ent window sizes depending on the spectrometer used and their respective
 231 spectral resolution. The VSN and MSC pretreatments did not give optimal
 232 results and do not appear in Table 2. This smoothing is combined with SNV
 233 pretreatment for $\mu\text{NIR2200}$, $\mu\text{NIR1700}$ and NIRscan in the case of CP pre-
 234 diction. SNV is also combined with smoothing on the $\mu\text{NIR2200}$, $\mu\text{NIR1700}$
 235 and NIRone and F750 for the TS variable.

236 Different pretreatments are obtained for micro-spectrometers, even to pre-
 237 dict the same response variable. This is due to different characteristics of the
 238 spectrometer used (spectral region, spectral resolution, noise). For a given
 239 spectrometer, pretreatments can be different depending on the variable to
 240 be predicted. Indeed, two chemical variables of different nature will impact
 241 differently reflectance spectrum shape.

242 3.2.2. Model evaluation

243 Once optimal pretreatment and LV number are chosen during the cross-

validation procedure, models are calibrated with the entire calibration set samples. (Tab. 2). These models are now applied to the test set. For the two chemical variables, performances of the prediction models are evaluated through sep and R^2_{test} values. These values are obtained for each spectrometer or micro-spectrometer and can be seen in table 3.

Table 3: Evaluation of prediction models on a test set. Spectrometers are ranked in order of best to worst model based on SEP value

Y	Spectrometer	sep (%DM)	bias (%DM)	R^2_{test}
CP	ASD	0.56	-0.13	0.935
	μ NIR1700	0.58	0.18	0.932
	μ NIR2200	0.67	0.20	0.908
	SCIO	0.72	-0.31	0.902
	NIRone	0.73	-0.027	0.88
	NIRscan	0.78	0.28	0.88
	F750	0.86	-0.30	0.87
TS	ASD	2.59	0.41	0.978
	μ NIR2200	2.99	0.31	0.970
	μ NIR1700	3.01	0.81	0.969
	NIRscan	4.40	0.55	0.939
	NIRone	8.04	-1.64	0.78
	F750	9.37	0.49	0.73
	SCIO	11.05	3.80	0.61

CP. For CP variable, R^2_{test} values range from 0.87 to 0.94 and error values range from 0.56 to 0.86%. The range of prediction error values needs to be compared with the protein content values, which range from 1 to 7%, but with the majority of values between 1 and 3% (Fig. 2a). The best model is obtained with the ASD (sep = 0.56%; bias=-0.13%; R^2_{test} = 0.935). The micro-spectrometers with values close to those obtained with the ASD are the μ NIR1700 (sep =0.58%; bias=0.18%; R^2_{test} =0.932) and the μ NIR2200

(sep =0.67%; bias=0.20%; R^2_{test} =0.908). Models with intermediate results are obtained with SCIO (sep =0.72%; bias=-0.31%; R^2_{test} =0.902), NIRone (sep =0.73%; bias=-0.0027%; R^2_{test} =0.88) and NIRscan (sep =0.78%; bias=-0.28%; R^2_{test} =0.88). The worst performance is obtained for the model using the F750 (sep =0.86%; bias=-0.30%; R^2_{test} =0.87)

The μ NIR1700 has a spectral region defined between 908 nm and 1676 nm. This spectral region contains a part related to overtones of the C-H, C-N, N-H bonds present between 1600-1700 nm and related to protein (Clark and Lamb, 1991). Besides, predictive quality obtained with the NIRone remains satisfactory despite a very small spectral range defined between 1750 nm and 2150 nm. Nitrogen-Hydrogen (N-H) bonds absorb at 2055 nm and 2180 nm (Wetzel, 1983). In addition, proteins contain mostly amide structures that possess nitrogen-hydrogen (N-H) bonds. The NIRone spectral region is therefore suitable to predict protein content, as absorption peak at 2055 nm can be observed as well as the beginning of the absorption peak at 2180 nm.

Almost equivalent results are reached with SCIO despite a restricted spectral range from 740 nm to 1070 nm. In this range, information is related to protein at 1007 nm or to primary amines at 1000 nm and 1020 nm (Workman and Springsteen, 1998) .

TS. For TS (Fig. 3), R^2_{test} and sep values have a wider range. These values range from 0.61 to 0.98 for R^2_{test} and from 1.81 to 11.05% for sep. Best models on the test set were obtained for the ASD (sep =2.59%; bias=0.41%; R^2_{test} =0.978) and the μ NIR2200 (sep =2.99%; bias=0.31%; R^2_{test} =0.970). Intermediate results were obtained for the μ NIR1700 (sep=3.01%; bias=0.81%; R^2_{test} =0.969) and the NIRscan (sep=4.40%; bias=0.55%; R^2_{test} =0.939). On

the other hand, models derived from the spectra measured by NIRone (sep=8.04%; bias=-1.64%; R^2_{test} =0.78), F750 (sep=9.37%; bias=0.49%; R^2_{test} =0.73) and SCIO (sep=11.05%; bias=3.80%; R^2_{test} =0.61) have a poor predictive quality.

Good and intermediate results (μ NIR2200, ASD, μ NIR1700 and NIRscan) are reached with spectrometers whose spectral ranges cover the region around O-H bond from sugar as crystalline sucrose (Kays et al., 1997) around 1441 nm (Workman and Springsteen, 1998). This is not the case for the NIRone, F750 and SCIO spectrometers (see 1), and may explain the high error values in TS prediction.

Best results are obtained with ASD and the μ NIR2200. These spectrometers cover both spectral regions around 1441 nm, as well as around 2100 nm. At 2100 nm, O-H bending and C-O stretching combination can be observed and can be related to sugar content (Workman and Springsteen, 1998) and could explain the good results obtained.

3.3. Regression model from a combination of spectrometers

Table 4 shows prediction model evaluations for CP and TS using ASD and using a combination of micro-spectrometers. Micro-spectrometers retained for the combination are the following: SCIO, NIRscan and NIRone. These micro-spectrometers were chosen because their combination covers approximately the same spectral range as the ASD while minimising the cost compared to other micro-spectrometers (see fig. 1). Pretreatments used for each micro-spectrometer correspond to those identified by the micro-spectrometers independently (see table 2).

Table 4: Evaluation of prediction performance for all variables using ASD and using the combination of three micro-spectrometers (SCIO; NIRscan; NIRone). The latent variables displayed in the format ‘../..’ correspond to the latent variables of the micro-spectrometers in the order: SCIO/NIRscan/NIRone

Y	Spectrometer(s)	pretreatment	LV	sec	secv	sep	bias	R_{cv}^2	R_{test}^2
CP content	ASD	savgol(40/0/0)'	10	0.40	0.57	0.56	-0.13	0.926	0.935
	Combination	Best each	3/2/10	0.29	0.47	0.69	0.15	0.952	0.910
TS content	ASD	savgol(40/0/0)	8	1.15	1.83	2.59	0.41	0.989	0.978
	Combination	Best each	0/6/6	1.67	2.56	2.38	-0.52	0.978	0.983

Results obtained previously with ASD are reported here as reference values. For CP variable, the optimal prediction model remains the one using spectra obtained with ASD (sep=0.56%; bias=-0.13 %; R_{test}^2 =0.935). Nonetheless, the micro-spectrometer combination provides a model with performances (sep=0.69%; bias=0.15 %; R_{test}^2 =0.910) close to those obtained with ASD.

For TS, results obtained with this micro-spectrometer combination (sep=2.38%; bias=-0.52%; R_{test}^2 =0.980) are better than those obtained with ASD (sep=2.59%; bias=0.41%; R_{test}^2 =0.978). Combining the three micro-spectrometers leads to lower prediction errors than using each micro-spectrometer separately, for both variables tested. Indeed, the best performances previously obtained for CP prediction were sep=0.72% and R_{test}^2 =0.88 with the NIRone, whereas TS prediction performances were sep=4.40% and R_{test}^2 =0.939 with the NIRscan. The combination of sensors greatly improves the predictive qualities for the variables studied. However, this proposed micro-spectrometer combination does not reach the performances obtained with μ NIR2200 for CP prediction (sep=0.65%; R_{test}^2 =0.926) as well as TS prediction (sep=2.36%; R_{test}^2 =0.985)

321 (see Tab. 3). Nevertheless, the three-spectrometer combination has a lower
322 cost than that of the μ NIR2200 alone.

323 In multi-block methods, the number of latent variables is defined by cross-
324 validation for each of the blocks (i.e. micro-spectrometers). This number
325 varies according to the relative importance of each block to predict a given
326 variable. Visualising the number of latent variables helps understanding the
327 relevance of each micro-spectrometer and would be a guided way to select the
328 best combination of micro-spectrometers according to predictive capabilities.
329 Indeed, if the number of latent variables is equal to zero, this means that the
330 micro-spectrometer is not considered in the multi-block model. This is the
331 case for the SCIO micro-spectrometer which is not used for TS prediction
332 (table 4). In this case study, the combination of only two micro-spectrometers
333 (NIRscan and NIRone) would be sufficient to predict TS at a considerably
334 lower cost.

335 Here we have chosen the pretreatments defined separately for these three
336 identified micro-spectrometers. However, it is recommended to integrate the
337 pretreatment choice into the cross-validation procedure of SO-PLS to ensure
338 better complementarity between blocks and thus improve the prediction ca-
339 pabilities. An alternative is to systematically add blocks corresponding to
340 relevant pretreatments for each micro-spectrometer. This alternative would
341 have the capacity to be automatic but would impose new constraints in terms
342 of computing time and memory space.

343 4. Conclusion

344 In this study, micro-spectrometers were evaluated individually to predict
345 Crude Protein (CP) and sugar content (TS) on sugarcane forage samples.
346 Optimal pretreatments were identified. For a micro-spectrometer, resulting
347 pretreatment may differ according to the chemical variable to be predicted
348 and depends on the measured phenomena. In a second step, a combination
349 of three micro-spectrometers (SCIO, NIRscan and NIRone) was proposed.

350 Model performances were compared to those obtained with the laboratory
351 spectrometer (ASD). Some models built from a single micro-spectrometer
352 (the most expensive) gave similar performances as the laboratory spectrom-
353 eter. For CP, the combination of micro-spectrometers gave a prediction
354 performance (sep=0.69%; bias=0.15%; R^2_{test} =0.910) close to that obtained
355 with the laboratory spectrometer (sep=0.56%; bias=-0.13%; R^2_{test} =0.935).
356 For TS, the results obtained with this combination of micro-spectrometers
357 (sep=2.38%; bias=-0.52%; R^2_{test} =0.983) are better than those obtained with
358 the laboratory spectrometer (sep=2.59%; bias=0.41%; R^2_{test} =0.978). For
359 both chemical variables, the combination of the micro-spectrometers signif-
360 icantly increases the performance of the predictive models compared to the
361 models obtained with the micro-spectrometers independently.

362 Using several low-cost micro-spectrometers, combined with a multi-block
363 method gave results as good as a single laboratory spectrometer. The overall
364 cost can be lower than a reference spectrometer. In this study, the SO-PLS
365 multi-block method with the number of latent variables selected per block
366 shows the usefulness of micro-spectrometers in the prediction results. It
367 guides the choice of the combination of micro-spectrometers by the variable(s)

368 to be predicted. A further study could thus define the cost benefit versus
369 the measurement efficiency. Trade-offs between prediction quality and device
370 cost can then be defined according to the objective and constraints of the
371 application, particularly as is the case with on-line monitoring applications
372 or outdoor measurements.

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379 **References**

- 380 Donald M. Ball, Mike Collins, G. D. Lacefield, N. P. Martin, D. A. Mertens,
381 K. E. Olson, D. H. Putnam, D. J. Undersander, and M. W. Wolf. Under-
382 standing forage quality. *American Farm Bureau Federation Publication*, 1
383 (01), 2001.
- 384 Michael Collins and J. Fritz. Forage quality. *Forages. Vol. 1. An Introduction*
385 *to Grassland Agriculture*, pages 363–390, 2003. Publisher: Iowa State Press
386 Ames, IA.
- 387 R. J. Wilkins. Forages and their role in animal systems. *Forage Evaluation*
388 *in Ruminant Nutrition, CAB International*, pages 1–14, 2000.

- 389 Jerry Stuth, Abdi Jama, and Doug Tolleson. Direct and indirect means
390 of predicting forage quality through near infrared reflectance spectroscopy.
391 *Field Crops Research*, 84(1):45–56, October 2003. ISSN 0378-4290. doi: 10.
392 1016/S0378-4290(03)00140-0. URL [https://www.sciencedirect.com/
393 science/article/pii/S0378429003001400](https://www.sciencedirect.com/science/article/pii/S0378429003001400).
- 394 E. R. Deaville and P. Ch Flinn. Near infrared (NIR) spectroscopy: an alter-
395 native approach for the estimation of forage quality and voluntary intake.
396 *Forage evaluation in ruminant nutrition*, pages 301–320, 2000. Publisher:
397 CABI Publishing Wallingford.
- 398 Franklin E Barton II and William R Windham. Determination of Acid-
399 Detergent Fiber and Crude Protein in Forages by Near-Infrared Re-
400 flectance Spectroscopy: Collaborative Study. *Journal of Association of*
401 *Official Analytical Chemists*, 71(6):1162–1167, November 1988. ISSN 0004-
402 5756. doi: 10.1093/jaoac/71.6.1162. URL [https://doi.org/10.1093/
403 jaoac/71.6.1162](https://doi.org/10.1093/jaoac/71.6.1162).
- 404 Heinz W. Siesler, Yukihiro Ozaki, Satoshi Kawata, and H. Michael Heise.
405 *Near-infrared spectroscopy: principles, instruments, applications*. John
406 Wiley & Sons, 2008.
- 407 Jerry Workman and Art W. Springsteen, editors. *Applied spectroscopy: a*
408 *compact reference for practitioners*. Academic Press, San Diego, 1998.
409 ISBN 978-0-12-764070-9.
- 410 Zongyin Yang, Tom Albrow-Owen, Weiwei Cai, and Tawfique Hasan. Minia-
411 turization of optical spectrometers. *Science*, 371(6528):eabe0722, January

412 2021. doi: 10.1126/science.abe0722. URL [https://www.science.org/](https://www.science.org/doi/10.1126/science.abe0722)
 413 [doi/10.1126/science.abe0722](https://www.science.org/doi/10.1126/science.abe0722). Publisher: American Association for the
 414 Advancement of Science.

415 Hui Yan and Heinz W Siesler. Hand-held near-infrared spectrometers:
 416 State-of-the-art instrumentation and practical applications. *NIR news*,
 417 29(7):8–12, November 2018. ISSN 0960-3360, 1756-2708. doi: 10.1177/
 418 0960336018796391. URL [http://journals.sagepub.com/doi/10.1177/](http://journals.sagepub.com/doi/10.1177/0960336018796391)
 419 [0960336018796391](http://journals.sagepub.com/doi/10.1177/0960336018796391).

420 Kerstin Wiesner, Karen Fuchs, Alexander M. Gigler, and Remigiusz Pastu-
 421 siak. Trends in Near Infrared Spectroscopy and Multivariate Data Anal-
 422 ysis From an Industrial Perspective. *Procedia Engineering*, 87:867–870,
 423 2014. ISSN 18777058. doi: 10.1016/j.proeng.2014.11.292. URL [https:](https://linkinghub.elsevier.com/retrieve/pii/S1877705814024072)
 424 [//linkinghub.elsevier.com/retrieve/pii/S1877705814024072](https://linkinghub.elsevier.com/retrieve/pii/S1877705814024072).

425 Svante Wold, Michael Sjöström, and Lennart Eriksson. PLS-regression: a ba-
 426 sic tool of chemometrics. *Chemometrics and intelligent laboratory systems*,
 427 58(2):109–130, 2001.

428 Jasper Engel, Jan Gerretzen, Ewa Szymańska, Jeroen J. Jansen, Ger-
 429 ard Downey, Lionel Blanchet, and Lutgarde M.C. Buydens. Break-
 430 ing with trends in pre-processing? *TrAC Trends in Analytical Chem-*
 431 *istry*, 50:96–106, October 2013. ISSN 01659936. doi: 10.1016/j.trac.
 432 2013.04.015. URL [http://linkinghub.elsevier.com/retrieve/pii/](http://linkinghub.elsevier.com/retrieve/pii/S0165993613001465)
 433 [S0165993613001465](http://linkinghub.elsevier.com/retrieve/pii/S0165993613001465).

434 Asmund Rinnan, Frans van den Berg, and Soren Balling Engelsen. Re-

view of the most common pre-processing techniques for near-infrared spectra. *TrAC Trends in Analytical Chemistry*, 28(10):1201–1222, November 2009. ISSN 01659936. doi: 10.1016/j.trac.2009.07.007. URL <http://linkinghub.elsevier.com/retrieve/pii/S0165993609001629>.

Puneet Mishra, Jean-Michel Roger, Delphine Jouan-Rimbaud-Bouveresse, Alessandra Biancolillo, Federico Marini, Alison Nordon, and Douglas N. Rutledge. Recent trends in multi-block data analysis in chemometrics for multi-source data integration. *TrAC Trends in Analytical Chemistry*, 137:116206, April 2021. ISSN 0165-9936. doi: 10.1016/j.trac.2021.116206. URL <https://www.sciencedirect.com/science/article/pii/S0165993621000285>.

T. Naes, O. Tomic, B.-H. Mevik, and H. Martens. Path modelling by sequential PLS regression. *Journal of Chemometrics*, 25(1):28–40, January 2011. ISSN 08869383. doi: 10.1002/cem.1357. URL <http://doi.wiley.com/10.1002/cem.1357>.

L. Awhangbo, R. Bendoula, J.M. Roger, and F. Béline. Multi-block data analysis for online monitoring of anaerobic co-digestion process. *Chemometrics and Intelligent Laboratory Systems*, 205:104120, October 2020. ISSN 01697439. doi: 10.1016/j.chemolab.2020.104120. URL <https://linkinghub.elsevier.com/retrieve/pii/S0169743920300198>.

Abdallah Zgouz, Daphné Héran, Bernard Barthès, Denis Bastianelli, Laurent Bonnal, Vincent Baeten, Sebastien Lurol, Michael Bonin, Jean-Michel Roger, Ryad Bendoula, and Gilles Chaix. Dataset of visible-near infrared handheld and micro-spectrometers – comparison of the prediction accuracy

459 of sugarcane properties. *Data in Brief*, 31:106013, August 2020. ISSN 2352-
 460 3409. doi: 10.1016/j.dib.2020.106013. URL [http://www.sciencedirect.](http://www.sciencedirect.com/science/article/pii/S2352340920309070)
 461 [com/science/article/pii/S2352340920309070](http://www.sciencedirect.com/science/article/pii/S2352340920309070).

462 SMRIDeterminationofthe reducing sugars in raw sugar bythe Luff Schoorl
 463 method. *SMRITest methods, TM050.*, 1997. URL [http://www.smri.](http://www.smri.org/rawsugar.php)
 464 [org/rawsugar.php](http://www.smri.org/rawsugar.php).

465 R. J. Barnes, Mewa Singh Dhanoa, and Susan J. Lister. Standard normal
 466 variate transformation and de-trending of near-infrared diffuse reflectance
 467 spectra. *Applied spectroscopy*, 43(5):772–777, 1989. Publisher: SAGE
 468 Publications Sage UK: London, England.

469 Gilles Rabatel, Federico Marini, Beata Walczak, and Jean-Michel Roger.
 470 VSN: Variable sorting for normalization. *Journal of Chemometrics*, 34(2),
 471 February 2020. ISSN 0886-9383, 1099-128X. doi: 10.1002/cem.3164. URL
 472 <https://onlinelibrary.wiley.com/doi/abs/10.1002/cem.3164>.

473 Abraham Savitzky and Marcel JE Golay. Smoothing and differentiation of
 474 data by simplified least squares procedures. *Analytical chemistry*, 36(8):
 475 1627–1639, 1964.

476 Bart M. Nicolaï, Thijs Defraeye, Bart De Ketelaere, Els Herremans,
 477 Maarten L.A.T.M. Hertog, Wouter Saeys, Alessandro Torricelli, Thomas
 478 Vandendriessche, and Pieter Verboven. Nondestructive Measurement of
 479 Fruit and Vegetable Quality. *Annual Review of Food Science and Tech-*
 480 *nology*, 5(1):285–312, February 2014. ISSN 1941-1413, 1941-1421. doi: 10.

481 1146/annurev-food-030713-092410. URL <http://www.annualreviews.org/doi/10.1146/annurev-food-030713-092410>.
 482

483 B. G. Osborne, T. Fearn, and P. T. Hindle. *Practical NIR spectroscopy with*
 484 *applications in food and beverage analysis*. Addison-Wesley Longman Ltd,
 485 Harlow UK, 1993. ISBN 978-0-582-09946-3. URL <http://discovery.ucl.ac.uk/267166/>.
 486

487 Maxime Ryckewaert, Nathalie Gorretta, Fabienne Henriot, Federico Marini,
 488 and Jean-Michel Roger. Reduction of repeatability error for analysis of
 489 variance-Simultaneous Component Analysis (REP-ASCA): Application to
 490 NIR spectroscopy on coffee sample. *Analytica Chimica Acta*, 1101:23–31,
 491 March 2020. ISSN 00032670. doi: 10.1016/j.aca.2019.12.024. URL <https://linkinghub.elsevier.com/retrieve/pii/S0003267019314606>.
 492

493 Akira Ishimaru. *Wave propagation and scattering in random media*, vol-
 494 ume 2. Academic press New York, 1978.

495 David H. Clark and Robert C. Lamb. Near Infrared Reflectance Spec-
 496 troscopy: A Survey of Wavelength Selection To Determine Dry Matter
 497 Digestibility1, 2, 3. *Journal of Dairy Science*, 74(7):2200–2205, July 1991.
 498 ISSN 0022-0302. doi: 10.3168/jds.S0022-0302(91)78393-8. URL <https://www.sciencedirect.com/science/article/pii/S0022030291783938>.
 499

500 David L. Wetzel. Near-infrared reflectance analysis. *Analytical chemistry*, 55
 501 (12):1165A–1176A, 1983. Publisher: ACS Publications.

502 Sandra E. Kays, Franklin E. Barton, William R. Windham, and David S.
 503 Himmelsbach. Prediction of Total Dietary Fiber by Near-Infrared Re-

504 flectance Spectroscopy in Cereal Products Containing High Sugar and
505 Crystalline Sugar. *Journal of Agricultural and Food Chemistry*, 45(10):
506 3944–3951, October 1997. ISSN 0021-8561, 1520-5118. doi: 10.1021/
507 jf9703260. URL <https://pubs.acs.org/doi/10.1021/jf9703260>.