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Response to Reviewers:	

Rapid estimation of natural pigments in olive and avocado oils using a colorimetric sensor

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Abstract

Chlorophylls and carotenoids are naturally existing pigments and play a crucial role in the chemical and sensory quality of vegetable oils. These compounds have at the same time substantial positive health impacts and can be useful in detecting adulteration. Therefore, this study evaluated the feasibility of a color sensor (RGB sensor) for predicting the total content of carotenoids and chlorophylls in avocado and olive oils, two of the vegetable oils that have well documented health effects. as well as their total spectrophotometric color (TSC). Different color parameters (RGB, HSV, or L*a*b*) and lighting conditions (white or 395 nm UV light) were compared in order to identify the best analytical condition. The least-square support vector machine (LS-SVM) models exhibited superior performance compared to the multiple linear regression (MLR) models. The use of UV light resulted in an enhanced predictive performance for the total chlorophylls content. In contrast, white lighting was found to be more suitable for the prediction of total carotenoids and TSC. The use of HSV or RGB values demonstrated better performance in predicting total chlorophylls ($R^2 > 0.9$, RMSE from 0.99 to 4.13 mg kg^{-1}, and RPD from 4.04 to 3.48). On the other hand, the L*a*b* values demonstrated the highest accuracy in predicting the total carotenoids content ($R^2 > 0.8$, RMSE from 0.42 to 0.92 mg kg^{-1}, and RPD from 2.02 to 2.22). In conclusion, this color sensor-based approach has been demonstrated as a cost-effective, accurate, and rapid method for predicting pigment content in vegetable oils, requiring minimal or no sample preparation.

Keywords: colorimetry, chemometrics, chlorophyll, carotenoids, edible oils, electronic sensor

1. Introduction

The quality of vegetable oils, such as olive and avocado oils, is correlated with their nutritional value, freshness, and functional properties, all of which can be linked to their natural pigment content (Jimenez-Lopez et al., 2020; Lazzerini & Domenici, 2017; Tena et al., 2015). These oils have been under intense research interests, due to their health positive effects, and their production has increased substantially (Chiavarini et al., 2024; Lin & Li, 2024). Their primary pigments, namely chlorophylls and carotenoids, play a significant role in the chemical and sensory quality of these vegetable oils (de Carvalho & Nunes, 2021; Tan, 2019). Chlorophylls are the primary green color pigments, while carotenoids are responsible for the yellowish or reddish color (Pérez-Gálvez et al., 2020; Tan, 2019; Wong et al., 2008). Chlorophylls have been reported to possess antioxidant, antimutagenic activity, and have the ability to prevent degenerative diseases (Ferruzzi & Blakeslee, 2007). Carotenoids are natural antioxidants that inhibit free radicals propagation (Fernando et al., 2021). The presence of carotenoids in foods is linked to a reduced risk of diseases of the skin, eyes, and cardiovascular problems, especially those based on oxidation of low-density cholesterol (LDL) (Fernando et al., 2021). Although limits for chlorophylls and carotenoids are currently absent in official guidelines or standards for vegetable oils (International Olive Council, 2024), the measurement of these pigments in virgin vegetable oils is considered of substantial importance, as they can provide information on the product stability. There are a important sensorial parameters as well, since the color is usually the first attribute evaluated by the consumer (Zegane et al., 2015). The pigment composition also has been used already for the detection of adulteration of olive oil with other edible oils (Lu et al., 2023).

There are several well-documented analytical techniques employed for the determination of natural pigments in oils mainly based on spectrophotometry and chromatography. These techniques are often time-consuming, costly, and labor-intensive, as they include a number of pre-treatment steps before their final analysis and chemical reagents (Borello et al., 2021; Jiménez-Sotelo et al., 2016). Nowadays methods based on smartphone cameras and colorimetric sensors have been

proposed as faster oil quality evaluation alternatives (de Carvalho & Nunes, 2021). Carvalho and Nunes (2021) have proposed a smartphone-based method for the prediction of both chlorophylls and carotenoids content in olive and avocado oils. The method proposed by them had a relatively good performance, presenting, for example, a limit of quantification of total chlorophyll (1.86 mg kg^{-1}). This limit is slightly higher than this of the AOCS Cc 13i-96 spectrophotometric method (1.0 mg kg^{-1}), which have been used as a reference. However, that method had the drawback of requiring a calibration transfer to mitigate errors from light effects and differences in smartphone cameras. In addition, image processing presents several challenges, such as interference from external factors, correction of internal artifacts, and precise definition of the region of interest (Fan et al., 2021), de Carvalho et al., 2023). These aspects require advanced knowledge to ensure the quality and reliability of the results. In contrast, portable sensors appear to be a more attractive alternative than smartphones.

Optical sensors are designed with a focus on "point-and-shoot" capabilities, with particular attention paid to their ruggedness (Rodriguez-Saona et al. 2020). These sensors can have some limitations, such as limited sensitivity and accuracy and the need to control external factors, such as lighting conditions and angle of measurement. They are also not sensitive to non-visible features and perform best when the food sample is relatively homogeneous in color (de Carvalho Pires et al., 2024). Nevertheless, these sensors are considered a promising and emerging from an analytical perspective approach, due to their significantly reduced size, low cost, and their integration of micro-electro-mechanical systems (Rodriguez-Saona et al., 2020). These color sensor-based approaches can offer advantages over traditional methods, such as spectroscopy and chromatography, including no chemical waste, portability, on-site measurement, remote monitoring, high-throughput testing with minimal effort, and on-site quality control. This approach facilitates the development of novel devices with a broad range of applications in food analysis, such as fluorescence-based devices for detecting oil mixtures (Bi et al., 2019), monitoring storage conditions, and adulteration of extra virgin olive oil (Lastra-Mejias et al., 2019), and the detection

of mixtures of vegetable oils in avocado oil (Lorenzo et al., 2024). To the best of authors' knowledge, there is an absence of documented data relevant to colorimetric sensors for natural pigments determination in vegetable oils.

The food industry uses widely well-established spectrophotometry and chromatography methods that have been validated over time, particularly in quality control. These methods are trusted by regulatory agencies and industry professionals, especially the chromatographic ones as they have low detection limits and they are able to discriminate compounds. Therefore, it is rather impossible these chromatographic methods to be entirely replaced from other currently available analytical technologies. Although colorimetric sensors are less expensive and easier to use, they present a lack of maturity to be considered viable replacements for these more established methods in contexts that require regulatory accuracy, consistency, or scientific validation. Therefore, studying the applicability of these sensors is essential for a transition to new analytical technologies, which can offer an initial quick in-site estimation of the oils quality.

In this context, the objective of this proof-of-concept study is to evaluate the feasibility of using a conventional and inexpensive color sensor for the simultaneous prediction of the carotenoids and chlorophylls content, in addition to the total spectrophotometric color of olive and avocado oils. This sensor's response with respect to the pigment content was evaluated against the responses of commonly employed methods for the determination of chlorophylls and carotenoids. The most appropriate modeling approach (linear or non-linear), color parameters (RGB, HSV, or L*a*b*), and the type of lighting (white or UV light) were investigated.

2. Material and Methods

2.1. Samples and instruments

Five virgin avocado oils (Hass, Breda, Margarida, Fortuna, and Quintal avocado cultivars) and two extra virgin olive oils (Koroneiki and Arbequina cultivars) were collected directly after extraction from Empresa de Pesquisa Agropecuária de Minas Gerais (EPAMIG, Brazil) with

guarantee of authenticity and purity. Four commercial extra virgin olive oils (Andorinha, Larambia, Herdade, and Irarema) and one refined soybean oil (Liza) were obtained from the local market. Prior to storage and analysis, the oils were filtered through qualitative paper filters (Unifil 80g). All oils were within their expiration dates and were stored in a fridge at 5°C until their analysis (within a period of three months).

In order to better represent a few common commercial available blends, such as olive and soybean or olive and avocado oils, as well as to increase the samples size and include a variety of calibration and validation points, a series of blends were prepared (Table S1) by combining the oil samples mentioned above, resulting in 43 additional samples. The proportions of the blends were defined after determining the pigment content of the pure oils in order to obtain a wide and varied range of concentrations, well distributed over the entire measurements range. The blending was performed by weighing the respective oils in 10 ml glass vials and then manually shaking them for approximately 30 seconds until a visually homogeneous mixture was produced. The analyses were conducted within four hours after the mixture preparation and ensuring that the mixture was bubble-free. The samples were analyzed in triplicate, resulting in a total of 129 points.

All the spectrophotometric analyses were conducted in a UV/Vis spectrophotometer (Drawell® DV-8200, UV-Pro software ver. 1.0.01) using a 1 cm glass cuvette.

2.2. Determination of total chlorophylls by spectrophotometry

The three most common spectrophotometric methods reported in the literature to determine the total chlorophylls content (Tchl) in oil samples were used.

In the first method, the chlorophylls were determined by direct (without solvent) measurement of the sample's absorbance at 670 nm, 630 nm, and 710 nm (Pokorny et al., 1995). This method was designated as Tchl – IUPAC. The Tchl value was calculated using the following equation:

$$Tchl(mg.kg^{-1}) = \frac{345.3(A_{670} - 0.5 \times A_{630} - 0.5 \times A_{710})}{L} \quad (1)$$

Where:

Tchl: content of chlorophylls in mg of pheophytin per kg of oil

A: absorbance at the respective wavelength (nm)

L: optical path length (1 cm)

In the second method, the standard AOCS Cc 13d-55, as described by Sabah (2007), was employed for the determination of total chlorophyll. This involved the measurement of the absorbance of the sample (without solvent) at 630 nm, 670 nm, and 710 nm. This method was designated as Tchl – AOCS. The calculation of Tchl was performed in accordance with the following equation:

$$Tchl\ (mg.kg^{-1}) = \frac{A_{670} - 0.5\ (A_{630} + A_{710})}{0.0964\ L} \qquad 2$$

Where:

Tchl: content of chlorophylls in mg of pheophytin per kg of oil

A: absorbance at the respective wavelength (nm)

L: optical path length (1 cm)

The third method employed the measurement of the absorbance at 670 nm to quantify the total chlorophylls and their derivatives in the sample (Minguez-Mosquera et al., 1991). This approach is based on the observation that the absorbance at 670 nm is exclusively attributed to the fraction of these pigments. The samples were prepared by mixing 0.6 g of oil with 2 ml of n-hexane. This method was designated as Tchl – MM. Tchl was calculated in accordance with the following equation:

$$Tchl\ (mg.kg^{-1}) = \frac{A_{670} \times 10^6}{613 \times 100 \times L} \qquad 3$$

Where:

Tchl: content of chlorophylls in mg of pheophytin per kg of oil

A: absorbance at the respective wavelength (nm)

168 *L: optical path length (1 cm)*

169

170 *2.3. Determination of total carotenoids*

171 The two most common spectrophotometric methods reported in the literature to determine the
172 total carotenoids content (Tcar) in oil samples were used.

173 In the first method, the samples were prepared by mixing 0.6 g of oil and 2 ml of n-hexane, as
174 described by Goodwin (1952) and adapted by Mba et al. (2017). The total carotenoids content was
175 determined from the absorbance at 445 nm. This method was designated as Tcar – GW. Tcar was
176 calculated using the following equation:

177 $$Tcar\ (mg.kg^{-1}) = \frac{A_{445} \times v \times 10^6}{2500 \times W \times 1000} \quad 4$$

178 Where:

179 *Tcar: total carotenoids content in mg per kg of oil*

180 *A: absorbance at the respective wavelength (nm)*

181 *v: volume of n-hexane in ml*

182 *W: weight of sample in g*

183

184 In the second method, the absorbance at 470 nm was employed to assess the total content of
185 carotenoids in virgin oils, given that absorbance at this wavelength is largely attributable to the
186 absorption of these pigments (Minguez-Mosquera et al. 1991). The samples were prepared by
187 mixing 0.6 g of oil and 2 ml of n-hexane. This method was designated as Tcar – MM. The Tcar
188 value was calculated using the following equation:

189 $$Tcar(mg.kg^{-1}) = \frac{A_{470} \times 10^6}{2000 \times 100 \times L} \quad 5$$

190 Where:

191 *Tcar: total carotenoids content in mg per kg of oil*

192 *A: absorbance at the respective wavelength (nm)*

193 *L: optical path length (1 cm)*

194

195 *2.4. Determination of total spectrophotometric color by spectrophotometry*

196 The total spectrophotometric color (TSC) determination was conducted in accordance with
197 the Standard PN-A-86934:1995 (Różańska & Namieśnik, 2017). The samples were prepared by
198 mixing 0.2 g of oil with 2 ml of n-hexane for the measurement at 442 nm and mixing 1.0 g of oil
199 with 1 ml of n-hexane for the measurement at 668 nm. TSC was calculated using the following
200 equation:

201 $$TSC = 1000\ (A_{442} + A_{668}) \qquad 6$$

202 Where:

203 *TSC: total spectrophotometric color*

204 *A_{442}: absorbance at the respective wavelength (nm)*

205 *A_{668}: absorbance at the respective wavelength (nm)*

206

207 *2.5. Analysis using the color sensor*

208 A TCS34725 color sensor (Texas Advanced Optoelectronic Solutions Inc.) was employed to
209 acquire digital readings of red, green, blue (RGB), and clear light (C) values. This sensor, which is a
210 color light-to-digital converter, was interfaced with an Arduino Uno (Figure 1). The integration time
211 was set at 24 ms, and the gain was set at 1x. A sample holder was constructed using white ethylene-
212 vinyl acetate (EVA) material, as previously described (Lorenzo et al., 2024). The samples were
213 analyzed in 4 ml glass cuvettes under two distinct lighting conditions: ultraviolet light (3V, 395 nm
214 LED) and white light from the color sensor's light source. The closed sample holder ensured the
215 lighting standardization. The raw readings for the red (R), green (G), blue (B), and clear light (C)
216 outputs were acquired by averaging 10 readings using Realterm software (version 2.0.0.70,
217 i2cchip). The raw RGB values were normalized by dividing them by the C value, resulting in the R,
218 G, and B values used as descriptors in the models. Furthermore, the RGB values were converted to

HSV and CIE L*a*b using the functions "rgb2hsv" and "rgb2lab" from the Image Processing package for Octave (Eaton et al., 2024).

2.6. Predictive models

The color parameters of the oil samples obtained using the color sensor (independent variables) were calibrated against the total chlorophylls, total carotenoids, and TCS values determined spectrophotometrically using the different methods (dependent variables). In order to identify the optimal descriptors, different color systems (RGB, HSV, or L*a*b*) and lighting conditions (white or UV light) were employed. The dataset is available as supplementary material.

Two modeling approaches were evaluated: Multiple Linear Regression (MLR) and Least-Square Support Vector Machine (LS-SVM) with a radial basis function. The dataset was split into a calibration set, which encompassed 75% (97 samples) of the total samples, and a test set, which comprised the remaining 25% (32 samples). This sample division was conducted employing the Kennard-Stone algorithm (Yun, 2022). The suitability of the model was assessed using the determination coefficient (R^2) and the root mean squared error (RMSE) for calibration, y-randomization, leave-one-out cross-validation, and test set, in addition to Relative Standard Deviation (RSD) and the ratio of performance to deviation (RPD) for the test set (Bellon Maurel et al., 2010).

The R^2m value was calculated (Equation 7) to confirm that the predicted values obtained through the test set demonstrate a strong correlation with the observed values and exhibit congruence as well. A threshold of 0.5 was used as the criterion for validity (Mitra et al., 2010).

$$R_m^2 = R^2 \left(1 - \sqrt{R^2 - R_0^2}\right) \qquad 7$$

where R^2 and R^2_0 represent the quadratic correlation coefficients between the actual and predicted values, with and without the intercept, respectively.

Furthermore, the robustness of the models was assessed by a y-randomization test, which consists of fixing the X matrix (independent variables) and shuffling the y vector (dependent

variable) to obtain new models. It is expected that the predictive performance will decrease as the response is truly related to its predictor, thus validating the relationship between independent and dependent variables. From this test, the cR^2p value was computed, which accounts for the distinction between the y-randomization R^2 (R^2rand) and calibration R^2 (R^2cal) (Equation 8). A cR^2p > 0.5 was established to attest to the absence of overfitting or random adjustment (Mitra et al., 2010).

$$cR_p^2 = R_{cal}^2 \left(\sqrt{R_{cal}^2 - R_{rand}^2}\right) \qquad 8$$

All computations were conducted using Octave version 9.2.0 (Eaton et al., 2024). The LS-SVM models were implemented via the LS-SVMlab toolbox version 1.8 (Suykens et al., 2002). The LS-SVMlab toolbox was chosen for its ease of use, mainly due to its automatic tuning of kernel parameters. Deep learning methods could be effective, but they are generally more suitable for high-dimensional and large datasets, and may not be able to generalize well and may result in poor performance when training on small datasets.

3. Results

The content of total chlorophylls and carotenoids in vegetable oils can be determined by different spectrophotometric methods. Therefore, the three most common methods for the determination of chlorophylls and the two most common methods for the determination of carotenoids were used to obtain the known values for the calibration of the sensor response. This allows the ability of the sensor to predict the content of these pigments in vegetable oils to be tested against different analytical approaches. The main performance parameters for calibration and test are summarized in Table 1(the detailed Tables with information for y-randomization and cross-validation can be found in the supplementary material; Tables S2 and S3).

The MLR models demonstrated good predictive capability for the determination of Tchl in olive and avocado oils based on both the IUPAC, AOCS, and MM methods, using both lighting (UV and white) and RGB values as descriptors, with R^2 values of approximately 0.8. For the test

set, R^2 values of approximately 0.9 were obtained, in addition to R^2m values greater than 0.5, indicating substantial congruence between actual and predicted values (Figure 2). The high RMSE values and low R^2 for the y-randomization test, in addition to the high cR^2p value (>0.5), indicated that there were no overfitting or random adjustments.

The LS-SVM models demonstrated better performance compared to the MLR models, particularly in models based on IUPAC and AOCS methods utilizing HSV values and UV lighting, as well as the model based on the MM method under white lighting with RGB values, with R^2 values > 0.90 for both calibration and test. The RMSE values resulting from the LS-SVM models were notably lower than those obtained from the MLR models. Moreover, the elevated R^2m values (R^2m > 0.90) indicated excellent congruence between actual and predicted values (Figure 3). The LS-SVM models exhibited poor performance in the y-randomization test, with cR^2p values exceeding 0.5, suggesting the robustness of these models without overfitting or random adjustments.

In general, the MLR models exhibited poor performance in predicting Tcar, with R^2 values for calibration ranging from 0.59 to 0.67 for white lighting and between 0.47 and 0.52 for UV lighting. Despite the relatively low R^2 values for the test set (ranging from 0.62 to 0.72), the R^2m values exceeded 0.5, indicating a certain degree of congruence between the actual and predicted values when using white light (Figure 2). In contrast, the models exhibited considerably poor performance when using UV light, with the R^2m values falling below 0.5 for the majority of the models. Furthermore, the cR^2p values, which were found to be lower than 0.5 in the y-randomization test, indicated a possible random adjustment when using UV lighting.

The LS-SVM models demonstrated better performance in predicting Tcar compared to the MLR models, particularly when using L*a*b* under white lighting. The R^2 values for the test set were close to 0.8 for the LS-SVM models, while the RMSE values were lower than those of MLR models in both lighting conditions. The R^2m value exceeded 0.5, indicating a valid congruence between the actual and predicted values (Figure 3). Additionally, the LS-SVM models exhibited

297 elevated RMSE and low R^2 in the y-randomization test, particularly when using L*a*b* and white
298 light, with cR^2p values exceeding 0.5, suggesting no overfitting or random adjustments.

299 The MLR models demonstrated satisfactory performance in predicting TSC when using white
300 lighting (Table 1), with calibration R^2 values close to or exceeding 0.8 for both the calibration and
301 test. The value of $R^2m > 0.5$ indicated congruence between actual and predicted values (Figure 2).
302 Additionally, the high RMSE and low R^2 values, accompanied by $cR^2p > 0.5$, indicated that the
303 models did not exhibit overfitting or random adjustments.

304 Similar to the results obtained with the Tchl and Tcar models, the LS-SVM models
305 demonstrated superior performance in predicting TSC compared to the MLR models. This was
306 particularly evident under white lighting conditions, where the use of RGB values as descriptors
307 resulted in an R^2 of 0.85 for the calibration set and 0.90 for the test set. The RMSE values obtained
308 from the LS-SVM models were considerably lower than those obtained from the MLR models. The
309 elevated R^2m values (approximately 0.80) indicated a high degree of congruence between actual
310 and predicted values (Figure 3). Additionally, the LS-SVM models had a poor performance in the y-
311 randomization test, with cR^2p values exceeding 0.5, indicating the robustness of these models
312 without overfitting or random adjustments.

313 In general, all predicted variables had residuals with apparently random patterns at all levels
314 of the variables predicted by the LS-SVM models (Figure S2), suggesting homoscedasticity. On the
315 other hand, some residuals for MLR models (Figure S1), especially for total chlorophylls based on
316 IUPAC and AOCS methods, had an increasing pattern towards higher values, suggesting some
317 heteroscedasticity.

318 The model performances based on RMSE and R^2 were confirmed by the RSD and RPD
319 values for the test set (Table 1), suggesting that the LS-SVM models had better precision (lower
320 RSD) compared to the MLR models. The best LS-SVM models presented RSDs between 9.9% and
321 14.6% for chlorophylls and between 21.3% and 29.2% for carotenoids. These findings are
322 comparable to those reported for a smartphone-based method, which presented RSDs of 10.3% for

chlorophylls and 25.4% for carotenoids (Carvalho and Nunes, 2021). In comparison, one of the collaborative studies reported as satisfactory in the IUPAC method for the determination of chlorophylls (Pokorny et al., 1995) achieved coefficients of variation up to 9.72% for repeatability and up to 57.69% for reproducibility. Some of the MLR models for chlorophylls and most for carotenoids had poor reliability due to RPDs < 2, as recommended by some authors (Bellon Maurel et al., 2010; Chang et al., 2001). In contrast, the LS-SVM models had RPD between 2.9 and 4 for chlorophylls and up to 2.7 for carotenoids.

4. Discussion

The proposed RGB sensor-based method for the determination of pigments in vegetable oils offers significant cost and time savings compared to conventional spectrophotometric methods. A typical RGB sensor can cost a few hundred USD depending on quality, brand, and features. These devices are relatively inexpensive compared to a spectrophotometer, which typically costs between a few thousand USD. Another advantage of RGB sensors is that they require minimal sample preparation, often without the need for dilution, resulting in instant analysis and fast results. Spectrophotometers also require relatively simple oils sample preparation, which may include dilution or filtration of samples. However, these procedures can increase analysis time.

Optical or colorimetric sensors have been employed to evaluate the properties of oils that depend on their chlorophyll or carotenoid content. The primary applications of this technology involve the authentication of oils, particularly blends of extra virgin oils (high natural pigment content) with other vegetable oils (commonly refined and with low or no pigment content). Lorenzo et al. (2024) demonstrated the same color sensor competence in detecting blends of vegetable oils in avocado oil. In another study by Huang et al. (2022), a colorimetric sensor array combined with linear discriminant analysis was employed to distinguish extra virgin olive oil from its mixtures with soybean and corn oil. A photonics sensor was utilized by Weesepoel et al. (2021) to differentiate between extra virgin olive oil adulterated with other edible oils using one-class

classification modeling. This study's results are in agreement with those of the studies mentioned earlier.

MLR is simpler to use than SVM methods, which are more complex and susceptible to overfitting for small datasets. Based on parsimonious principles, complex modeling methods should be considered as a last option, preferring simpler and more robust approaches when these are sufficient. However, a better performance of LS-SVM over MLR was supported for all the predictive models of this study, including Tchl, Tcar, and TSC. SVM-based algorithms can offer advantages over MLR in terms of regularization, stability, and robustness to outliers. SVM is generally more robust to outliers due to its regularization and penalty mechanisms, which reduce the influence of extreme data points. On the other hand, MLR is more sensitive to outliers, as it minimizes the sum of squared residuals, meaning large outliers can disproportionately affect the model. Its ability to produce reliable solutions can make SVM a good choice in many regression scenarios, especially when noisy data is present (Othman et al., 2023). Indeed, the potential of machine learning or deep-learning techniques, such as SVM, to enhance the implementation of cost-effective sensors, compensating for their inherent limitations in terms of design and manufacture has been highlighted in the literature (Payette et al., 2023; Lorenzo et al., 2024), which have been a trend in food product quality evaluation based on spectroscopy techniques (Ahmed et al., 2025; Chang et al., 2001; Zhang et al., 2021).

The performance of a color-based predictive model can be influenced by the color space used to predict the desired response (Anconi et al., 2022; de Carvalho & Nunes, 2021; Resende et al., 2023). This effect occurs due to the manner in which the color space describes the observed color. For instance, L*a*b* is a three-dimensional color space that encompasses the entire range of human color perception. The L* value (lightness) is a scale that ranges from black to white. The a* and b* values represent chromatic components, with a* representing green-red opponent colors and b* representing blue-yellow opponent colors (Ibraheem et al., 2012). The RGB system describes a color by an additive model, in which the linear combination of the three primary colors, red (R),

green (G), and blue (B), is used. Consequently, the diverse systems employed to describe a color influence its correlation with a particular property, such as the content of pigments in oils. This effect results in discrepancies in modeling performance depending on the color system utilized as a descriptor, which is consistent with the findings of other studies. Carvalho and Nunes (2021) presented several effective models for predicting Tchl in olive and avocado oils using RGB or HSV values obtained with a smartphone camera. Moyano et al. (2008) found that L*a*b* had a strong correlation with carotenoids content in olive oils when using complex regression models, with $R^2 > 0.86$. These reports are in line with the results of the present study.

The models for predicting Tchl based on solvent-free methods (IUPAC and AOCS) exhibited superior performance when UV light was used. In contrast, the predictive models for Tcar or TSC (which encompass carotenoids absorption) demonstrated enhanced performance when employing white light. When chlorophylls molecules in oils are exposed to UV light (including 400 nm), they absorb the UV radiation and transit into an excited state. After a very short period (typically nanoseconds), the molecules return to their ground state and release the absorbed energy in the form of fluorescence, typically in the red region (around 650–750 nm) of the electromagnetic spectrum (Fan et al., 2021). This effect was indeed captured by the sensor, as can be seen by comparing the redder color of one of the olive oil samples under UV light (R = 238, R = 95, R = 98) with a browner color under white light (R = 223, G= 132, B= 96). As reported by Hakonen and Beves (2018), fluorescence may cause inner-filter effects when detected at a 90° angle from the excitation light due to the presence of particles in a liquid medium. This effect would be even more pronounced in oils rich in chlorophylls (fluorescent species), such as olive and avocado oils. The researchers reported that this phenomenon when employing an excitation light with a wavelength of approximately 400 nm, could provide supplementary information for differentiating vegetable oils based on color parameters. This hypothesis may explain the enhanced performance observed when predicting Tchl based on solvent-free methods, given that the more concentrated medium may be

more susceptible to inner-filter effects, thereby contributing to a stronger correlation between the color parameters and the chlorophylls content.

The prediction of Tchl based on solvent-free methods also demonstrated superior outcomes when using the HSV values as descriptors, which can also be attributed to the effects of fluorescence. As demonstrated by Hakonen and Beves (2018), the hue (H) parameter (from the HSV color model) has been identified as a reliable signal for optical chemical sensors, particularly when analyzing samples exhibiting fluorescence effects. The researchers observed that oils rich in chlorophylls, such as olive oils, exhibited significantly higher hue values than those with low chlorophylls content when illuminated by LED at approximately 400 nm, indicating a strong correlation between hue and the content of fluorescent species, such as chlorophylls.

5. Conclusion

This proof-of-concept study demonstrated that the device based on a conventional color sensor and chemometrics models was able of predicting the levels of carotenoids and chlorophylls in olive and avocado oils, in addition to their TSC. Despite a relatively small dataset, the validation techniques, such as y-randomization, cross-validation, and predictions for a test set, suggested that the models provided reliable predictions for pigment content in olive and avocado oils.

A better performance of LS-SVM over MLR was observed for all the predictive models. This can be attributed to the mathematical assumptions of each method regarding data processing abilities to describe the predicted response. The use of UV lighting was demonstrated to improve the performance of these models in respect to total chlorophylls content, when the response is based on solventless methods (IUPAC and AOCS methods). White lighting was appropriate in the rest cases.

The color space used as a descriptor also influenced the predictive accuracy, depending on the type of variable and reference method. HSV predicted better total chlorophylls referenced on solventless methods. RGB was found to be a more suitable color space for predicting TSC and total

chlorophylls referenced on solvent dilution methods. Finally, total carotenoids content was better predicted using L*a*b* values as descriptors.

The color sensor-based approach has been demonstrated to provide a viable and cost-effective alternative to traditional methods for predicting pigment content in vegetable oils. This technique requires negligible sample preparation, thereby indicating significant potential for implementation in industrial applications that require a fast, reliable, and cheap estimation of food based on colorful compound concentrations. The improvement of the predictivity for carotenoids is necessary in near future additional studies, perhaps considering the use of more powerful modeling methods and additional color descriptors. This study can further expand and include oils from various olive and avocado cultivars and investigate the effect of interferences from other color sources, including artificial colorants. These points that future studies should address, they could contribute to the implementation of such techniques in food quality control and simplify the analytical procedures, once they proven robust with these additional considerations.

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Supplementary material

Tables and figures with model performance, and data file with color parameters, total chlorophylls, total carotenoids, and total spectrophotometric color of the oil samples were available.

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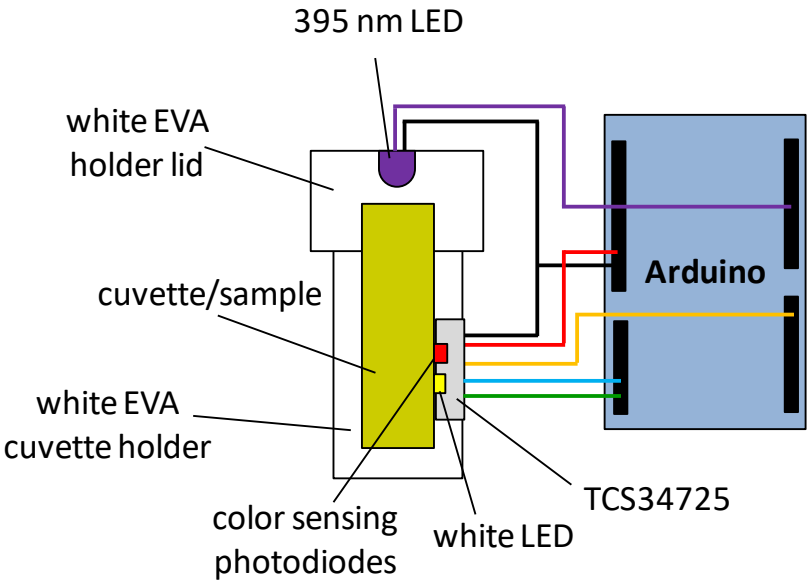
Tables

Table 1. Performance parameters for the best MLR and LS-SVM models to predict the total chlorophylls (Tchl), total carotenoids (Tcar), and total spectrophotometric color (TSC) in olive and avocado oils based on different methods using the color sensor.

		MLR	LS-SVM	MLR	LS-SVM
		Tchl – IUPAC (mg kg^{-1})		Tcar – GW (1951) (mg kg^{-1})	
calibration	lighting	white	uv	white	white
	color system	RGB	HSV	HSV	Lab
	RMSE	6.68	2.1	0.57	0.53
	R^2	0.77	0.98	0.61	0.67
test	RMSE	5.32	4.13	0.59	0.42
	R^2	0.89	0.94	0.67	0.79
	RSD	12.83	9.97	41.32	29.24
	RPD	2.7	3.48	1.43	2.02
		Tchl – AOCS (mg kg^{-1})		Tcar – MM (mg kg^{-1})	
calibration	lighting	white	uv	white	white
	color system	RGB	HSV	RGB	Lab
	RMSE	2.01	0.64	1.21	1.06
	R^2	0.77	0.98	0.63	0.7
test	RMSE	1.6	1.23	1.12	0.92
	R^2	0.89	0.94	0.72	0.82
	RSD	12.83	9.9	33.12	27.22
	RPD	2.7	3.5	1.83	2.22
		Tchl – MM (mg kg^{-1})		TSC	
calibration	lighting	white	white	white	white
	color system	RGB	RGB	RGB	RGB
	RMSE	1.63	1.31	326.6	268.5
	R^2	0.81	0.88	0.78	0.85
test	RMSE	1.54	0.99	300	251.2
	R^2	0.88	0.94	0.86	0.9
	RSD	22.84	14.65	25.49	21.34
	RPD	2.59	4.04	2.3	2.75

IUPAC: based on Pokorny et al. (1995). AOCS: based on AOCS Cc 13i-96 method.
MM: based on Minguez-Mosquera et al. (1991).

Figure 1. Device used to read color parameters of oils based on the TCS34725 color sensor interfaced with an Arduino.

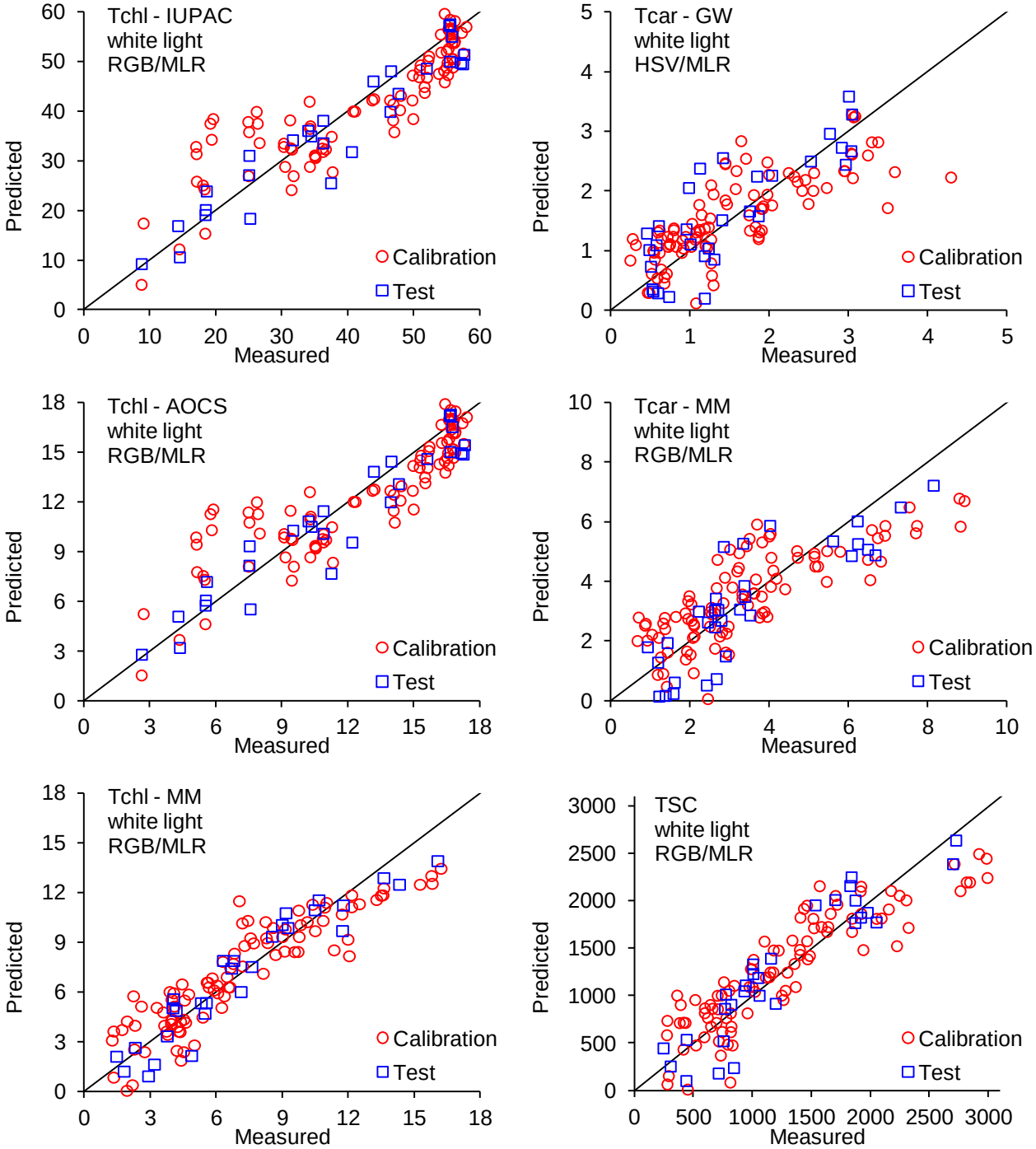


Device pinout

TCS34725	Arduino	Wire
LED	D7	
SCL	A5	
DAS	A4	
GND	GND	
VIN	3.3V	

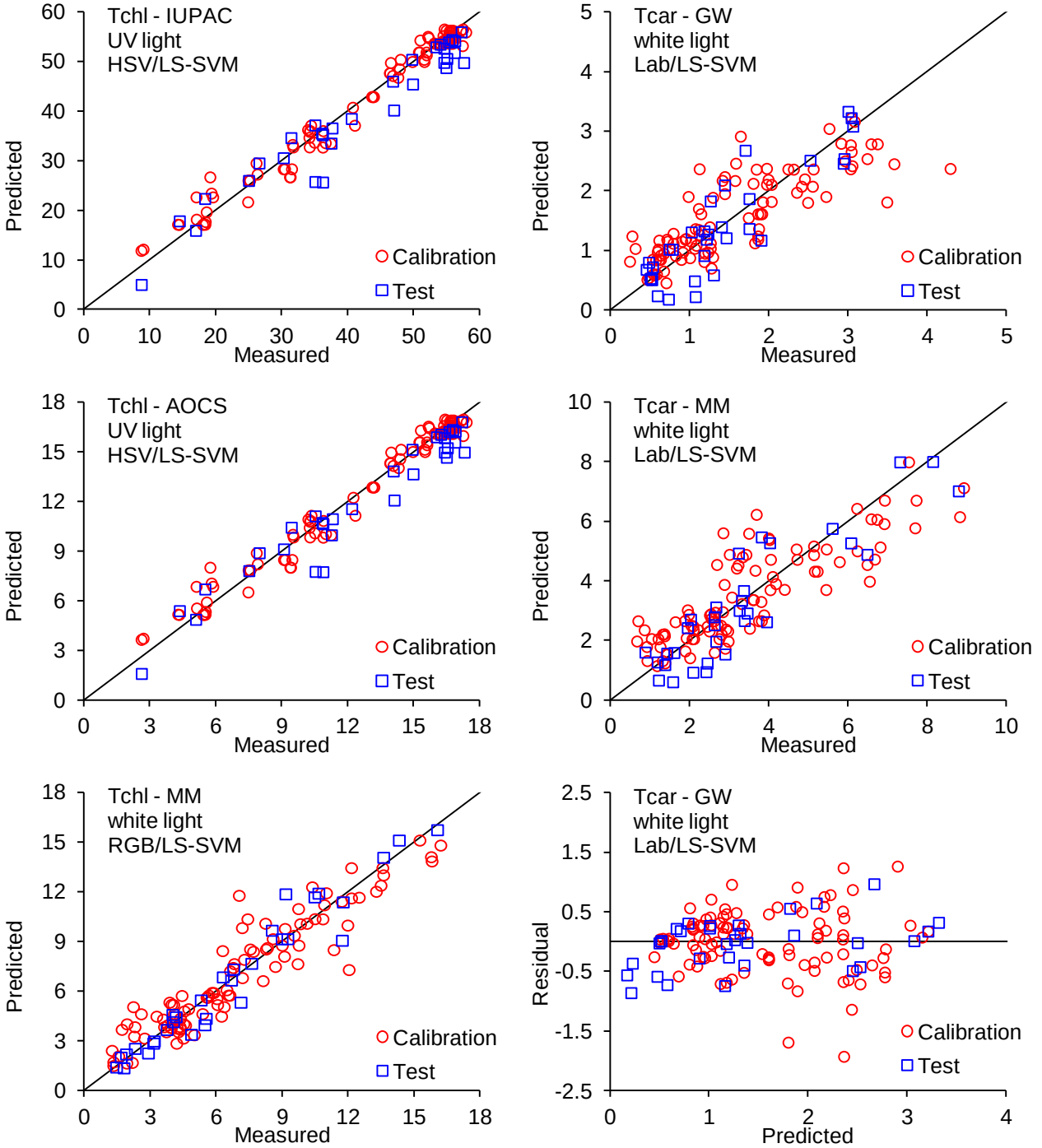
395nm LED	Arduino	Color
+	D9	
-	GND	

Figure 2. Measured vs. predicted total chlorophylls (Tchl), total carotenoids (Tcar), and total spectrophotometric color (TSC) in olive and avocado oils based on different methods using the color sensor and the best MLR models.



IUPAC: based on Pokorny et al. (1995) method. AOCS: based on AOCS Cc 13i-96 method. MM: based on Minguez-Mosquera et al. (1991) method. GW: based on Goodwin (1952) method.

Figure 3. Measured vs. predicted total chlorophylls (Tchl), total carotenoids (Tcar), and total spectrophotometric color (TSC) in olive and avocado oils based on different methods using the color sensor and the best LS-SVM models.



IUPAC: based on Pokorny et al. (1995) method. AOCS: based on AOCS Cc 13i-96 method. MM: based on Minguez-Mosquera et al. (1991) method. GW: based on Goodwin (1952) method.

		white light			UV light	
oil	% m/m	R	G	B	R	G
avocado breda	100	178	106	81	249	116
avocado breda	100	178	106	82	248	116
avocado breda	100	179	107	83	249	117
avocado margarida	100	180	107	85	249	121
avocado margarida	100	172	102	80	249	121
avocado margarida	100	172	102	80	249	120
avocado fortuna	100	191	114	88	248	117
avocado fortuna	100	180	107	82	247	102
avocado fortuna	100	193	115	89	247	103
avocado quintal	100	183	109	86	250	114
avocado quintal	100	174	105	82	249	110
avocado quintal	100	184	110	87	249	107
avocado hass	100	189	113	86	248	111
avocado hass	100	183	109	83	248	111
avocado hass	100	191	114	88	247	111
olive A	100	185	112	87	249	118
olive A	100	178	107	83	249	117
olive A	100	184	111	86	249	118
olive B	100	179	108	84	250	120
olive B	100	180	109	85	249	118
olive B	100	183	111	87	249	119
olive andorinha	100	211	126	92	241	101
olive andorinha	100	218	130	95	241	105
olive andorinha	100	208	123	91	241	104
olive larambia	100	218	129	95	241	101
olive larambia	100	214	126	91	240	102
olive larambia	100	222	131	96	240	101
olive herdade	100	223	132	96	238	95
olive herdade	100	223	132	95	237	94
olive herdade	100	214	127	93	238	93
olive Irarema	100	215	127	94	241	103
olive Irarema	100	209	124	92	240	101
olive Irarema	100	215	127	95	240	100
margarida + andorinha	25:75	181	108	84	248	106
margarida + andorinha	25:75	184	109	85	248	106
margarida + andorinha	25:75	177	106	82	248	111
margarida +Larambia	50:50	185	110	85	246	110
margarida +Larambia	50:50	188	112	86	247	107
margarida +Larambia	50:50	183	109	85	246	105
margarida + herdade	75:25	199	117	88	244	101
margarida + herdade	75:25	197	117	87	243	101
margarida + herdade	75:25	186	110	82	244	96
margarida +Larambia	80:20	197	120	87	237	91
margarida +Larambia	80:20	196	119	88	237	91

margarida +Larambia	80:20	204	123	90	237	91
oliva A + Irarema	25:75	179	108	83	248	104
oliva A + Irarema	25:75	186	112	85	248	104
oliva A + Irarema	25:75	175	106	80	248	104
oliva A +herdade	50:50	185	111	83	246	101
oliva A +herdade	50:50	191	115	86	246	101
oliva A +herdade	50:50	182	110	83	247	102
oliva A + andorinha	75:25	189	114	83	245	98
oliva A + andorinha	75:25	194	117	86	244	102
oliva A + andorinha	75:25	197	119	88	246	97
oliva A + soybean	50:50	185	111	83	245	100
oliva A + soybean	50:50	183	110	82	245	101
oliva A + soybean	50:50	186	113	85	245	101
oliva A +herdade	80:20	187	112	82	245	96
oliva A +herdade	80:20	189	113	84	244	96
oliva A +herdade	80:20	191	115	86	245	96
oliva B + larambia	24:75	175	105	81	248	118
oliva B + larambia	24:75	176	106	81	248	119
oliva B + larambia	24:75	173	105	81	248	117
oliva B + soybean	50:50	183	111	84	247	116
oliva B + soybean	50:50	180	109	82	247	114
oliva B + soybean	50:50	181	109	82	247	113
oliva B + herdade	50:50	178	108	81	247	113
oliva B + herdade	50:50	181	109	83	247	117
oliva B + herdade	50:50	186	113	86	247	118
oliva B + soybean	85:15	192	115	85	242	98
oliva B + soybean	85:15	189	113	84	242	98
oliva B + soybean	85:15	192	115	86	241	98
fortuna + irarema	50:50	194	116	87	244	122
fortuna + irarema	50:50	191	114	86	244	123
fortuna + irarema	50:50	192	114	85	245	128
fortuna + larambia	75:25	206	122	90	242	119
fortuna + larambia	75:25	203	121	91	242	117
fortuna + larambia	75:25	196	116	85	242	116
fortuna + andorinha	75:25	197	118	88	243	116
fortuna + andorinha	75:25	202	120	89	242	116
fortuna + andorinha	75:25	197	117	88	243	116
fortuna + soybean	50:50	192	114	86	243	120
fortuna + soybean	50:50	192	114	86	243	117
fortuna + soybean	50:50	201	119	89	243	117
fortuna + herdade	80:20	193	116	84	243	95
fortuna + herdade	80:20	195	117	86	243	95
fortuna + herdade	80:20	195	118	88	242	94
fortuna + irarema	80:20	197	117	87	241	100
fortuna + irarema	80:20	194	116	87	242	99
fortuna + irarema	80:20	195	116	86	242	99

quintal + herdade	25:75	174	104	81	248	122
quintal + herdade	25:75	180	108	84	248	121
quintal + herdade	25:75	174	104	81	248	122
quintal + andorinha	50:50	182	110	85	248	119
quintal + andorinha	50:50	179	108	83	247	117
quintal + andorinha	50:50	180	108	82	247	118
quintal + soybean	50:50	188	113	86	247	117
quintal + soybean	50:50	181	108	83	247	116
quintal + soybean	50:50	189	113	87	247	115
quintal + larambia	50:50	185	111	85	248	117
quintal + larambia	50:50	188	112	86	247	116
quintal + larambia	50:50	182	109	84	247	118
quintal + larambia	85:15	193	115	86	244	101
quintal + larambia	85:15	187	112	84	244	100
quintal + larambia	85:15	190	113	84	244	102
breda + herdade	50:50	192	115	86	245	116
breda + herdade	50:50	180	107	81	245	122
breda + herdade	50:50	185	111	83	245	121
breda + irarema	25:75	182	109	84	247	119
breda + irarema	25:75	185	111	85	247	121
breda + irarema	25:75	180	108	83	246	120
breda + soybean	50:50	188	113	85	245	121
breda + soybean	50:50	190	113	85	245	119
breda + soybean	50:50	195	117	89	244	119
breda + andorinha	50:50	185	110	83	245	122
breda + andorinha	50:50	186	111	84	245	122
breda + andorinha	50:50	192	115	88	246	118
breda + andorinha	85:15	202	120	89	241	99
breda + andorinha	85:15	198	118	88	242	99
breda + andorinha	85:15	193	115	85	241	99
breda + soybean	85:15	194	115	85	241	98
breda + soybean	85:15	193	115	85	241	96
breda + soybean	85:15	203	121	89	241	97
hass + soybean	50:50	200	118	88	243	105
hass + soybean	50:50	196	116	86	244	107
hass + soybean	50:50	198	117	87	244	109
hass + herdade	75:25	196	116	85	243	104
hass + herdade	75:25	198	117	84	243	104
hass + herdade	75:25	192	114	85	243	104

	Tchl (mg/kg)			Tcar (mg/kg)		TSC
B	IUPAC	AOCS	MM	GW	MM	
112	57.53	17.28	12.01	3.06	6.83	2324.50
112	57.31	17.22	11.74	3.04	6.75	2306.10
113	58.00	17.42	12.18	3.05	6.93	2248.50
116	53.18	15.98	16.09	3.01	8.16	2727.90
117	53.48	16.07	14.35	3.05	7.33	2701.90
116	54.01	16.22	15.29	3.05	7.55	2714.50
114	57.19	17.18	9.28	2.95	6.50	1921.10
98	57.68	17.33	8.57	2.96	6.09	1873.10
99	57.49	17.27	9.02	2.97	6.25	1978.30
109	54.69	16.43	15.81	3.09	8.94	2986.10
105	54.40	16.34	15.84	3.04	8.84	2993.20
102	54.69	16.43	16.24	3.07	8.81	2922.40
108	54.72	16.44	12.07	1.45	4.19	1403.60
108	54.61	16.41	9.13	1.58	3.20	1465.00
108	55.13	16.56	8.61	1.59	3.02	1408.50
114	55.47	16.66	10.69	2.04	3.35	1703.30
113	55.53	16.68	11.04	1.98	3.51	1706.50
114	55.44	16.66	10.95	2.00	3.44	1721.00
115	54.69	16.43	13.52	1.45	4.01	1918.50
112	54.72	16.44	13.64	1.45	4.04	1923.50
114	54.55	16.39	13.64	1.42	4.03	1841.60
102	18.44	5.54	2.94	0.54	1.62	441.40
106	18.41	5.53	2.21	0.49	1.42	453.50
105	18.64	5.60	2.34	0.49	1.44	443.80
102	14.30	4.30	1.83	0.51	1.20	308.30
103	14.56	4.37	1.94	0.53	1.23	305.30
102	14.49	4.35	1.96	0.52	1.19	280.90
98	8.78	2.64	1.70	0.47	1.39	280.50
98	8.75	2.63	1.59	0.52	1.39	282.90
97	9.06	2.72	1.36	0.59	1.33	292.60
104	18.49	5.55	1.49	0.55	0.94	247.60
103	18.07	5.43	1.29	0.54	0.93	276.90
101	18.31	5.50	1.36	0.46	0.89	280.40
100	55.70	16.73	12.53	2.92	6.60	2176.60
101	55.84	16.77	11.80	2.77	6.24	1830.50
106	55.40	16.64	10.51	2.53	5.62	1874.80
106	55.00	16.52	7.21	1.71	3.83	1437.80
102	55.01	16.53	7.58	1.85	4.06	1587.30
102	55.25	16.60	7.07	1.65	3.70	1571.60
98	36.33	10.91	5.57	1.47	3.40	944.60
98	36.69	11.02	4.55	1.27	2.98	959.40
93	36.29	10.90	5.34	1.41	3.27	933.10
91	37.72	11.33	4.42	1.07	2.46	814.30
92	37.57	11.29	5.41	1.30	2.99	818.50

92	37.48	11.26	4.90	1.19	2.68	844.50
99	54.11	16.26	7.46	0.99	2.70	1517.80
99	53.81	16.17	8.72	1.15	3.08	1406.00
99	54.18	16.28	9.58	1.24	3.33	1487.90
98	46.42	13.94	6.65	0.95	2.63	1003.30
98	46.48	13.96	7.15	1.02	2.80	1061.60
98	46.58	13.99	6.82	0.96	2.66	1006.40
95	36.28	10.90	5.03	0.74	2.10	733.50
100	36.15	10.86	4.38	0.68	1.90	716.90
95	36.27	10.90	4.40	0.68	1.93	746.10
98	43.72	13.13	5.69	0.72	1.89	975.80
98	44.01	13.22	5.92	0.75	1.96	1022.60
98	43.90	13.19	6.72	0.83	2.23	1051.10
94	26.64	8.00	3.82	0.71	2.02	593.90
94	26.36	7.92	4.12	0.75	2.11	645.30
94	26.20	7.87	3.91	0.73	2.05	706.70
114	55.56	16.69	9.19	1.13	2.86	1535.90
115	55.67	16.72	10.52	1.30	3.24	1523.30
112	55.45	16.66	10.40	1.27	3.25	1464.20
113	51.05	15.34	6.85	0.80	1.99	1011.00
110	50.94	15.30	6.80	0.79	2.04	996.80
110	50.83	15.27	6.67	0.80	1.96	988.90
110	51.99	15.62	7.64	1.01	2.72	1009.50
114	52.34	15.72	8.36	1.12	2.89	1103.80
115	52.23	15.69	7.72	1.03	2.68	1181.80
95	19.39	5.82	1.97	0.25	0.68	385.10
96	19.19	5.76	2.62	0.32	0.87	393.50
96	19.62	5.89	2.26	0.28	0.71	363.40
120	46.89	14.09	6.09	1.88	3.89	1282.00
121	46.92	14.10	5.84	1.87	3.82	1298.10
126	47.07	14.14	6.27	1.91	3.96	1265.10
117	31.49	9.46	4.23	1.19	2.64	792.70
115	31.70	9.52	4.08	1.19	2.64	776.20
114	31.80	9.55	4.54	1.31	2.91	832.90
114	34.48	10.36	4.05	1.22	2.64	769.00
114	34.27	10.30	4.31	1.24	2.76	823.10
113	34.28	10.30	4.77	1.26	2.85	848.30
117	40.83	12.27	5.60	1.90	3.61	1178.10
114	41.13	12.36	5.65	1.92	3.63	1153.60
115	40.64	12.21	5.51	1.83	3.53	1198.50
94	25.06	7.53	3.21	1.08	2.43	715.30
94	25.10	7.54	3.79	1.28	2.91	756.90
94	24.93	7.49	4.00	1.27	2.93	708.60
97	31.58	9.49	4.03	1.07	2.51	818.20
96	31.28	9.40	4.09	1.08	2.52	805.20
96	31.37	9.43	4.63	1.20	2.82	780.20

118	55.99	16.82	12.18	3.30	6.94	2817.10
118	56.25	16.90	13.31	3.25	7.71	2764.80
119	56.33	16.92	13.60	3.38	7.74	2845.40
115	56.01	16.83	9.77	2.36	5.80	2157.20
114	55.89	16.79	10.88	2.73	6.50	2053.70
114	56.20	16.88	11.38	2.50	6.56	2226.40
114	55.21	16.59	9.74	3.50	5.46	1941.50
113	55.29	16.61	9.16	3.59	5.15	2095.90
112	55.51	16.67	11.76	4.30	6.69	2052.90
114	55.92	16.80	9.03	2.42	5.17	1633.60
112	55.94	16.81	8.30	2.32	4.73	1644.10
115	55.84	16.78	8.27	2.25	4.71	1664.50
98	34.36	10.32	4.58	1.13	2.56	740.50
97	34.22	10.28	4.47	1.12	2.55	760.00
99	34.02	10.22	4.20	1.09	2.46	822.10
113	49.94	15.00	6.39	1.87	3.76	1250.80
120	49.87	14.98	6.32	1.81	3.67	1223.70
119	49.81	14.96	6.58	1.87	3.83	1368.60
116	56.17	16.88	10.16	2.57	5.47	1924.30
118	55.91	16.80	9.79	2.56	5.24	1845.60
117	56.26	16.90	9.86	2.46	5.15	1847.40
119	48.07	14.44	6.51	1.76	3.47	1115.60
116	47.93	14.40	6.06	1.75	3.33	1144.70
117	47.70	14.33	6.34	1.76	3.38	1158.70
120	51.68	15.53	8.16	2.04	4.41	1358.50
119	51.65	15.52	7.22	1.93	4.05	1469.40
115	52.02	15.63	7.31	1.98	4.11	1340.20
97	30.52	9.17	3.76	0.92	2.12	651.00
97	30.33	9.11	3.62	0.91	2.10	663.50
97	30.32	9.11	3.67	0.90	2.08	697.00
96	17.09	5.13	1.74	0.58	1.05	418.00
94	17.02	5.11	2.33	0.62	1.22	434.40
95	17.13	5.15	2.30	0.64	1.27	416.60
104	35.13	10.55	3.98	0.61	1.37	598.50
105	35.02	10.52	4.26	0.64	1.38	623.50
108	35.12	10.55	3.98	0.60	1.33	598.00
103	24.98	7.50	2.77	0.56	1.44	523.20
103	25.23	7.58	3.18	0.60	1.59	551.70
103	25.05	7.53	3.32	0.62	1.65	516.90

Rapid estimation of natural pigments in olive and avocado oils using a colorimetric sensor

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Table S1. Samples of avocado and olive oil with their respective blends.

Oil	% m/m
Breda (avocado)	100
Margarida (avocado)	100
Fortuna (avocado)	100
Quintal (avocado)	100
Hass (avocado)	100
Olive A	100
Olive B	100
Andorinha (olive)	100
Larambia (olive)	100
Herdade (olive)	100
Irarema (olive)	100
Margarida + Andorinha	25:75
Margarida +Larambia	50:50
Margarida + Herdade	75:25
Margarida +Larambia	80:20
Olive A + Irarema	25:75
Olive A +Herdade	50:50
Olive A + Andorinha	75:25
Olive A + Soybean	50:50
Olive A +Herdade	80:20
Olive B + Larambia	24:75
Olive B + Soybean	50:50
Olive B + Herdade	50:50
Olive B + Soybean	85:15
Fortuna + Irarema	50:50
Fortuna + Larambia	75:25
Fortuna + Andorinha	75:25
Fortuna + Soybean	50:50
Fortuna + Herdade	80:20
Fortuna + Irarema	80:20
Quintal + Herdade	25:75
Quintal + Andorinha	50:50
Quintal + Soybean	50:50
Quintal + Larambia	50:50
Quintal + Larambia	85:15
Breda + Herdade	50:50
Breda + Irarema	25:75
Breda + Soybean	50:50
Breda + Andorinha	50:50
Breda + Andorinha	85:15
Breda + Soybean	85:15
Hass + Soybean	50:50
Hass + Herdade	75:25

Table S2. Performance parameters for MLR and LS-SVM models to predict the total chlorophylls (Tchl) in olive and avocado oils based on different methods using the color sensor.

Tchl – IUPAC (mg kg^{-1})													
		MLR						LS-SVM					
		white light			uv light			white light			uv light		
		RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab
calibration	RMSE	6.68	6.46	6.47	6.08	5.63	5.96	5.30	5.00	4.82	2.03	2.10	1.94
	R^2	0.77	0.78	0.79	0.82	0.85	0.82	0.86	0.87	0.88	0.98	0.98	0.98
y-rand	RMSE	18.75	18.59	19.03	18.95	19.87	19.13	12.35	11.57	12.80	13.03	13.53	12.09
	R^2	0.01	0.01	0.01	0.02	0.01	0.02	0.34	0.46	0.25	0.30	0.19	0.45
	cR^2p	0.77	0.78	0.79	0.81	0.84	0.81	0.67	0.60	0.75	0.81	0.88	0.73
loo-cv	RMSE	6.95	6.70	6.72	6.46	6.05	6.35	6.68	6.19	6.22	3.68	5.00	3.27
	R^2	0.75	0.77	0.77	0.79	0.82	0.80	0.77	0.80	0.81	0.93	0.88	0.95
test	RMSE	5.32	7.01	7.06	7.25	9.24	7.26	5.03	4.85	4.90	4.21	4.13	4.49
	R^2	0.89	0.85	0.83	0.77	0.64	0.77	0.90	0.91	0.91	0.93	0.94	0.91
	R^2m	0.86	0.81	0.78	0.62	0.57	0.68	0.85	0.88	0.90	0.76	0.90	0.81
	RSD	12.83	16.91	17.02	17.49	22.27	17.51	12.14	11.70	11.81	10.16	9.97	10.83
	RPD	2.70	2.05	2.04	1.98	1.56	1.98	2.86	2.96	2.94	3.41	3.48	3.20
Tchl – AOCS (mg kg^{-1})													
		MLR						LS-SVM					
		white light			uv light			white light			uv light		
		RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab
calibration	RMSE	2.01	1.94	1.94	1.83	1.69	1.79	1.59	1.50	1.45	0.61	0.64	0.59
	R^2	0.77	0.78	0.79	0.82	0.85	0.82	0.86	0.87	0.88	0.98	0.98	0.98
y-rand	RMSE	5.64	5.51	5.76	5.74	5.89	5.67	3.52	3.83	3.52	3.72	4.16	3.67
	R^2	0.01	0.01	0.01	0.00	0.02	0.01	0.39	0.37	0.39	0.43	0.23	0.41
	cR^2p	0.76	0.78	0.79	0.81	0.84	0.82	0.64	0.66	0.66	0.73	0.89	0.75
loo-cv	RMSE	2.09	2.01	2.02	1.94	1.82	1.91	2.01	1.85	1.86	1.12	1.51	0.98
	R^2	0.75	0.77	0.77	0.79	0.82	0.80	0.77	0.80	0.81	0.93	0.88	0.95
test	RMSE	1.60	2.11	2.12	2.18	2.77	2.18	1.51	1.46	1.47	1.27	1.23	1.34
	R^2	0.89	0.85	0.83	0.77	0.64	0.77	0.90	0.91	0.91	0.93	0.94	0.91
	R^2m	0.86	0.81	0.78	0.62	0.57	0.68	0.86	0.88	0.90	0.75	0.90	0.81
	RSD	12.83	16.91	17.02	17.49	22.27	17.52	12.12	11.73	11.81	10.22	9.90	10.78
	RPD	2.70	2.05	2.04	1.98	1.56	1.98	2.86	2.96	2.94	3.39	3.50	3.22
Tchl – MM (mg kg^{-1})													
		MLR						LS-SVM					
		white light			uv light			white light			uv light		
		RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab
calibration	RMSE	1.63	1.40	1.46	1.78	1.63	1.69	1.31	1.06	1.33	0.82	0.79	1.06
	R^2	0.81	0.85	0.84	0.77	0.81	0.78	0.88	0.91	0.87	0.95	0.96	0.91
y-rand	RMSE	4.95	4.79	4.98	4.93	5.01	4.82	3.62	3.06	3.18	3.51	3.60	3.16
	R^2	0.00	0.01	0.01	0.01	0.02	0.01	0.19	0.51	0.31	0.24	0.14	0.32
	cR^2p	0.81	0.84	0.84	0.77	0.80	0.77	0.77	0.60	0.70	0.82	0.88	0.74
loo-cv	RMSE	1.72	1.46	1.53	1.89	1.73	1.79	1.51	1.45	1.42	1.16	1.33	1.28
	R^2	0.79	0.83	0.83	0.74	0.79	0.75	0.84	0.84	0.85	0.90	0.88	0.87
test	RMSE	1.54	1.89	2.05	2.10	2.36	2.33	0.99	1.40	1.56	1.44	1.40	1.16
	R^2	0.88	0.86	0.83	0.72	0.66	0.72	0.94	0.91	0.88	0.89	0.88	0.94
	R^2m	0.82	0.79	0.74	0.55	0.56	0.49	0.91	0.89	0.83	0.85	0.87	0.81
	RSD	22.84	28.00	30.36	31.12	35.09	34.50	14.65	20.78	23.10	21.35	20.76	17.21
	RPD	2.59	2.11	1.95	1.90	1.69	1.71	4.04	2.85	2.56	2.77	2.85	3.44

y-rand: y-randomization test. loo-cv: leave-one-out cross-validation

IUPAC: based on Pokorny et al. (1995). AOCS: based on AOCS Cc 13i-96 method. MM: based on Minguez-Mosquera et al. (1991).

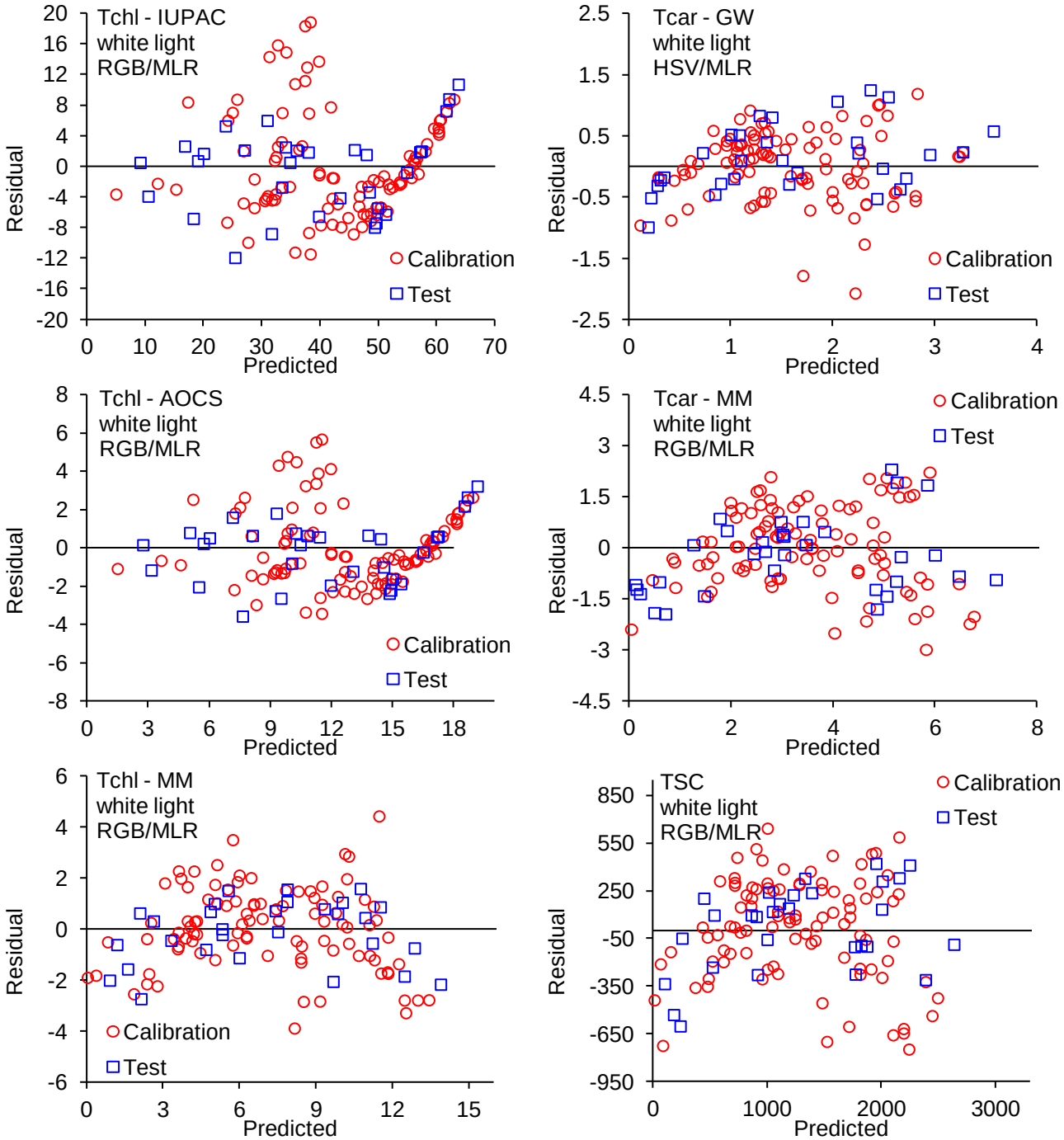
Table S3. Performance parameters for MLR and LS-SVM models to predict the total carotenoids (Tcar) and total spectrophotometric color (TSC) in olive and avocado oils based on different methods using the color sensor.

Tcar – GW (1951) (mg kg^{-1})													
		MLR						LS-SVM					
		white light			uv light			white light			uv light		
		RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab
calibration	RMSE	0.56	0.57	0.57	0.64	0.66	0.66	0.48	0.50	0.53	0.41	0.51	0.44
	R^2	0.59	0.61	0.61	0.50	0.48	0.47	0.70	0.70	0.67	0.80	0.69	0.76
y-rand	RMSE	1.11	1.16	1.17	1.11	1.11	1.06	0.76	0.75	0.87	0.85	0.84	0.77
	R^2	0.00	0.01	0.01	0.01	0.01	0.02	0.44	0.46	0.24	0.24	0.31	0.48
	cR^2p	0.59	0.60	0.61	0.50	0.47	0.47	0.43	0.41	0.54	0.67	0.51	0.46
loo-cv	RMSE	0.59	0.59	0.60	0.66	0.68	0.68	0.57	0.57	0.59	0.60	0.65	0.57
	R^2	0.55	0.58	0.58	0.47	0.44	0.44	0.59	0.61	0.59	0.57	0.49	0.59
test	RMSE	0.62	0.59	0.62	0.70	0.66	0.64	0.61	0.44	0.42	0.72	0.57	0.49
	R^2	0.62	0.67	0.64	0.39	0.48	0.50	0.63	0.77	0.79	0.50	0.62	0.73
	R^2m	0.49	0.62	0.62	0.12	0.28	0.24	0.50	0.64	0.79	0.40	0.50	0.53
	RSD	43.57	41.32	43.79	49.07	46.27	44.98	42.80	30.88	29.24	50.37	40.11	34.54
	RPD	1.36	1.43	1.35	1.21	1.28	1.31	1.38	1.91	2.02	1.17	1.47	1.71
Tcar – MM (mg kg^{-1})													
		MLR						LS-SVM					
		white light			uv light			white light			uv light		
		RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab
calibration	RMSE	1.21	1.09	1.15	1.31	1.36	1.29	1.03	0.92	1.06	0.76	0.93	1.01
	R^2	0.63	0.67	0.65	0.52	0.52	0.52	0.73	0.77	0.70	0.85	0.77	0.71
y-rand	RMSE	2.40	2.47	2.59	2.32	2.42	2.25	1.70	1.72	1.73	1.81	1.87	1.70
	R^2	0.01	0.01	0.01	0.01	0.01	0.00	0.38	0.34	0.35	0.29	0.18	0.25
	cR^2p	0.62	0.67	0.65	0.52	0.51	0.51	0.50	0.58	0.50	0.69	0.68	0.57
loo-cv	RMSE	1.27	1.14	1.21	1.37	1.41	1.34	1.18	1.16	1.18	1.18	1.20	1.37
	R^2	0.58	0.64	0.62	0.48	0.48	0.48	0.64	0.64	0.64	0.62	0.63	0.47
test	RMSE	1.12	1.33	1.29	1.62	1.50	1.65	1.02	1.09	0.92	1.28	1.13	1.11
	R^2	0.72	0.67	0.70	0.44	0.48	0.48	0.76	0.76	0.82	0.65	0.71	0.78
	R^2m	0.68	0.61	0.68	0.13	0.28	0.17	0.73	0.62	0.81	0.41	0.63	0.51
	RSD	33.12	39.32	38.23	47.81	44.36	48.66	30.17	32.06	27.22	37.87	33.38	32.91
	RPD	1.83	1.54	1.58	1.27	1.36	1.24	2.01	1.89	2.22	1.60	1.81	1.84
TSC													
		MLR						LS-SVM					
		white light			uv light			white light			uv light		
		RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab	RGB	HSV	Lab
calibration	RMSE	326.6	285.9	298.6	366.8	369.7	365.6	268.5	258.8	267.8	206.5	206.4	233.3
	R^2	0.78	0.82	0.81	0.70	0.71	0.70	0.85	0.85	0.85	0.91	0.91	0.88
y-rand	RMSE	922.9	936.2	912.6	862.3	884.7	867.5	632.4	629.8	603.5	623.9	627.5	625.1
	R^2	0.01	0.01	0.02	0.01	0.01	0.00	0.28	0.19	0.36	0.36	0.27	0.21
	cR^2p	0.78	0.82	0.80	0.70	0.71	0.69	0.70	0.75	0.64	0.70	0.77	0.76
loo-cv	RMSE	345.9	299.4	313.0	384.2	386.6	383.2	307.9	298.2	289.0	303.6	287.4	347.3
	R^2	0.76	0.80	0.79	0.67	0.68	0.67	0.81	0.81	0.82	0.80	0.83	0.73
test	RMSE	300.0	366.3	391.3	464.1	456.2	458.6	251.2	263.9	294.4	363.1	296.1	263.7
	R^2	0.86	0.83	0.82	0.63	0.64	0.67	0.90	0.90	0.88	0.79	0.85	0.89
	R^2m	0.79	0.77	0.70	0.39	0.51	0.44	0.85	0.89	0.80	0.75	0.81	0.77
	RSD	25.49	31.12	33.24	39.43	38.76	38.96	21.34	22.42	25.01	30.84	25.16	22.40
	RPD	2.30	1.88	1.76	1.49	1.51	1.50	2.75	2.61	2.34	1.90	2.33	2.62

y-rand: y-randomization test. loo-cv: leave-one-out cross-validation

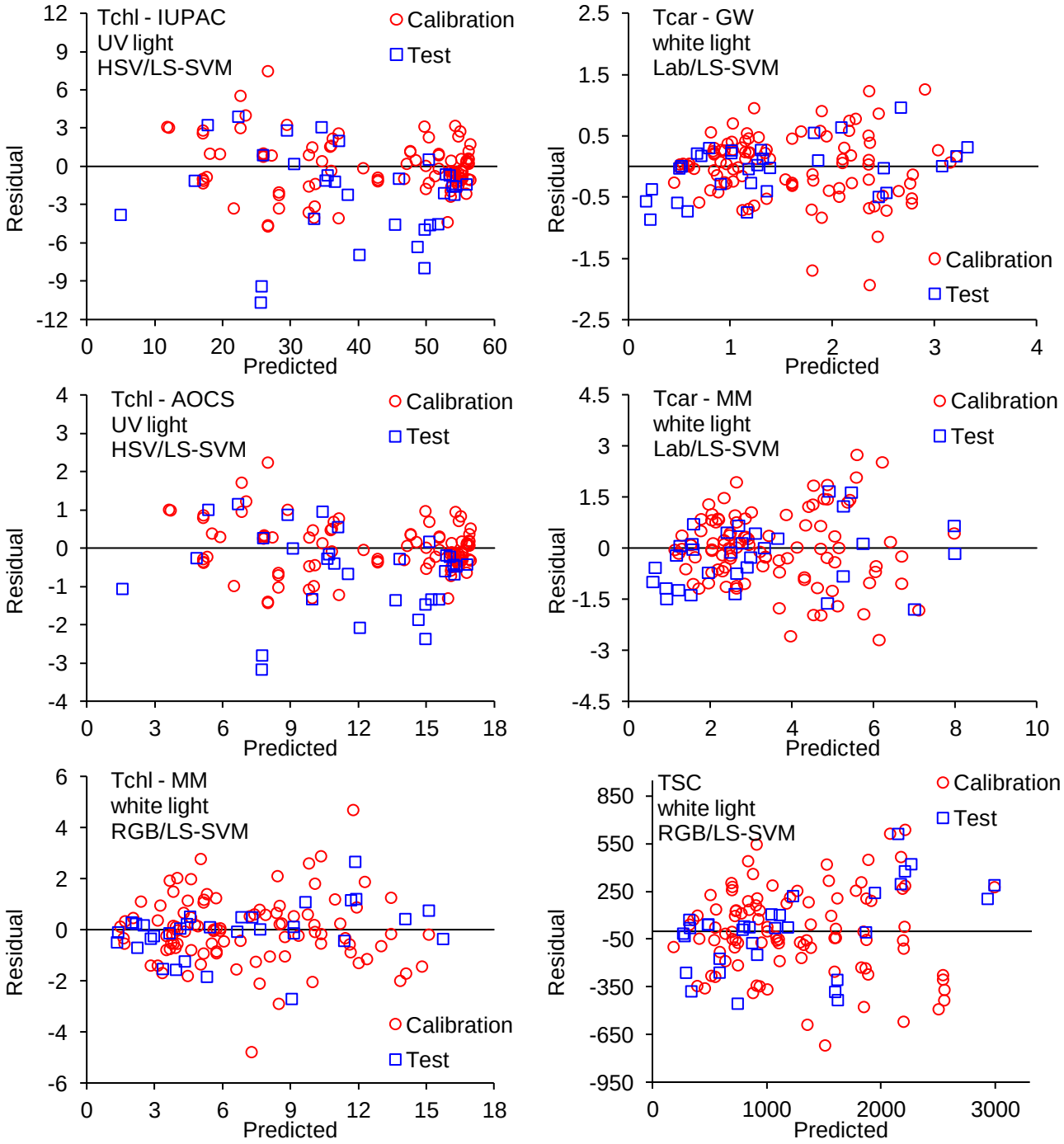
GW: based on T.W. Goodwin (1951). MM: based on Minguez-Mosquera et al. (1991).

Figure S1. Residuals vs. predicted for total chlorophylls (Tchl), total carotenoids (Tcar), and total spectrophotometric color (TSC) in olive and avocado oils based on different methods using the color sensor and the best MLR models.



IUPAC: based on Pokorny et al. (1995) method. AOCS: based on AOCS Cc 13i-96 method. MM: based on Minguez-Mosquera et al. (1991) method. GW: based on Goodwin (1952) method.

Figure S2. Residuals vs. predicted for total chlorophylls (Tchl), total carotenoids (Tcar), and total spectrophotometric color (TSC) in olive and avocado oils based on different methods using the color sensor and the best LS-SVM models.



IUPAC: based on Pokorny et al. (1995) method. AOCS: based on AOCS Cc 13i-96 method. MM: based on Minguez-Mosquera et al. (1991) method. GW: based on Goodwin (1952) method.

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