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Abstract: Non-destructive tools to evaluate the lycopene content in tomatoes is of large interest for the whole fruit chain because of the increasing demand for health beneficial products. With the aim to develop compact low-cost reflectance sensors for lycopene determination, we compared prediction Partial Least Squares (PLS) models by using either directional or total reflectance in the 500-750 nm range. Directional reflectance at 45° with respect to the LED lighting direction was acquired by a compact spectrometer sensor. Total reflectance was acquired through a 50-mm integrating sphere connected to a spectrometer. The analysis was conducted on two hydroponic greenhouse cultivated red tomato varieties, large round 'Dometica' (average diameter of 57 mm) and small cherry 'Juanita' (average diameter 26 mm). For both varieties, the spectral variance of directional reflectance was well correlated to that of total reflectance. Performances of PLS prediction models were also similar, with R2 of cross-validation between 0.73 and 0.81. The prediction error, relative to the mean lycopene content of full ripe tomatoes, was similar and around 16-17% for both varieties and sensors. Our results showed that directional reflectance measured by portable, low-cost and compact LED-based sensors can be used with a fair precision for the non-destructive assessment of lycopene in tomatoes.

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Sesto Fiorentino (Florence), 13 October 2015

Editor-in-Chief
J. Harnly
U.S. Department of Agriculture (USDA)
Beltsville, Maryland, USA

Dear Editor,

the manuscript entitled

Directional versus total reflectance spectroscopy for the in situ determination of lycopene in tomato fruits

by

Leonardo Ciaccheri, Lorenza Tuccio, Andrea A. Mencaglia, Anna G. Mignani, Ewelina Hallmann, Kalina Sikorska-Zimny, Stanislaw Kaniszewski, Michèl J. Verheul, Giovanni Agati

we are submitting for publication in JFCA is based on results of a multidisciplinary collaboration within the frame of an ERA-NET SUSFOOD European project.

The aim was that to test the performance of a new developed reflectance optical sensor for the non-destructive estimate of lycopene in tomatoes. We wanted to compare directional versus total reflectance by using destructive analysis of lycopene as reference and PLS regression analysis. We think that this can be a useful step to design new compact sensors to control rapidly the lycopene level of tomatoes in the field and during storage.

As reviewers for the present manuscript, I would suggest:

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Best regards

Dr. Giovanni Agati

Directional versus total reflectance spectroscopy for the in situ determination of lycopene in tomato fruits

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ABSTRACT

Non-destructive tools to evaluate the lycopene content in tomatoes is of large interest for the whole fruit chain because of the increasing demand for health beneficial products. With the aim to develop compact low-cost reflectance sensors for lycopene determination, we compared prediction Partial Least Squares (PLS) models by using either directional or total reflectance in the 500-750 nm range. Directional reflectance at 45° with respect to the LED lighting direction was acquired by a compact spectrometer sensor. Total reflectance was acquired through a 50-mm integrating sphere connected to a spectrometer. The analysis was conducted on two hydroponic greenhouse cultivated red tomato varieties, large round 'Dometica' (average diameter of 57 mm) and small cherry 'Juanita' (average diameter 26 mm). For both varieties, the spectral variance of directional reflectance was well correlated to that of total reflectance. Performances of PLS prediction models were also similar, with R^2 of cross-validation between 0.73 and 0.81. The prediction error, relative to the mean lycopene content of full ripe tomatoes, was similar and around 16-17% for both varieties and sensors.

Our results showed that directional reflectance measured by portable, low-cost and compact LED-based sensors can be used with a fair precision for the non-destructive assessment of lycopene in tomatoes.

Keywords

Lycopene; *Lycopersicon esculentum;* Non-destructive assessment; Optical Sensor; Partial Least Squares regression; Reflectance; Tomato.

Abbreviations

PLS, Partial Least Squares; RMSEC, Root Mean Square Error of Calibration; RMSECV, Root Mean Square Error of Cross-Validation.

1. Introduction

Lycopene, possessing high oxygen-radical scavenging properties, is the main antioxidant compound present in ripe tomato (*Lycopersicon esculentum* Mill.) fruits (Shi and Maguer, 2000). Because of this, its assumption can significantly reduce the risk of cancer and cardiovascular diseases (Müller et al., 2016; Rao and Agarwal, 2000). Therefore, it should be of large interest in producing tomatoes with the largest content of lycopene and to quantify this compound as quality added-value.

Usually, the concentration of lycopene is determined destructively on sample extracts by means of unsafe solvents and time-consuming methods (Davis et al., 2003a; Fish et al., 2002). To improve this procedure, several non-destructive spectroscopic methods have been proposed (Baranska et al., 2006; Choudhary et al., 2009; Clément et al., 2008). Other more sophisticated techniques concerned tomato spectral imaging that, besides the prediction of lycopene, can give information of the spatial heterogeneity of it (Liu et al., 2015; Polder et al., 2004). However, a standardized system and procedure for the fast estimate of lycopene to be transferred to tomato producers is not available yet.

Reflectance spectroscopy has been used for a long time to assess in situ fruit quality (Cozzolino, 2014; Nicolai et al., 2007). The method is rapid, non-destructive and can be applied both in the laboratory and in the field. The information that can be obtained from a reflectance spectrum depends on the absorbance and scattering properties of the sample and on the spectral range investigated. Highly pigmented fruits absorb visible light within the first few micron of tissue, then reflectance between 400 and 700 nm can provide data only on the superficial part of the sample. NIR, instead, penetrates deeper into the fruit tissues and can provide information on internal compounds and pulp structure.

Specificity of reflectance spectroscopy can be limited when, as usual, a high number of overlapping bands occur. For this, chemometrics can be used to extract information from the spectral data concerning sample quality features (Wang et al., 2015).

82 The geometry of the irradiation and detection system is also important. In a directional-
83 hemispherical system, irradiation occurs within a solid angle oriented with respect to the normal to
84 the sample surface and the reflected radiation is collected over the whole hemispherical space above
85 the sample surface.
86 Bidirectional reflectance of samples can be fully characterized by using a spectrogoniophotometer
87 that allows measurements as function of the irradiation and detection angles (Combes et al., 2007).
88 Since fruit and vegetable surfaces are far to be Lambertian, the angle of detection with respect to the
89 irradiation direction can significantly affect the reflectance values. Including or excluding the
90 specular reflection is also fundamental especially for glossy samples (Combes et al., 2007).
91 In principal, collecting all the radiation reflected by the sample by using an integrating sphere, with
92 internal diameter ≥150 mm and port fraction below 4%, should be the ideal in order to get the
93 highest accuracy and sensitivity. However, with the aim to develop low-cost, user-friendly sensor as
94 much compact as possible the choice can go towards a simpler configuration (Mignani et al., 2015).
95 In this study, we compared directional versus diffuse reflectance spectroscopy for the prediction of
96 lycopene in tomatoes. The two non-destructive techniques were correlated to the real content in
97 lycopene extracted from the very same samples measured spectroscopically and quantified by
98 HPLC. We used two tomato varieties with quite different size, in order to investigate if this could
99 have an effect on the method performance.
100

101 **2. Materials and Methods**

102 *2.1. Fruit material*

103 Fully developed round tomatoes (*Lycopersicon esculentum* Mill. 'Dometica') and cherry tomatoes
104 (*Lycopersicon esculentum* Mill. 'Juanita') were harvested at different ripening stages at the
105 beginning of August 2014 from two commercial greenhouses, Orre Gartneri – Orre and Lauvsnes
106 Gartneri – Finnøy, respectively, in southwestern Norway.

All the different maturity stages: “green”, “breakers”, “turning”, “pink”, “light red” and “red” (USDA, 1975) were represented (Fig. 1). Twenty-seven fruits for each variety were used in the study.

Plants were grown as hydroponic greenhouse cultures under optimal standard growth conditions in Norway (Verheul, 2012). Tomatoes were harvested from greenhouse compartments with and without the use of artificial light (280 µmol $m^{-2}s^{-1}$ PAR for maximum 18h per day). Fruits from trusses 10-12 (Dometica) or 2-3 (Juanita) were harvested. Global radiation outside of the greenhouse the last 14 days before harvesting was on average 19.5 MJ m^{-2} d^{-1}. Daily mean temperatures in the greenhouse were 21 °C (Dometica) or 21.5 °C (Juanita). Plants were irrigated when needed with a standard nutrient solution for tomato, keeping a EC of 4.0 dS m^{-1} (Dometica) or 4.5 dS m^{-1} (Juanita) in the rockwool slabs.

2.2. Reflectance sensors

Directional reflectance spectra of tomatoes were measured by the LED-based sensor (hereafter LED-sensor) described in Mignani et al. (Mignani et al., 2015).

Briefly, it consisted of a group of LEDs for illumination and a compact spectrometer for detection. The light source was made of three sets of four LEDs sequentially placed in a twelve-element circular-array. Each set was made of a white LED and other three LEDs emitting at 740 nm, 420 nm, and 680 nm, respectively. Lighting of the samples occurred at 45° with respect to the axis of detection. This opto-geometric arrangement minimizes the influence of any surface texture or roughness effects.

The detector was an Ocean Optics STS-VIS spectrometer (Ocean Optics, Dunedin, FL, USA) with optical fibre input, operating in the 350-800 nm spectral range, with a resolution of 1.5 nm. The sensor was USB-connected to a notebook and operated through a custom Labview® software interface. The sampled zone of tomatoes at the exit port of the sensor was 5 mm in diameter.

Total reflectance spectra of tomatoes were acquired by the compact spectrometer BRC112E-USB-VIS (B&W Tek, Lübeck, Germany) working in the visible range (380-750 nm), with a 25 µm slit and a resolution at 546 nm of 1 nm, connected through an optical fibre to a 50-mm integrating sphere (AvaSphere-50-LS-HAL, Avantes, The Netherlands), hereafter IS-sensor. An external halogen lamp (LS-1 Tungsten Halogen Light Source, Ocean Optics, Dunedin, FL, USA) connected to the integrating sphere by an optical fibre was used to illuminate directly the tomato samples at an 8° angle of incidence. The integrating sphere sensor, hereafter IS-sensor, sampled a zone of tomatoes of 10 mm in diameter.

The same day of harvesting, the reflectance spectra of each tomato were measured by the two sensors on four different points, at 90° to each other, along the equatorial zone. The average spectrum of the four measurements was then calculated.

A white Spectralon® standard was used as reference.

After reflectance measurements, each 'Dometica' tomato was finely homogenized in a blender and then immediately frozen in liquid nitrogen. Aliquots 8-10 g were freeze-dried to get about 1 g dried powder. 'Juanita' tomatoes were cut in 4 pieces and immediately frozen in liquid nitrogen and then freeze-dried.

2.3. Lycopene extraction and analysis

Lycopene extraction and analysis of 'Juanita' tomatoes were performed according to Hallmann (2012) with some adjustment. Fifty mg of powdered freeze-dried samples were weighted to plastic tubes, to which magnesium carbonate ($MgCO_2$) and cold n-hexane (5 ml) were added. Samples were shaken on vortex and extracted in ultrasonic cold bath (15 min in the dark) and then centrifuged at 6,000 rpm, 0°C, for 10 min. One ml of supernatant was transferred to Eppendorf tubes and centrifuged again (12,000 rpm, 0°C, 5 min). Nine hundred µl of supernatant were injected into the HPLC column (Max-RP 80i, 250 x 4.60 mm). The HPLC set-up consisted of two LC-20AD pumps, a CMB-20A system controller, SIL-20AC autosampler, ultraviolet–visible SPD-20AV

158 detector, and CTD-20AC oven. Acetonitrile and deionized water with ethyl acetate (90:10:100) at a
159 flow rate of 1 mL min^{-1} was used as a gradient solvent. The time of analysis was 27 min., with
160 detection at 471 nm. Carotenoids were identified on the basis of external standards (Sigma-Aldrich)
161 with purity of 99.9%.
162 Lycopene extraction and analysis of 'Dometica' tomatoes were performed according to the AOAC
163 method (Latimer, 2012). Five hundred mg of freeze-dried tomato samples were re-suspended with
164 12 ml of water containing butylated hydroxytoluene (BHT, 0.01g). Samples were shaken in
165 ultrasonic bath (30 min), then added with ethanol (16 ml) and dichloromethane (DCM) to a final
166 volume of 40 ml and stored in the dark for 2 h. Twenty µl of supernatant were inject into the HPLC
167 column (Suplex pKb-100 250x4.6 mm, 5 µm) kept at 30°C. Methanol with the addition of BHT
168 (0.005% w:v), 2-propanol (2% v:v), N-ethyldiisopropylamine (0.02% v:v), ammonium acetate
169 (2.5% v:v) and acetonitrile (45.5% v:v) at a flow rate of 0.8 mL min^{-1} was used as an isocratic
170 solvent. The time of analysis was 20 min with detection at 488 nm for lycopene, identified by an
171 external standard (Sigma-Aldrich).
172
173 *2.4. Statistical analysis*
174 Before statistical analysis, reflectance spectra were smoothed by mobile average. The smoothing
175 window was 15 and 11 points for IS- and LED-sensor spectra, respectively, with a width of about 5
176 nm, in both cases. Spectra were then converted to apparent absorbance units by taking the natural
177 logarithm of the reciprocal of reflectance and corrected for the offset.
178 To better compare reflectance data from the two systems, spectra were re-sampled at 2 nm step and
179 analysed by using the same wavelength range (500-750 nm). Wavelengths below 500 nm were
180 discarded because they showed a saturated absorption. The new sampling step was more than
181 adequate in comparison with the average width of spectral features, and provided a further damping
182 of high frequency noise.

Partial Least Squares (PLS) regression analysis was used for lycopene content prediction. PLS is a widely used regression method when many co-linear variables are present. It provides a strong reduction in the number of predictors, thus reducing the probability of overfitting, while maximizing the covariance between the predictor set and the target variable (Esbensen et al., 2002). The accuracy of the calibration and validation models was described by the coefficient of determination (R^2), the Root Mean Square Error of Calibration (RMSEC) and the Root Mean Square Error of Cross-Validation (RMSECV).

The RMSEC was calculated as follows:

$$RMSEC = \sqrt{\frac{\sum_{n=1}^{N} (y_n - z_n)^2}{N - K}} \quad (1)$$

where y_n are the reference values, z_n are the predicted values, N is the number of samples and K is the number of statistical parameters estimated in calibrating the model.

The expression of RMSECV was similar considering at the denominator simply the number of samples, N.

The R^2 was a measure of the size of RMSEC relative to the standard deviation of *y* variable given by:

$$R^2 = 1 - \left(\frac{RMSEC}{s_y}\right)^2 \quad (2)$$

where s_y is the standard deviation of *y*. A similar coefficient can be estimated for RMSECV.

The data processing was carried out by means of CAMO-Unscrambler software. Because of the limited number of samples available, it was not possible to divide the entire set into two sets for calibration and validation, respectively, and the validation was carried out using the Leave-One-Out (LOO) method (Esbensen et al., 2002).

3. Results and Discussion

The two varieties of tomato fruits differed significantly in weight and size. The average weight was 93 ± 11 g for 'Dometica' and 10 ± 2 g for 'Juanita'. The average diameter of 'Dometica' fruits was almost double that of 'Juanita' (56.7 ± 2.7 versus 25.9 ± 1.5 mm).

The concentration of lycopene in tomato fruits resulting from the destructive chemical extraction and HPLC analysis ranged from 0 to 79 mg/100 g DW and from 1 to 49 mg/100 g DW for the 'Dometica' and 'Juanita' varieties, respectively. These data were used as references for the calibration and cross validation of the PLS models.

At the full ripe "red" stage the lycopene concentration was 68.1 ± 7.7 and 41.1 ± 5.1 mg/100g DW for 'Dometica' and 'Juanita', respectively. Considering a dry matter for 'Dometica' of 6%, ripe tomatoes had a concentration of about 4 mg/100 g fresh weight that is in line with that found early for this variety cultivated in Norwegian greenhouses (Verheul et al., 2015). Lycopene content for 'Juanita' fruits was almost half than that found by Verheul in the same variety in 2013 (data not shown). Nassar et al. (Nassar et al., 2015) found also higher lycopene concentrations in 'Juanita' hydroponically grown (76.7 mg/100 g DW). This difference can be partially explained by a different ripening stage at harvest, by the fact that fruits were harvested from young plants and, likely, by a difference in the methods of analysis.

Figure 2 shows representative directional and total reflectance spectra measured on 'Dometica' and 'Juanita' tomatoes at different ripening stages by both the LED- and IS- sensors. As expected, reflectance values recorded by the IS-sensor were higher than those recorded by the LED-sensor. This was because: i) specular reflectance was measured by the IS-sensor but not the LED-sensor; ii) tomato fruits are non Lambertian surfaces so that directional reflectance is depending on the view angle of detector and cannot equal hemispherical reflectance. The IS-sensor detected a larger portion of light scattered inside the tomato samples than the LED-sensor.

For both varieties, the absorbance band of chlorophyll was clearly evident as a reflectance minimum at around 675 nm for samples at breakers-turning stages. With ripening, reflectance in the blue-yellow decreased due to the accumulation of lycopene, while reflectance in the red increased because of chlorophyll degradation.

The absorbance bands of chlorophyll and lycopene for the same fruit appeared slightly more evident in the IS-sensor spectra than in the LED-sensor. This is likely due to a possible multi-pass effect present in the integrating sphere.

Partial Least Square regression analysis of reflectance spectra showed that for both tomato varieties and reflectance sensors the first PLS factor was able to explain more than 95% of X-variance (i.e. the summed variance of all column of the spectra matrix). Therefore, the different shapes observed in the directional and total reflectance spectra did not change significantly the analysis of variance.

The good correlation found between the scores of first PLS factors, reported in Fig. 3A and B for 'Dometica' and 'Juanita' tomatoes respectively, demonstrated that such factors were related to a common cause. It was also evident that such cause was the increase of lycopene (and simultaneous decrease of chlorophyll) during ripening.

The slope of the regression line between the first factor scores of LED-sensor and IS-sensor data in 'Dometica' was very close to 1 (0.95), while for 'Juanita' the same slope was about 0.6. This is explainable by a similar X-variance for both sensors in the former case, while in the latter, the X-variance of IS-sensor was significantly lower than LED-sensor. The effect was likely due to the different sizes of interacting area and angular detection range possessed by the two detectors in relation with the small size of 'Juanita' tomatoes. In fact, such effect was not observed for the larger 'Dometica' fruits.

The PLS calibration models explained 77% or more of Y-variance by using just a single factor for LED-sensor data and IS-sensor 'Dometica' data. Two factors were instead necessary for IS-sensor 'Juanita' data (Table 1). This could be due to the skewed distribution of the spectral data, which tend to reduce the representativeness of estimated statistical parameters.

The PLS regression coefficients spectra for lycopene prediction are reported in Figure 4. Regression coefficients for 'Dometica' derived from both LED- and IS- sensors data were quite similar (Fig. 4A), showing a negative peak at around 675 nm corresponding to the chlorophyll absorbance maximum in the red, and a positive peak at around 560 nm often used in the past for spectrophotometric determination of lycopene content in turbid media (Davis et al., 2003b). For 'Juanita' fruits (Fig. 4B), the regression coefficients pattern for data from LED-sensor was comparable to the 'Dometica' ones, while the 2-factors coefficients from IS-sensor data showed a sharp positive peak at around 600 nm, beside the negative chlorophyll peak at 675 nm.

The performance of PLS regression models to predict lycopene from directional and total reflectance spectroscopy can be evaluated from the scatter plots reported in Figures 5 and 6 for the 'Dometica' and 'Juanita' varieties, respectively, and from the statistics data reported in Table 1. For 'Dometica', lycopene prediction was slightly better by using directional than total reflectance, while the opposite occurred for 'Juanita'. Considering the prediction relative error, calculated as the ratio between RMSECV and the mean lycopene content found in full ripe "red" tomatoes, it was similar and around 16-17% for both varieties and sensors. These data suggested that both spectral sensors utilized to estimate tomato lycopene performed similarly and that the prediction models were not significantly affected by the size of the fruits.

The accuracy of the prediction model can be limited because of the heterogeneity of lycopene distribution on fruits, especially for the early stages of ripening, when the reflectance spectrum taken as average on four equatorial points might not be representative of the whole fruit. A saturation of reflectance at the very full ripe stage may also occur. This could be related to the skin to pulp distribution of lycopene. In fact, the ratio of lycopene content between skin and pulp depends on the cultivar and changes during ripening (Kaur et al., 2006; Toor and Savage, 2005). Since visible light does not penetrate much in highly pigmented samples, it is possible that the correlation between optical signals and lycopene concentration can markedly change according to the tomato fraction considered. This aspect will be investigated in future work.

Several different non-destructive spectroscopic techniques along with chemometrics have been used in the past to predict lycopene content in tomato fruits. Liu et al. (Liu et al., 2015) used multispectral imaging and multivariate analyses on cv. Wanza 15 tomatoes, finding higher or lower precision in assessing lycopene according to different quantitative models. PLS regression gave RMSEP of 6.5 mg/kg over the highest values of lycopene of about 36 mg/kg (that is about 18%). The error reduced to 2.3-2.6 mg/kg (6.4-7.2%) when new chemometric analysis such as least square-support vector machine (LS-SVM) and back propagation neural network (BPNN) were used. Clement et al. (Clément et al., 2008) presented an accurate prediction of lycopene ($R^2 = 0.98$, relative error at maturity of about 5%) on different (var. Trust, Blitz and DRK 453) not completely identified tomato varieties by using a bench spectrophotometer equipped with an integrating sphere and PLS analysis with 12 latent variables. A relative error of about 21% of prediction on the most red tomatoes cv. Momotaro was found by using a portable NIR sensor in the 600-1100 nm spectral range (Kusumiyati et al., 2008). Similar results were obtained by measuring the fruits directly on the plant or at postharvest. Imaging spectrometry between 396 and 736 nm along with PLS regression analysis was used on greenhouse cultivated tomatoes cv. Capita obtaining 8-9% relative error of prediction at the full ripe stage (Polder et al., 2004).

The level of performance of the different techniques depend on several aspects, such as the instrumentation used to obtain spectral data, more or less sophisticated algorithms of data elaboration, the spectral range considered, tomato cultivars and growing conditions, the destructive analysis for lycopene determination. For this, comparison of results from different methods is difficult and a conclusive indication of the best procedure to be used is still lacking. Yet, for practical purposes, it is often useful to find an optimal compromise between the precision of the techniques and the cost and user-friendliness of it.

4. Conclusion

Our results showed that portable, low-cost and compact LED-based sensors measuring directional reflectance can be used with a fair precision for the non-destructive assessment of lycopene in tomatoes. Although this approach can be limited in accuracy with respect to more sophisticated spectroscopic techniques and statistical analyses, it can be useful for practical applications and to facilitate transfer of the methodology to tomato producers. Calibrated portable sensors can be employed directly into the field (or greenhouses) to predict the best time of harvesting in order to get the highest level of lycopene. This is an important issue considering the marked dependence of lycopene content on the environmental conditions (Brandt et al., 2006).

Furthermore, there will be interest in applying the reflectance technique to control the level of lycopene in tomatoes during their travelling from producers to consumers and during storage conditions (Schouten et al., 2014; Verheul et al., 2015), or to evaluate its seasonal variation (Toor et al., 2006). The spread of non-destructive tools, as those presented here, will have also a positive environmental impact reducing the use of time-consuming and costly destructive analyses. Lastly, another remarkable application of reflectance sensors could concern the monitoring of lycopene stability during tomato processing (Seybold et al., 2004; Shi and Maguer, 2000).

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Figure Captions

Figure 1. Tomato fruits of the ‘Dometica’ and ‘Juanita’ variety used in the study.

Figure 2. Representative spectra of directional (A,C) and total reflectance (B,D) acquired on ‘Dometica’ (A,B) and ‘Juanita’ (C,D) fruits with different lycopene content by the LED-sensor and the IS-sensor.

Figure 3. Correlation between scores of the PLS regression first factors from reflectance (R) data recorded by the LED-sensor and the IS-sensor for ‘Dometica’ (A) and ‘Juanita’ (B) tomatoes. Different symbols and colors indicate different ranges of the lycopene content (mg/100g DW): for ‘Dometica’, 0-15 (circles, green); 15-30 (squares, yellow); 30-50 (triangles, orange); 50-79 (diamonds, red). For ‘Juanita’, 0-10 (circles, green); 10-15 (squares, yellow); 15-32 (triangles, orange); 32-49 (diamonds, red).

Figure 4. Regression coefficients spectra for prediction of lycopene content in ‘Dometica’ (A) and ‘Juanita’ (B) tomatoes. ‘Dometica’ data and LED-sensor ‘Juanita’ data refer to PLS models with 1 factor, IS-sensor data refer to a PLS model with 2 factors.

Figure 5. PLS prediction of lycopene content from reflectance spectroscopy in the 500-750 nm range on ‘Dometica’ large round tomatoes by using directional reflectance (A, LED-sensor) or total reflectance (B, IS-sensor). Dotted lines represent the identity lines.

Figure 6. PLS prediction of lycopene content from reflectance spectroscopy in the 500-750 nm range on ‘Juanita’ small cherry tomatoes by using directional reflectance (A, LED-sensor) or total reflectance (B, IS-sensor). Dotted lines represent the identity lines.

Tables

Table 1. Regression statistics for the prediction of lycopene in tomatoes						
Variety/Device	PLS Factors	RMSEC (mg/100g DW)	R^2 cal.	RMSECV (mg/100g DW)	R^2 cross-val.	Relative error (%)*
'Dometica'						
LED-sensor	1	10.0	0.79	11.0	0.77	16.2
IS-sensor	1	11.0	0.77	12.0	0.73	17.6
'Juanita'						
LED-sensor	1	6.2	0.80	6.6	0.77	16.0
IS-sensor	2	5.7	0.83	6.5	0.81	15.8

*Relative error was calculated as ratio between RMSECV and the mean lycopene concentration of full ripe "red" tomatoes.

Figure 1

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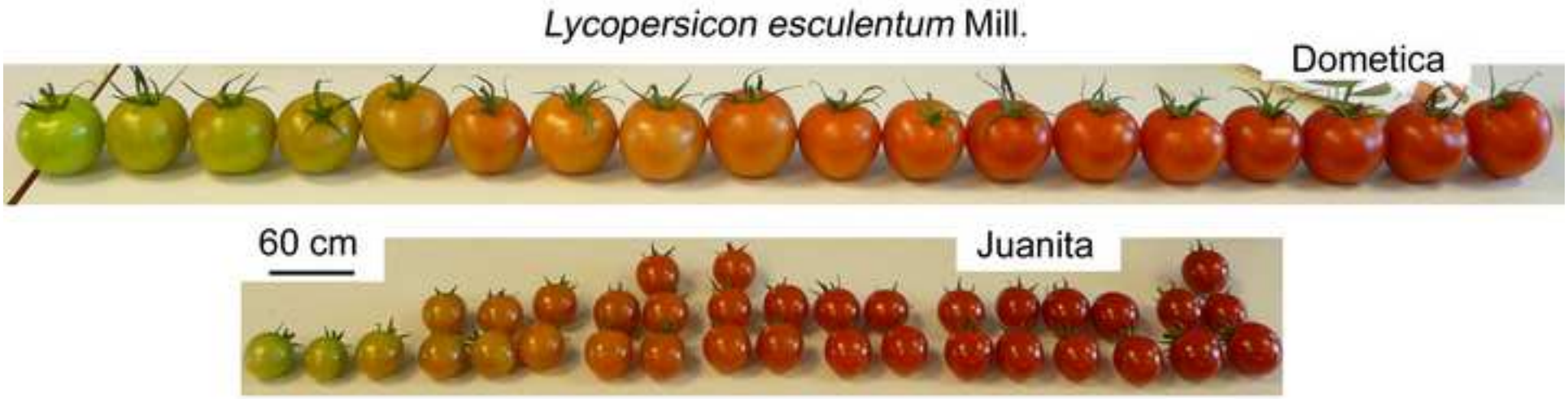

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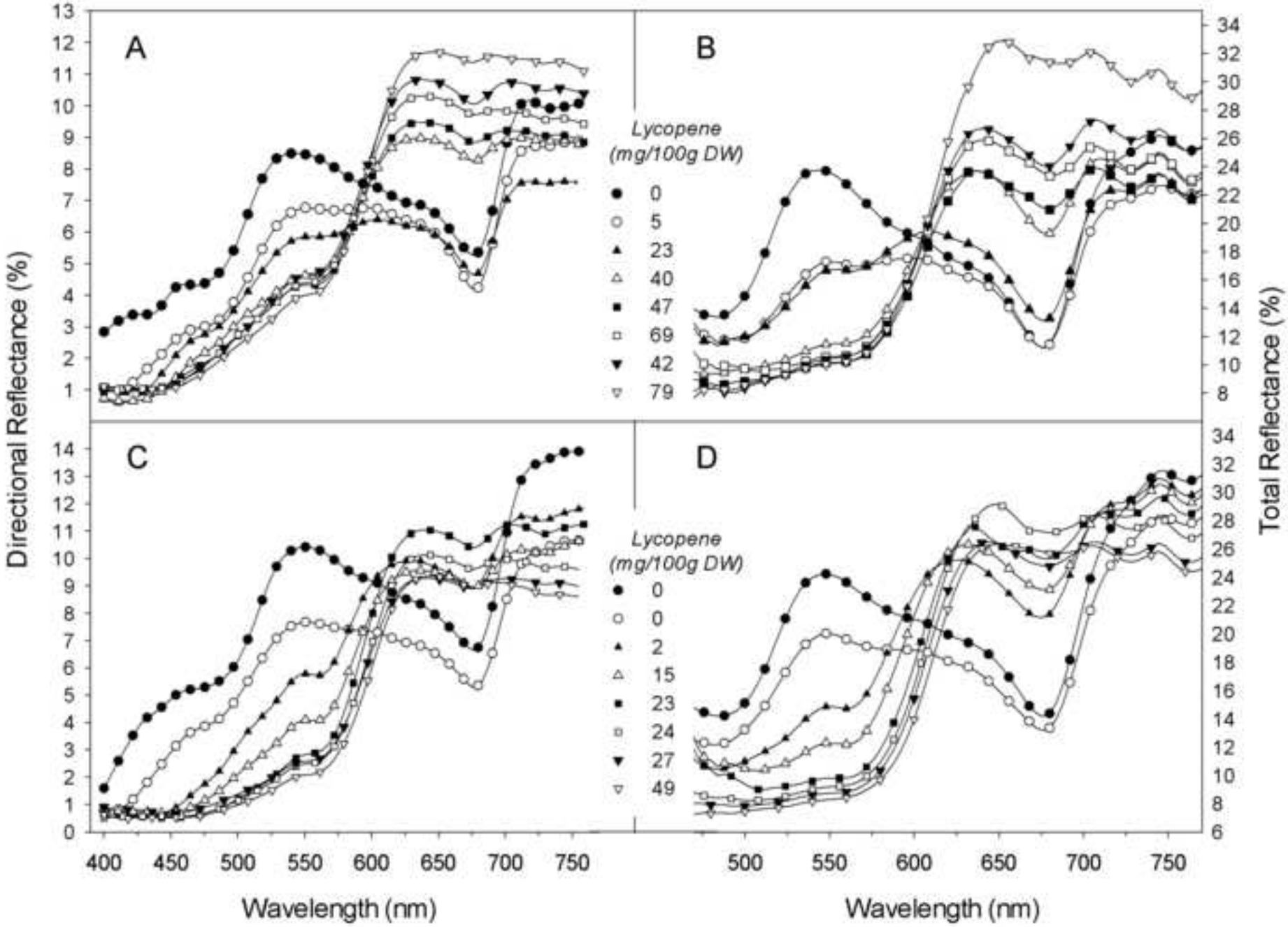

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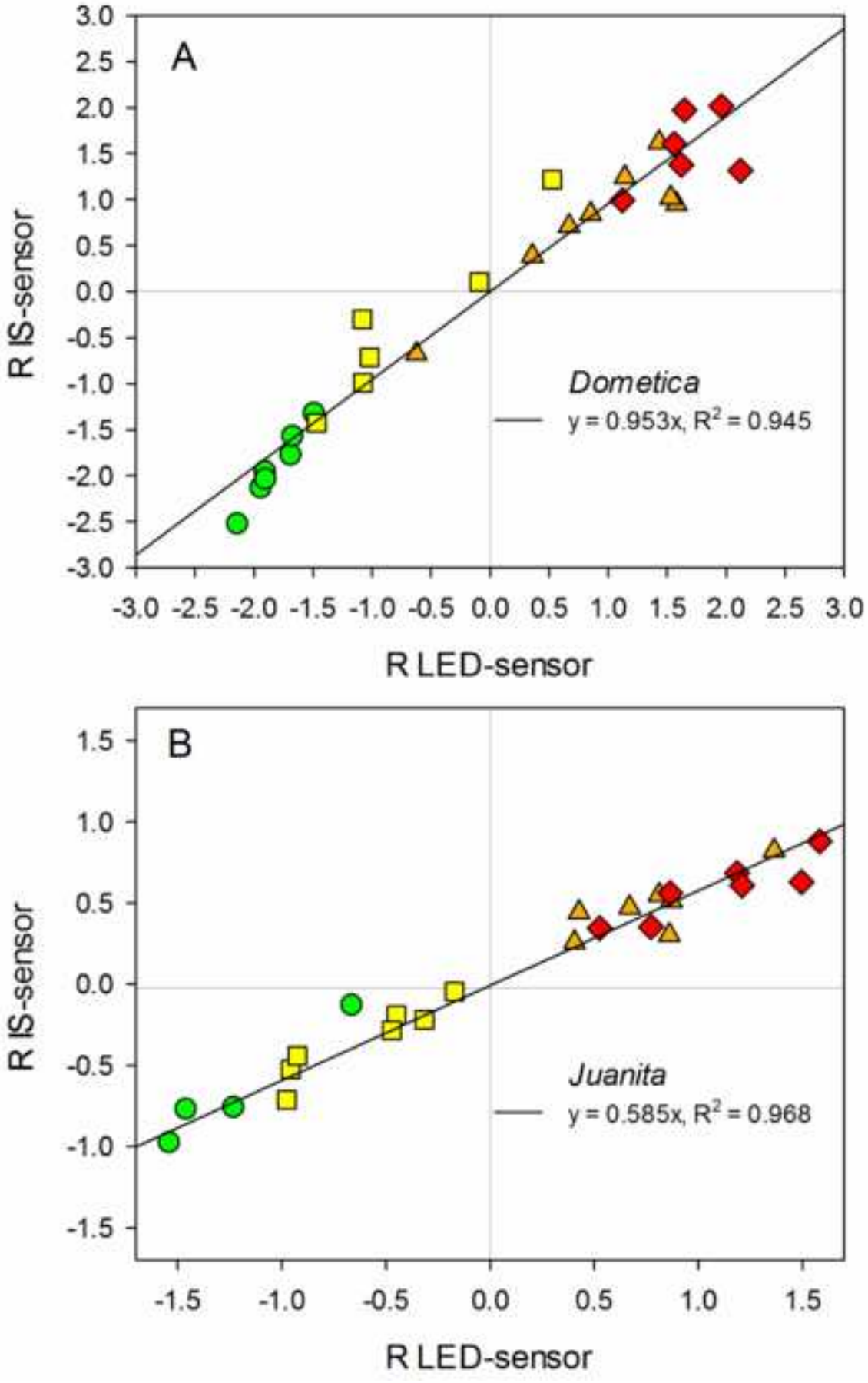

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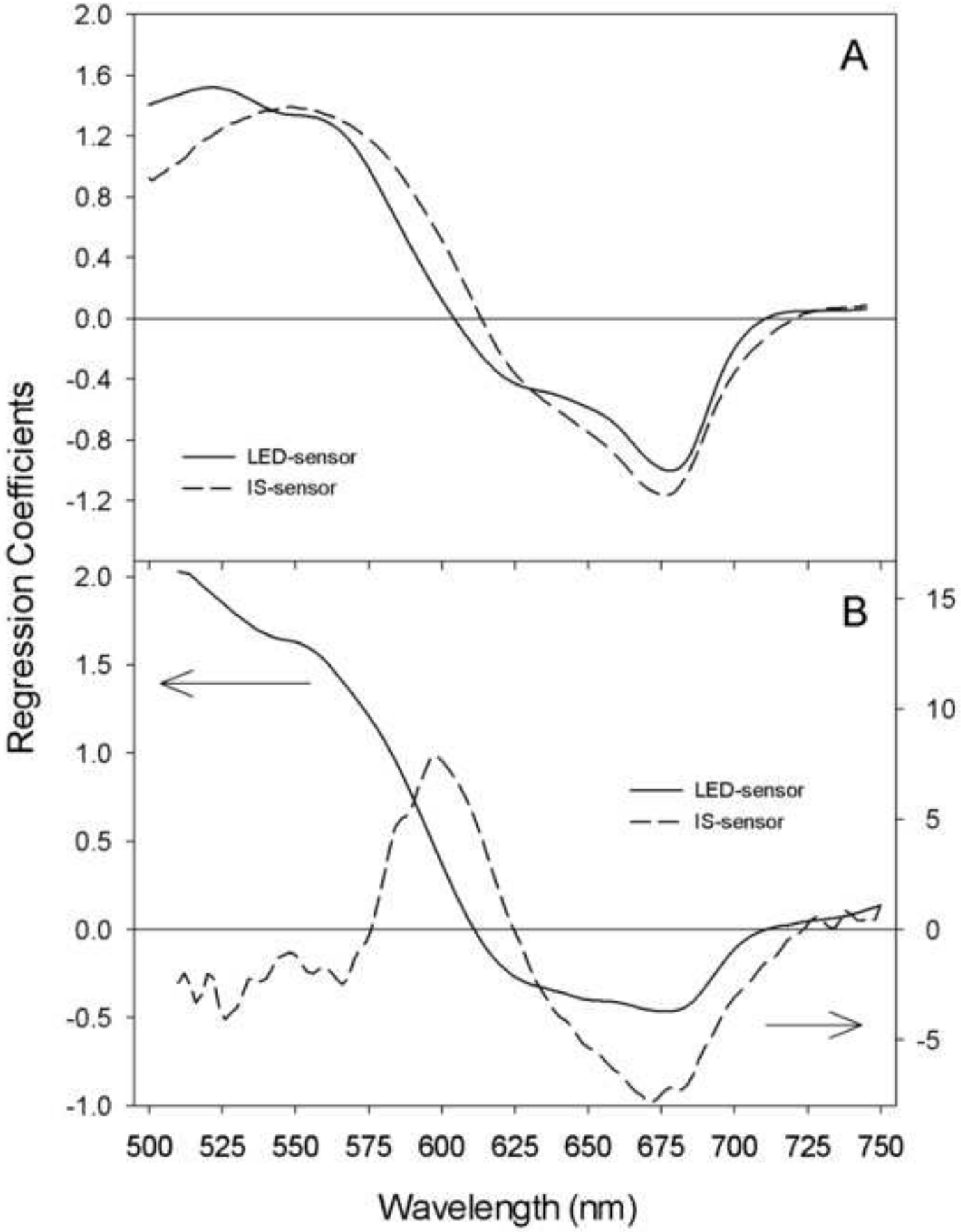

Figure 5

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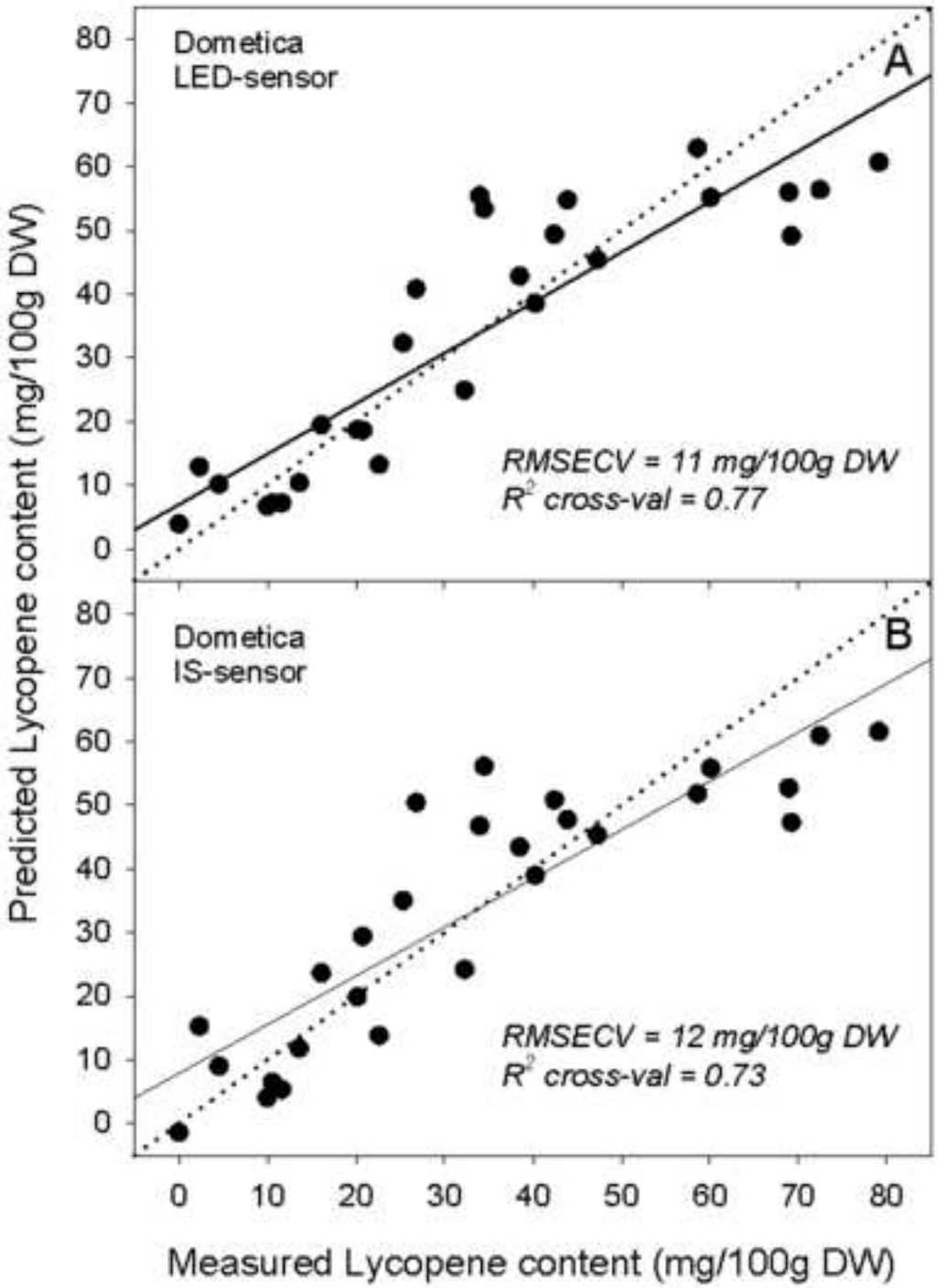

Figure 6

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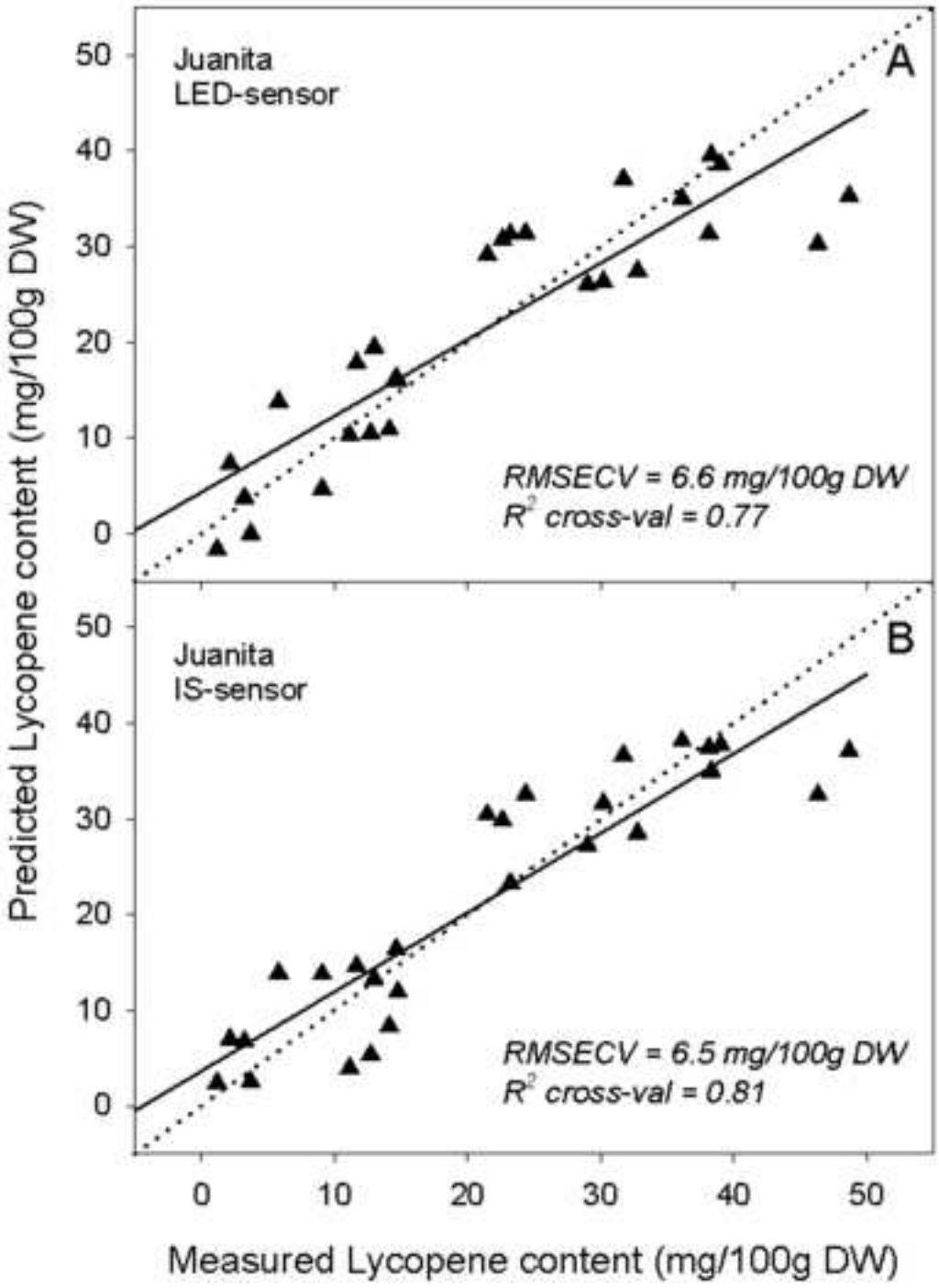
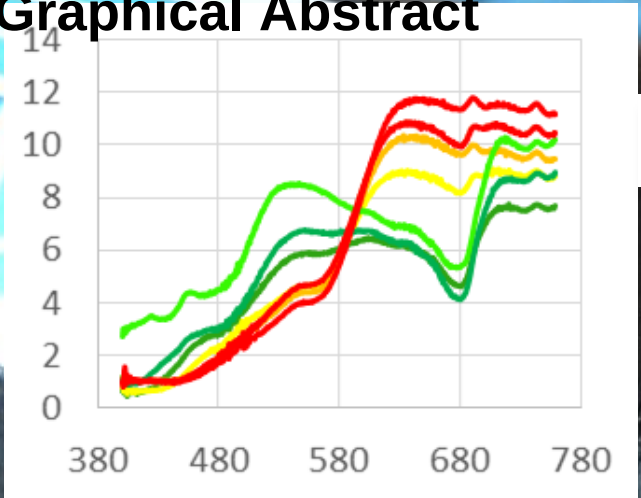


***Highlights**

- Integrating-sphere and LED-based sensors for tomato spectral reflectance detection
- Directional and total reflectance spectra of whole tomatoes are highly correlated
- Tomato lycopene was predicted non-destructively by reflectance and PLS regression
- Directional and total reflectance similarly predict tomato lycopene (16% error)

Graphical Abstract



Reflectance predicted Lycopene