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Feasibility studies and engineering of optical simplified and stand-alone devices for agri-food applications

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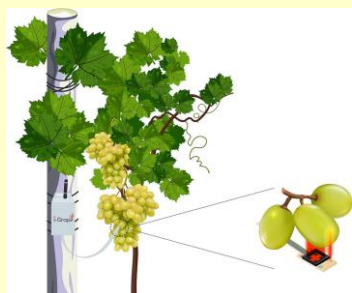
Extended Abstract

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Preface

The food industry needs to comply with stricter rules (from regulatory agencies) and meet customers' demands for higher-quality production. To achieve these objectives, the integration of emerging technologies has become essential.

Among these, optical techniques stand out as the most versatile and widely employed across various sectors, notably including agriculture and the food industry. Such methods offer unparalleled effectiveness during crucial stages like harvest, post-harvest and food processing. They enable rapid monitoring of critical quality parameters without the need for extensive sample preparation and with minimal environmental impact perfectly aligning with sustainable practices.



This PhD project explored different applications of non-destructive optical techniques for assessing the quality of agri-food products. Additionally, it involved the development of tailor-made optical devices to address the requirements of the agri-food industry within the context of Industry 4.0. A significant focus of the research has been on developing a comprehensive autonomous grape maturation monitoring system, which is elaborately described below. This system has been selected to be presented in the "Giuseppe Pellizzi Prize 2024" under the topic of "Automation and Electronics."

1. Introduction

In the wine sector, monitoring grape ripeness is a complex and crucial process for the production of high-quality wines. However, current methods are cumbersome and inefficient and could cause a decrease in the quality and value of the wine.

Such methods rely on labor-intensive and time-consuming wet-chemistry assays, which are destructive and based on complex sampling processes. To revolutionize this process, a new technology has been proposed that offers real-time, stand-alone monitoring at a low cost without the use of chemicals. This technology should also drastically reduce the need for manpower and offer information with both temporal and spatial resolution.

2. Scope

This work focused on the development of a fully integrated stand-alone optical device for grape quality monitoring directly in the field. The main steps to fulfil the project purpose were:

- Setting up of a miniaturized low-cost and stand-alone optical prototype composed by LEDs suitable for diffuse reflectance measurements, photodetectors (PDs, CMOS), sensors controller and power management;
- Multivariate predictive models' development for the prediction of the main grape ripening parameters;
- Test the prototype in field conditions.

3. Materials and methods

3.1 Sensor specs

Concerning miniaturization and usability requirements in the field, it was developed a "stripe" design in which the spectrometric components were mounted on a long flexible substrate which can be placed onto or inside the grape bunch. The multiple spectrometers were placed along the stripe (currently 2, module 1 (M1) and module 2 (M2)), enabling simultaneous measurements at different parts of the grape bunch. Figure 1a shows the four optical bands associated to the evolution of the maturation parameters of the grapes such as the development of anthocyanins and sugars, chlorophyll degradation, and decrease of water content. Therefore, four light-emitting diodes (LEDs) were used for illumination of the grape (530 nm, 630 nm, 690 nm and 730 nm). Placed close to these, but optically isolated using an opaque barrier, four photodiodes (with an active area of $520 \times 520 \mu\text{m}^2$) assembled to allow intensity measurements at the desired wavelengths (the relative spectra sensitivity is reported in figure 1b) have been used.

The light emitted from each LED hits the sample and the diffuse reflectance light is collected by each PD. The electromagnetic signal is converted into electronic signal and expressed in arbitrary units from 0 to 4095. From each sample, 20 readouts were obtained (one readout from each PD at each LED on and one with LEDs off for background info).

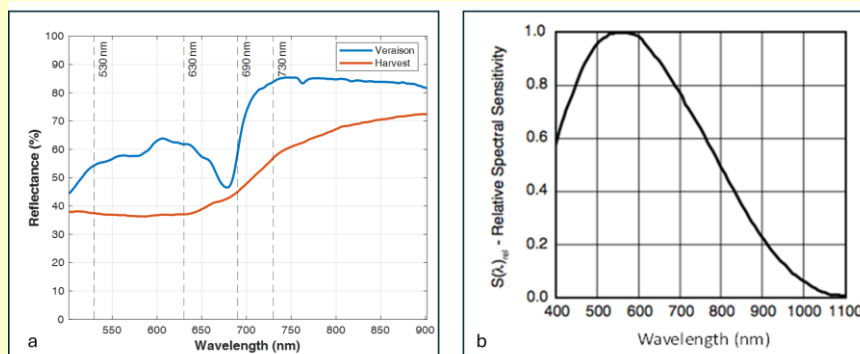


Figure 1. a) Reflectance spectra from veraison to harvest of grape samples acquired with a benchtop spectrophotometer (Perkin Elmer 950). b) Spectral sensitivity of each PD.

Concerning the data transmission, the sensors were configured in order to share the optical outputs coming from the sensors placed in a target parcel to a local IoT gateway LoRaWAN. Then, the local server broadcasts the data to a web app (IoT database) in order to process the data with the chemometric models developed during the sampling campaign 2020 using samples analysed in lab and direct in field (Figure 2).

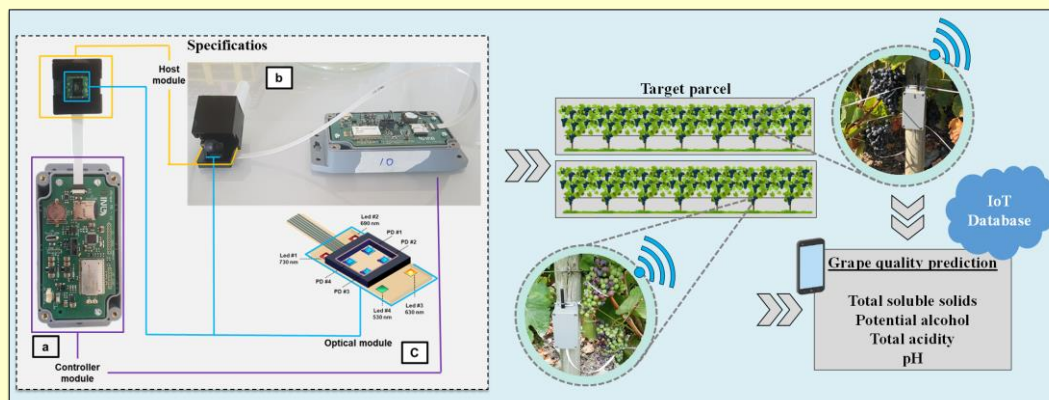


Figure 2 Sensor technical specifications (spectral sensing system with optical sensing head (a), operative representation of the system for lab data acquisition (b), and schematic representation of the optical head structure (c)), installation and data transmission.

3.2 Reference analysis

The experimental activity took place in the viticulture area of the Douro Valley (Sogrape's owned Quinta do Seixo, Portugal) from the end of July to mid-September for a total of six sampling dates. Sampling was performed on cv. Touriga Nacional (TN) and Touriga Franca (TF) (from 18 parcels) using the optical prototype without any sample preparation.

The reference analyses performed were: (i) Total Soluble Solids (TSS, °Brix) using a digital refractometer (PAL-1 ATAGO, Japan), (ii) Potential Alcohol (PA, % vol), (iii) Titratable Acidity (TA, g of tartaric acid L-1) using an automatic titrator (TitroMatic KF 1S, Crison Instruments, Italy) and (iv) pH (pH meter, PCE Inst. GmbH, Germany).

3.3 Optical analysis

Optical acquisitions were managed with careful consideration of various factors: environmental noise, physical characteristics of the berries, bunch size increase, variable optical gap, and changing sensor positions during ripening. To mitigate these issues and maximize sensor data, measurements were conducted overnight for in-field analysis and in a dark room for in-lab analysis. Each PD readout was analyzed individually to extract maximum information. Thus, a total of 16 optical variables (light emitted by 4 LEDs read by 4 PDs) were utilized for model building.

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3.4 Models development

A multivariate analytical approach was followed exploring the information using PCA. A latent variable (LV) modelling using the PLS method, which maximizes the covariance among the sensor readouts and the reference qualitative parameters (TSS, PA, TA and pH), was performed. Model accuracy was evaluated (in calibration, cross-validation and prediction) using the RMSE, as well as bias and R².

4. Results

4.1 Sensor output

Figure 3 depicts the optical results obtained from both laboratory and field sensors. It presents the overall readings captured by each PD across all LEDs, including when the LED is switched off. To streamline the presentation, the average optical profile for each sampling time in the lab data (Figure 3a), and the complete acquisitions spanning from late July to mid-September (Figure 3b) for the field data have been reported.

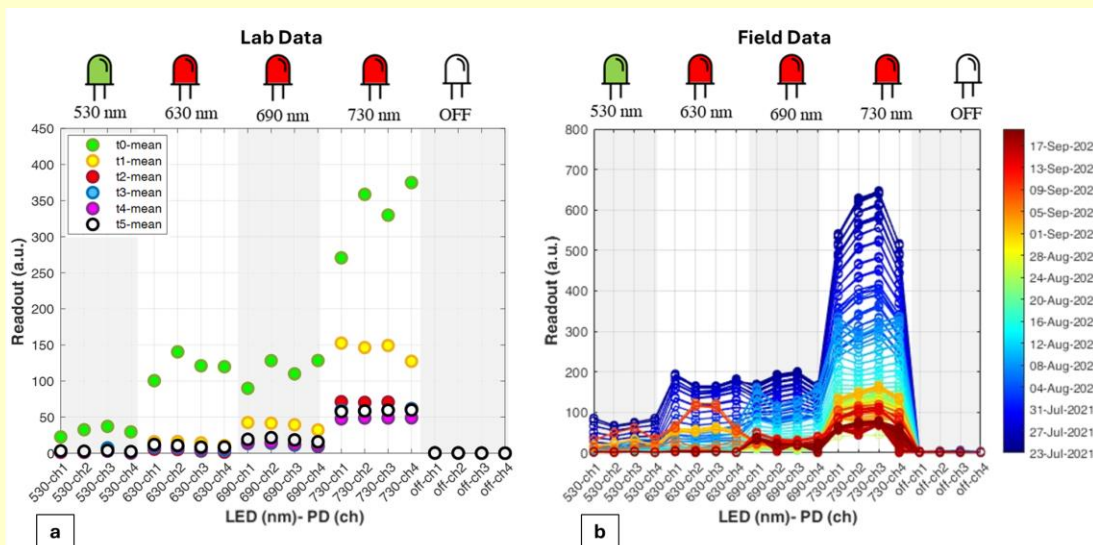


Figure 3 Sensor readouts of each LED read by each PD. a) mean optical outputs obtained each sampling time; (b) field readouts (samples labelled according to the date of acquisition).

4.2 Modelling

The wet-chemical descriptive statistics are summarized in figure 4. Overall, the technological maturation curve of TN and TF grapes is well described by the sampling campaign performed during the crop season 2020. Each sample was analysed optically (by lab sensor) and chemically (by the reference instruments) to proceed with the model's calculation.

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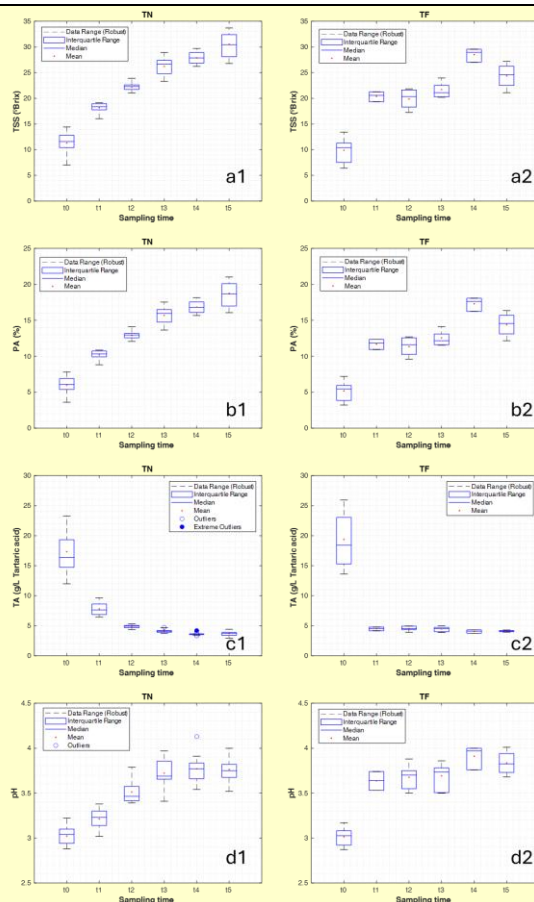


Figure 4 Descriptive statistics of the reference analysis of TSS (a), PA (b), TA (c) and pH (d) obtained from cv. Touriga Nacional (TN) and cv. Touriga Franca samples at each sampling time.

PLS models were developed for the prediction of the qualitative parameters of interest. The 70% of the total amount of the data was used for calibration and 30% for the external validation (prediction).

Figure 5 and Table 1 summarize the models figure of merit both in cross-validation and in prediction. The external validation samples set were labelled in red (TF) and in green (TN). In detail, it was concluded that:

- The best models were obtained for TSS, and PA considering an $R^2 \sim 0.90$ and RMSEP of 2.41 and 1.68, respectively using 4 LVs.
- A very promising model was also obtained for TA with an RMSEP of 1.61 (using 4 LVs) and an $R^2 \sim 0.9$.
- The pH model (using 4 LVs) showed a lower performance than previous parameters ($R^2 \sim 0.8$ and RMSEP 0.13) but still with potential for being used with further improvements.

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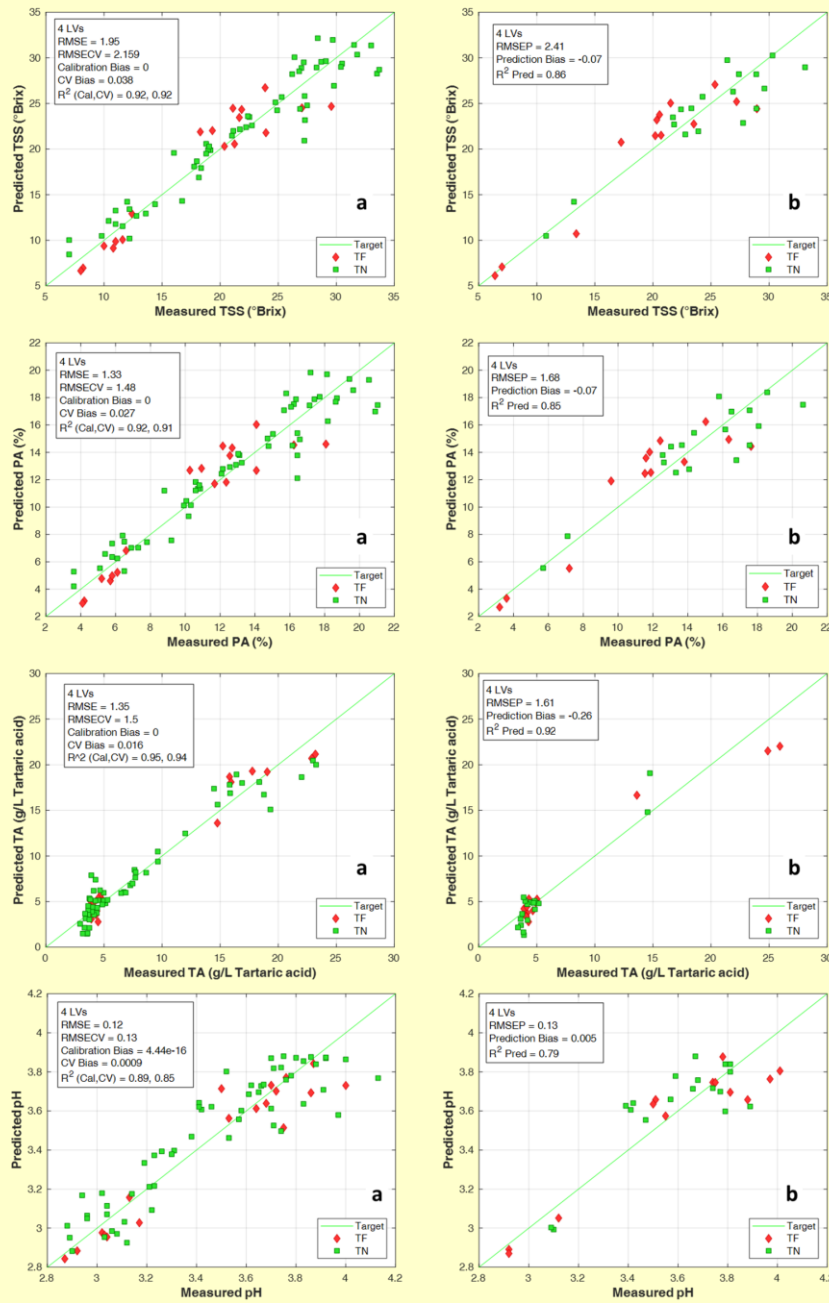


Figure 5. Models figure of merits of the calibration/cross-validation (a) and prediction (b) datasets related to the technological parameters of maturation.

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Table 1- Figures of merit of the PLS models. *

Qualitative parameter	LVs	RMSE	R ²	RMSEP	R ² Pred	Bias Pred	RPD
TSS (°Brix)	4	1.95	0.92	2.41	0.86	-0.07	2.76
PA (%)	4	1.33	0.92	1.68	0.85	0.03	2.58
TA (g/L Tartaric acid)	4	1.35	0.95	1.61	0.92	-0.26	3.65
pH	4	0.12	0.89	0.13	0.79	0.005	2.27

*LVs = number of latent variables; RMSE = root mean square error of calibration; R² = coefficient of determination; RMSEP= root mean square error of cross-validation; R² Pred= coefficient of determination in Prediction; Bias Pred= Prediction Bias; RPD = residual prediction deviation.

4.3 Field test

The lab-developed models were used in the 2021 field campaign to assess sensor performance in monitoring the maturation process. At the beginning of the campaign 2021, 8 sensors were deployed (Figure 6) to perform 11 measurements during the night (one measurement every 30 minutes) from midnight to 5:00 a.m.

However, external factors like environmental conditions could cause variations in the optical data and, consequently, on the predicted values over time. To counter this, a data filtering procedure and a harmonization approach was introduced, involving the application of a multivariate filtering strategy and a moving-average function to daily mean prediction values. This smoothing technique reduced the impact of external effects on the maturation curve, ensuring a more accurate trend in predictions.

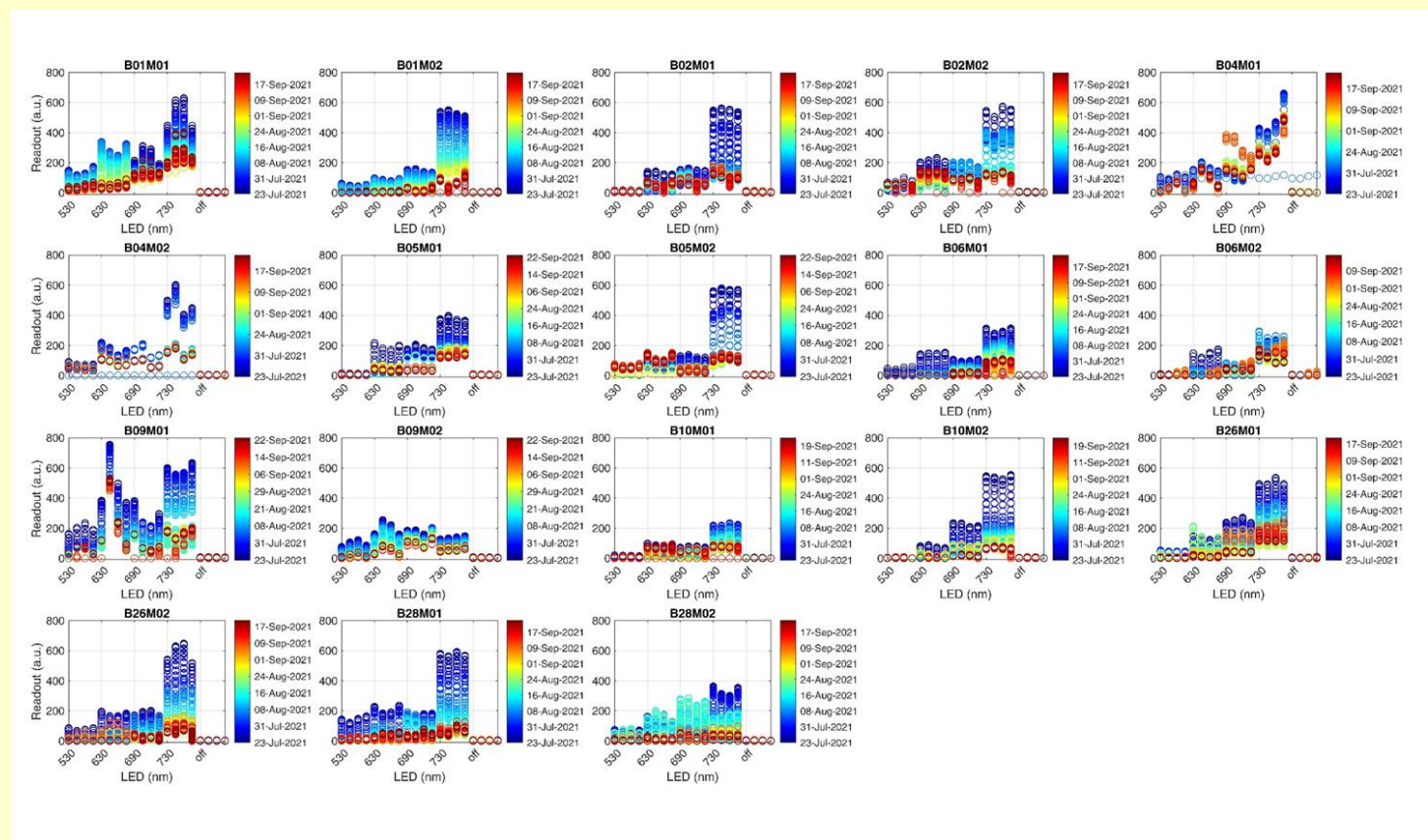


Figure 6. Raw optical data collected in the field during the 2021 campaign. The 16 scatter plots correspond to optical spots from the 8 deployed sensors. Data labelled according to the day of the year.

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Figure 7 shows the average and harmonized output of PLS models using field data compared to the average value of the reference analysis performed on the same plots at Quinta do Seixo (cv. Touriga Nacional, red grapes). Eight sampling sessions were performed during the 2021 campaign. The comparison shows a significant high correlation ($r=0.99$ and $p<0.05$) between the mean predicted values and the reference analysis, demonstrating the reliability of the laboratory models combined with the new data processing and filtering procedure for the prediction of the four technological parameters under evaluation. The pH is the only parameter that shows lower performance at the end of the season underestimating the real condition of 0.2 ($r=0.97$ and $p<0.05$).

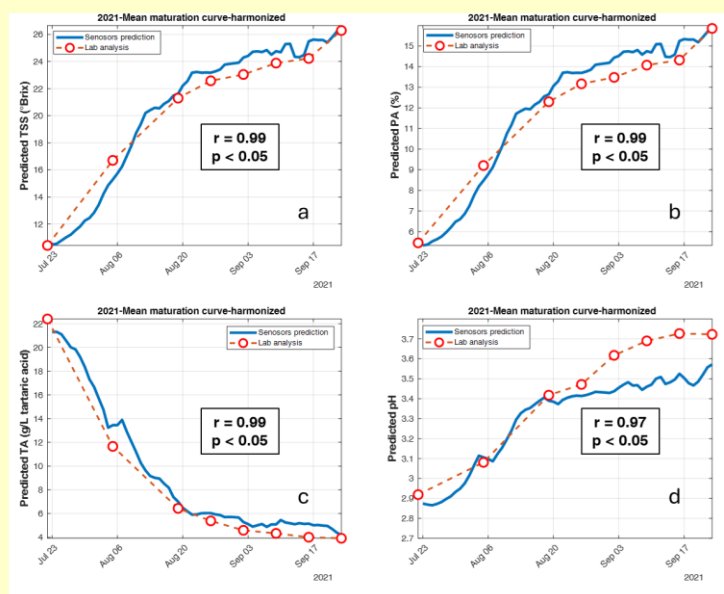


Figure 7. Average and harmonized prediction of PLS models using of the 2021 field campaign compared to the average value of the reference analysis performed on the same parcel (TSS (a), PA (b), TA (c) and pH (d)).

5. Conclusions

To conclude, a good prediction capability has been reached for each qualitative parameter envisaging a real application of this device in a more sophisticated network of sensors in order to give the possibility to the wine industry to bring the laboratory to the field. However, further experiments must be carried out and different operational strategies to obtain reliable optical data need to be fine-tuned.

In order to spread the application of this sensor for the whole viticulture sector, other models for the prediction of qualitative parameters need to be calibrated to include white grape varieties into the package of potential applications of this new type of sensors. Moreover, given the low capability of these sensors (which work in diffuse reflectance in the vis/NIR range) to give back optical outputs strongly related to the concentration of polyphenols and anthocyanins (performance is consistent with previous works reported in literature), the development of a fluorescence module is currently under study, and it will be taken in consideration for a future sensor upgrade.

Final remarks concerning benchmarks and strength points of the Pellizzi Prize 2024

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The Ph.D. thesis focuses on "Automation and Electronics," designing a standalone optical device for real-time grape monitoring. It offers the "Agricultural Machines and Mechanization" sector a new perspective via a wireless proximal sensing sensor network. With its standalone design and affordable components, it suits viticultural areas where the use of bulky machinery is critical. The method also aims to synergize with machines for precision viticulture, managing info remotely for more effective planning. Its transferability for assessing plant water stress is being explored. A paper titled "Optical specifications for proximal sensing to monitor vine water status autonomously" was published during the Ph.D. to pave the way for a dedicated sensor with the same concept.

In conclusion, the general approach seeks to revolutionize vineyard management by bringing laboratory-level analysis to the field, replacing traditional wet-chemistry assays with a non-destructive, sustainable method.