# AGRICULTURAL AND FOOD CHEMISTRY

## Nondestructive Measurement of Fresh Tomato Lycopene Content and Other Physicochemical Characteristics Using Visible–NIR Spectroscopy

Alain Clément,\*<sup>,†</sup> Martine Dorais,<sup>§</sup> and Marcia Vernon<sup>#</sup>

Food Research and Development Centre, Agriculture and Agri-Food Canada, 3600 Casavant Boulevard West, St-Hyacinthe, QC J2S 8E3, Canada; Horticultural Research Centre, Agriculture and Agri-Food Canada, Université Laval, Québec, QC G1V 0A6, Canada; and Institut National d'Optique, Parc technologique du Québec métropolitain, 2740 rue Einstein, Québec, QC G1P 4S4, Canada

Measurement of fresh tomato fruit overall quality, and particularly lycopene content, is challenging in the context of high-volume production. An experiment was conducted to simultaneously measure various quality parameters of tomato in a nondestructive manner using vis–NIR reflectance spectroscopy and chemometrics. The sampling set included different cultivars that are obtainable from both retailers' shelves and two greenhouse producers. Results indicate that lycopene content was accurately predicted [ $r^2 = 0.98$ ; root mean square error of cross-validation (RMSECV) = 3.15 mg/kg], along with color variables such as Hunter a ( $r^2 = 0.98$ ), L, and b ( $r^2 = 0.92$ ). Tomato color index (TCI) was better predicted ( $r^2 = 0.96$ ) than the a/b ratio ( $r^2 = 0.89$ ). Firmness prediction, with an  $r^2$  of 0.75, is comparable to what is reported in the literature for other fruits and may have a practical interest. Prediction of internal quality such as pH, soluble solids, titratable acidity, and electrical conductivity was less accurate, partly due to a low variability of these parameters among samples. Predictions were robust with regard to cultivars, except for pink variety tomato. The 400–1000 nm range gave results almost as accurate as the 400–1500 nm range.

KEYWORDS: Color; firmness; lycopene; *Lycopersicon esculentum*; fruit quality; soluble solids; taste; titratable acidity

### INTRODUCTION

Lower prices, and greater availability of year-round products, in tandem with increasing incomes, have enhanced the array of fruits and vegetables in the global consumer's basket of goods. On the other hand, despite advances in electronic sorting systems, fruit and vegetable quality inspection is still largely a manual operation using simple tools such as color charts and national standards based on appearance and feel. Recently, quite a lot of research work has been published on rapid and nondestructive measurement of fruit and vegetable quality, using near-infrared (NIR) spectroscopy (1, 2). NIR is characterized by a relatively high light penetration inside fruits that allows quantitative analysis of various physicochemical characteristics. Despite its importance in terms of production and trade, there is relatively scant information available on the rapid and nondestructive measurement of tomato quality, particularly for simultaneous analysis of various quality parameters (3-5).

Lycopene content has received much attention lately, particularly because the antioxidant properties and health benefits of this pigment are documented. These benefits include anticarcinogenic and antiatherogenic effects (6, 7). The reference method for lycopene content measurement is tedious, involving a mixture of solvents for pigment solubilization and precautions to avoid pigment oxidation during extraction (8, 9). Some rapid methods of analysis have been proposed for tomato. Very good results were obtained on pureed samples using a xenon flash colorimeter/spectrophotometer (10, 11) or a NIR spectrometer (12). Measurement of lycopene content in whole tomato, based on color data and using a HPLC reference method, resulted in a nonlinear model involving either  $a^*$  or  $a^*/b^*$  ( $r^2 = 0.96$ ) (13).

Color is a major determinant of quality, which may influence consumer acceptability of fruits and vegetables. In the case of tomato, color is an indicator of maturity, and it is used as a basis for classification (14). Measurements with a colorimeter, using the  $L^*$ ,  $a^*$ , and  $b^*$  color space, are a convenient way to automatically classify tomato, particularly using indices such as the  $a^*/b^*$  ratio or the "tomato color index" (TCI) (15, 16). Spectral analysis may have the additional advantage to distinguish mature green fruit from those that will not ripen because they have not reached the climacteric respiration rise (17).

<sup>\*</sup> Corresponding author [telephone (450) 768-3239; fax (450) 773-8461; e-mail clementa@agr.gc.ca].

<sup>&</sup>lt;sup>†</sup>Food Research and Development Centre, Agriculture and Agri-Food Canada.

<sup>&</sup>lt;sup>§</sup> Horticultural Research Centre, Agriculture and Agri-Food Canada. <sup>#</sup> Institut National d'Optique.

Firmness evolution through the ripening process is a complex phenomenon that involves modifications in cell turgor, cell anatomy, relative importance of intercellular spaces, and chemical composition of the cell wall and middle lamella, as well as spatial arrangement of all of the polymer constituents of the cell wall structure (18, 19). Nondestructive measurement of fruit firmness using optical methods (NIR spectroscopy or scattering profiles) has been tested on a number of fruit, including apple, peach, mango, tomato (3, 20), cherry, and green pea. Results obtained are in the 0.60-0.80 coefficient of determination range, somewhat low in absolute terms, but still useful, considering that firmness is a quality criteria of major importance.

Using an interactance probe, Slaughter et al. (4) were able to measure soluble solids (SS) of tomato with good accuracy [standard error of prediction (SEP) = 0.33 °Brix,  $r^2 = 0.79$ ]. Walsh et al. (5) obtained a SEP of 0.20 °Brix ( $r^2 = 0.59$ ), pointing out that SS variability among fruits was low. Khuriyati and Matsuoka (21) found that near-infrared transmittance readings can be used to measure SS on growing tomato fruit with good accuracy ( $r^2 = 0.83$ ). Direct optical measurement of other quality parameters related to the chemical composition of tomato, such as pH, titratable acidity, and electrical conductivity, has received little attention. The objective of this study was to determine if lycopene content can be measured directly on intact tomato fruit while simultaneously estimating the basic physicochemical characteristics: color, firmness, soluble solids, acidity, and pH.

#### MATERIALS AND METHODS

Tomato Samples. Ninety-six tomato fruits were obtained from various sources in Quebec, Canada (longitude 71° W, latitude 46° N). They were bought directly at grocery stores (28 fruits) or from public markets (15 fruits) or obtained from local greenhouse growers (53 fruits) (2). Sampling was done in such a way that all levels of maturity were represented, from immature green to red and soft fruit. Whereas some tomatoes were analyzed within 12 h of acquisition, some green mature fruits were kept in the laboratory at ambient conditions for as long as 24 days, in order to generate further diversity in maturity levels. Although not all fruit cultivars were identified, they were mostly beefsteak-type red tomato (cv. Trust, Blitz), except for six pink variety samples (cv. DRK 453). Care was taken to maintain the tomatoes at room temperature prior to analysis at the Institut National d'Optique facility (Quebec City, Canada). Fruit surface temperature immediately before the start of physicochemical analyses was measured with an infrared meter (Cole Parmer Instruments, Vernon Hills, IL; model 39750-40) and averaged 21.7  $\pm$  0.3 °C.

After measurement of fresh weight, four equidistant spots were identified at the fruit equator. These were areas where both spectroscopic and near-surface physicochemical analyses were successively done. After measurement of near-surface quality variables (color, firmness, soluble solids, and pH), fruits were homogenized for a minute using a stainless steel blender (Toastess International, Markham, ON, Canada; model TB-50GS). The slurry was used directly for lycopene content determination, before filtering with a nylon-type cotton cheesecloth for soluble solids, pH, electrical conductivity, and titratable acidity measurements.

**Spectral Measurements.** The reflectance spectra of tomato were measured with a Varian Cary 500 UV–vis–NIR scanning spectrophotometer (Varian Inc., Palo Alto, CA) equipped with an integration sphere (Labsphere Inc., North Sutton, NH). The whole tomato was placed in such a way that the incident tungsten halogen light beam reached the selected sampling area, prior to the closing of a stray-light protection cover. The selected wavelength range used was from 400 to 1500 nm, with an integration time of 0.3 s and a reading at every 2 nm, for a total of 551 reflectance readings per sampled area. Calibration was done once a day, before starting measurements. Zero reflectance was adjusted by blocking the light path, and a poly(tetrafluoroethylene) (PTFE) diffuse reflectance standard was used for 100% reflectance. **Physicochemical Measurements.** Lycopene content was determined according to the reduced volumes of organic solvents method of Fish et al. (22). About 0.6 g of unfiltered whole tomato puree was weighed precisely, added to a 40 mL amber vial containing 5 mL of acetone with 0.05% butylated hydroxytoluene, 5 mL of ethanol, and 10 mL of hexane. The mixture was put on an orbital shaker at 180 rpm for 15 min. Three milliliters of water was then added, prior to an additional 5 min on the shaker. Afterward, the vial was left in an upright position at room temperature for 5 min to allow for phase separation. The upper phase (hexane) was sampled to obtain an absorbance reading at 503 nm using a Varian Cary 500. The following relationship was then used for estimation of lycopene content: lycopene (mg/kg) = ( $A_{503} \times 31.2$ )  $\div$  quantity of tissue used (22).

Color readings were made using a hand-held color meter (Miniscan XE, Hunterlab Associates Laboratory Inc., Reston, VA). It was configured for Hunterlab's L, a, and b scale with daylight (D65) and a 10° observer. The three color variables were used to compute the TCI  $[TCI = 2000a/(L(a^2 + b^2)^{1/2})]$  (23). Tomato pericarp firmness was measured with a mechanical probe (24) (Bareiss HP, Heinrich Bareiss, Oberdischingen, Germany). The device measures local pericarp movement upon application of a constant 12.5 N force, using a 0.25 cm<sup>2</sup> cylindrical flat-ended probe. Soluble solids were measured in two different ways using a refractometer. For tomato near-surface measurements, a drop of liquid was obtained after local removal of the cuticle and breakage of the peripheral pericarp cells with a Pasteur pipet; SS were measured with an Atago ATC 1E (Tokyo, Japan). A benchtop device (ABBE Mark II, Reichert Analytical Instruments, Depew, NY) was used for whole tomato extract soluble solids. Near-surface pH was measured with a pH-meter (Orion Research Inc., Beverly, MA), with a spear-type probe (Cole Parmer Instruments) inserted at a depth of 5 mm in the pericarp. A standard combination probe was used to measure whole tomato extract pH. Electrical conductivity was determined directly using an Orion Research specific probe. Titratable acidity was measured using 15 mL of the whole tomato extract, titrated to pH 8.1 using 0.100 N NaOH. The following formula was used for calculation:  $Z = (V \times N \times \text{Meq} \times 100) \div Y$ , where Z = titratable acidity (as percent citric acid), V = volume of NaOH used, N = normality of NaOH, Meq = weight of a milliequivalent of citric acid (0.064 g), and Y = volume of tomato extract used.

**Data Analysis.** Spectral analysis was done either on raw percent reflectance or log (1/reflectance) data. Partial least-squares (PLS) regressions were computed using the Unscrambler, version 9.2 (Camo Inc., Woodbridge, NJ). Model performance was determined using the full cross-validation approach, which measures the root mean square of error of cross-validation (RMSECV) and a coefficient of determination ( $r^2$ ) for prediction. The ratio of variable standard deviation to RMSECV (SDR) (25) was calculated. A SDR above 3.0 is considered sufficient for practical spectroscopy applications. A number of data transformations were tested, such as standard normal variate (SNV), and the Savitsky–Golay (SG) algorithm, using first or second derivatives and first- or second-degree polynomials.

#### **RESULTS AND DISCUSSION**

Physicochemical Quality Parameters. Of the raw tomato color parameters measured in this study (Table 1), the Hunter a value was the most variable, with a coefficient of variation (CV) of 64%. This variable is expected to be related to tomato maturity, because its scale ranges from green (negative values) to red (positive values). Hunter L and b were less variable, with CVs of 16 and 28%, respectively. The color indices that were computed, alb and TCI, are more variable (CVs of 80 and 71%, respectively) than raw color values. Lycopene content varied from 1.78 to 72.31 mg/kg, with a CV of 59%, whereas firmness, electrical conductivity (EC), titratable acidity (TA), and the SS (extract)/TA ratio had CVs ranging from 13 to 21%. Soluble solids and pH values were least variable, with CVs ranging from 7.7 to 8.1% and from 2.3 to 5.1%, respectively. A parameter that shows a large sample variation is likely to be better predicted by vis-NIR spectroscopy (26).

Table 1. Descriptive Statistics (n = 93-95) and Vis-NIR Prediction Statistics for Various Tomato Quality Parameters under Study (Computed with the Average of Four Spectra per Fruit)

variable	min	max	mean	CV <sup>a</sup>	outliers	PLS LV <sup>b</sup>	prediction statistics		
							RMSECV <sup>c</sup>	r <sup>2</sup>	SDR <sup>d</sup>
Hunter L	23.5	47.0	32.1	16.0	0	5	1.456	0.919	3.54
Hunter a	-5.9	25.3	12.9	63.9	0	5	1.126	0.981	7.32
Hunter b	10.8	48.6	28.3	28.1	1	9	2.134	0.924	3.40
a/b	-0.33	1.49	0.46	80.4	1	8	0.121	0.887	3.09
TCI <sup>e</sup>	-15.7	65.0	26.0	71.1	1	8	3.431	0.964	5.40
lycopene (mg/kg)	1.8	72.3	34.0	58.9	2	12	3.150	0.975	6.35
firmness	40.8	94.8	68.4	19.1	1	8	6.440	0.750	2.03
EC <sup>f</sup> (mS/cm)	4.06	7.54	5.40	13.0	0	5	0.637	0.181	1.10
SS <sup>g</sup> (surface) (°Brix)	3.17	5.07	4.18	8.1	0	13	0.354	0.100	0.96
SS (extract) (°Brix)	3.50	5.60	4.52	7.7	1	6	0.308	0.159	1.12
pH (surface)	3.86	4.97	4.51	5.1	0	15	0.196	0.350	1.17
pH (extract)	4.11	4.56	4.27	2.3	0	8	0.078	0.416	1.28
TA <sup>h</sup> (% citric acid)	0.239	0.657	0.418	20.6	0	11	0.070	0.362	1.23
SS (extract)/TA	7.09	17.58	11.24	20.3	0	11	1.759	0.417	1.30

<sup>a</sup> CV, coefficient of variation. <sup>b</sup> PLS LV, partial least-squares latent variables. <sup>c</sup> RMSECV, root mean square of error of cross-validation. <sup>d</sup> SDR, standard deviation to RMSECV ratio. <sup>e</sup> TCI, tomato color index. <sup>f</sup> EC, electrical conductivity. <sup>g</sup> SS, soluble solids. <sup>h</sup> TA, titratable acidity.

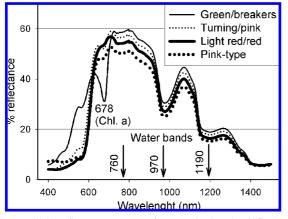
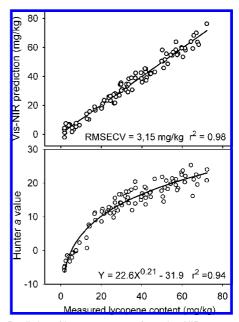


Figure 1. Light reflectance pattern of tomato in the vis-NIR spectral regions.

Better predictions were obtained when results were expressed in terms of log 1/R (without further preprocessing), as compared to raw percent reflectance data, and are thus reported here. In the specific case of firmness, best prediction was obtained after a SG smoothening of log 1/R data, first derivative, and secondorder polynomial.

Spectra of Fresh Fruits. Fruits were divided into four categories to outline differences in spectral signatures (Figure 1); three maturity stages and a specific category for pink tomato variety, a specialty cultivar grown almost exclusively in Canada. There is a general increase in reflectance from 400 nm to about 800 nm, followed by a decrease to low values, in the 4-8%range, at wavelengths higher than 1400 nm. In general, reflectance is higher in the case of less mature (green/breakers) tomato, particularly in the 400-600 nm range. This explains why Hunter L (luminosity) has been reported to be higher in less mature tomato fruit (2). There is a noticeable reflectance shoulder at 552 nm in green/breakers fruit, a region where chlorophyll does not absorb. Absorption at 678 nm represents the high content in chlorophyll a (Chl a) in green fruit, and some remaining green pigments in turning/pink fruit. The reflectance pattern of pink tomato variety is characterized by a generally lower reflectance throughout the spectrum, except at short wavelength values (400-500 nm). As the water content of tomato fruit is around 95% (2), there is a small but noticeable absorption band at 760 nm (Figure 1), caused by the third overtone of OH stretching (27), and wide absorption bands at

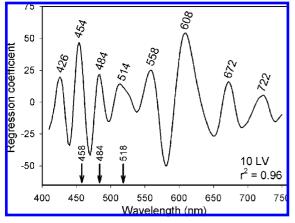


**Figure 2.** Prediction of lycopene content from vis—NIR spectroscopy (top) or from Hunter *a* value (bottom). RMSECV, root mean square error for prediction.

970 and 1200 nm, corresponding to H-O-H stretching and bending absorbance (27, 28).

Prediction of lycopene content was very accurate, with an  $r^2$  of 0.98 and an SDR of 6.35 (**Figure 2**). The RMSECV value of 3.15 mg/kg is small for direct measurements on raw fruits, as compared, for instance, to an RMSECV of 140 mg/kg obtained for the determination of anthocyanin content in raw grapes (29). The lycopene spectral signature is thus very distinctive. Because measurements were made at the equator and are a mean of four values, surface measurements are closely related to whole fruit lycopene content. Using a different approach, data derived from hyperspectral imaging also provide very good estimates of lycopene content in fresh tomato (30).

The spectral signature of pure lycopene in various nonpolar solvents is known to be limited to the 400-600 nm region, with three absorption peaks at 458, 484, and 518 nm in a chloroform solvent (*31*). A regression model for prediction of lycopene limited to the visible region was computed to determine if the regression equation reflects the known characteristics of pure



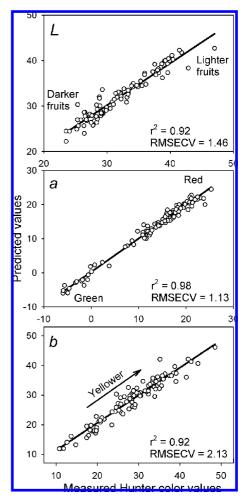
**Figure 3.** Regression coefficients for prediction of lycopene content from the visible spectrum (410–750 nm). Data smoothed with the Savitszky–Golay algorithm (11 nm range, second-order polynomial). LV, latent variables. Arrows indicate peak absorption of pure lycopene in chloroform (*31*).

lycopene (**Figure 3**). In PLS analysis, direct interpretation of regression coefficients is not always conclusive, because many latent variables are combined. In this case, however, the pattern of regression equations was consistent, even with the inclusion of 10 latent variables, a relatively large number. The 454, 484, and 514 nm wavelengths turned out to be influential in the model (**Figure 3**), as in pure solution. However, there were many other spectral regions of importance, at 426, 558, 608, 672, and 722 nm. These wavebands are likely related to lycopene due to the interaction of the molecule with its surrounding environment. Lycopene, being nonpolar, interacts with membranes within chromoplasts, causing spectral shifts (*32*). Hence, for instance, absorbance at 560 nm minus absorbance at 700 nm is linearly related to lycopene content (*33*).

Because the visible range was included in this study, prediction of color from spectral analysis is equivalent to matching two sets of spectrophotometric data. Best results were obtained for Hunter *a*, with a coefficient of determination  $(r^2)$ of 0.98 (Table 1; Figure 4). Values at the lower left of the graph represent green/breakers fruits, with more mature fruits in the upper right direction. Hunter L and b prediction, measuring "lightness" and "yellowness", respectively, were also accurately predicted, with  $r^2$  values of 0.92 in both cases and SDR values above 3.0 (Table 1; Figure 4). TCI ( $r^2 = 0.96$ ) was better predicted than the a/b ratio ( $r^2 = 0.89$ ; Figure 5). The *a/b* ratio has been identified as a suitable variable for color definition of tomato (13, 34). However, in our study, predictions for the pink tomato variety tend to be overestimated by the model. This suggests that spectroscopic calibrations are robust with regard to cultivars, but only within the red variety fruits. The pink tomato variety has been little studied. It appears to lack a yellow pigment, because Hunter b values are low, as compared to the other cultivars (data not shown).

Predicting the lycopene content from color measurements is feasible, with best results obtained with a power fit, using Hunter a values (**Figure 2**). Molyneux et al. (35) mention that prediction of lycopene from CIE  $a^*$  values did not work for all cultivars, and that the  $(a^*/b^*)^2$  ratio is a more reliable predictor (13, 35). In our case, this ratio did not allow satisfactory predictions due to the pink variety tomato, which behaves as a distinct set of data (**Figure 5**). Vis–NIR spectroscopy thus appears to be a more reliable predictor of lycopene content in fresh tomato as compared to regressions from color data.

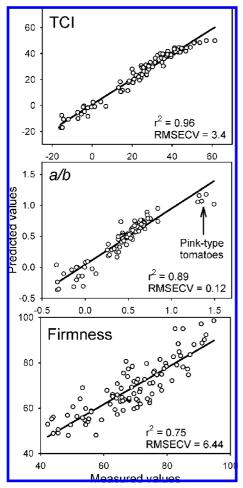
Tomato firmness was predicted with a coefficient of determination of 0.75 (**Figure 5**) and an SDR of 2.03. These results



**Figure 4.** Validation scatter plots of Hunter *L*, *a*, and *b* color variables. Predicted values were obtained by vis-NIR spectroscopy.

are comparable to what was reported in the literature for firmness prediction on tomato and other fruits. On tomato, using a Magness-Taylor puncture test as a reference, He et al. (36) obtained an  $r^2$  of 0.76, better than a compression reference test  $(r^2 = 0.67)$ . Tu et al. (37) obtained an  $r^2$  of 0.66 when calibrating laser scattering profiles with pericarp deformation under a 3 N constant force; lower values were obtained when calibration was performed with acoustic measurements ( $r^2 =$ 0.62). Using multispectral scattering data and a Magness-Taylor probe reference method on peach,  $r^2$  values were 0.76 on a single orchard, but 0.67 when combining data from two orchards (38). Results on apple are in the 0.60–0.70  $r^2$  value range, reaching 0.85 with an acoustic reference method (39, 40). The complexity of biological factors involved in firmness evolution as maturation proceeds and the diversity of approaches for reference measurements are noteworthy. This complicates development of a widely accepted optical method for firmness measurement of fruits. The SDR of 2.03 obtained in this study for tomato firmness measurement may not be sufficient for numerical quantification of tomato firmness. However, a rank scale with two or three categories could have a practical interest for online applications. It that case, definition of acceptable firmness for marketing purposes should be defined by calibration with sensory data.

The other quality parameters under study, soluble solids, pH, titratable acidity, electrical conductivity, and the soluble solids/ titratable acidity ratio (SS/TA), could not be accurately predicted from reflectance data (**Table 1**). Best results were obtained for tomato extract pH and SS/TA, with an  $r^2$  of 0.42. The result



**Figure 5.** Validation scatter plots of tomato color index, Hunter *a/b*, and firmness. Predicted values were obtained by vis—NIR spectroscopy.

for SS ( $r^2 = 0.16$ ) is very low as compared to what is reported by Slaughter et al. (4) ( $r^2 = 0.79$ ) or by Khuriyati et al. (21) ( $r^2 = 0.83$ ), probably because their data set included fruits with very high SS content (°Brix > 7.0). However, the RMSECV values of 0.31–0.35 obtained in this study are comparable with these reported results. Our sampling data show that the range of values was narrow (3.2–5.6, **Table 1**), making predictions more challenging. The configuration of illumination and light capture in other studies was different, with use of an interactance (4) or transmittance probe (21). These may be more suitable approaches for measurement of soluble solids, with a possibly deeper light penetration in tomato tissues.

Data Processing Approach. There are two possible approaches to the modeling of physicochemical characteristics from spectral data using PLS regression. The average spectra on each tomato can be used for prediction (Table 1), or individual values at each of the four sampling spots can be considered for computation. Variability within a tomato can be important, as color can vary from green to various shades of red on a single fruit during maturation, particularly at the breakers and turning stages of maturity. In general, better results were obtained when the average spectrum per fruit was considered. The coefficient of determination  $(r^2)$  was particularly higher with combined spectra as compared to individual spectra in the case of Hunter b (0.92 vs 0.62), firmness (0.75 vs 0.69), Hunter a/b (0.89 vs 0.85), TCI (0.96 vs 0.92), Hunter L (0.92 vs 0.90), and Hunter a (0.98 vs 0.96). However, individual spectra provided better prediction for near-surface pH (0.35 vs 0.39) and near-surface SS (0.10 vs 0.22). In these two cases,

Table 2. Effect of Wavelength Range on Tomato Calibration Statistics

	400-1	000 nm	900-1500 nm		
variable	r <sup>2</sup>	SDR <sup>a</sup>	r <sup>2</sup>	SDR	
Hunter L	0.918	3.52	0.682	1.78	
Hunter a	0.981	7.22	0.561	1.50	
Hunter b	0.895	3.10	0.265	1.16	
a/b	0.872	2.81	0.564	1.51	
TCI <sup>b</sup>	0.964	5.37	0.653	1.71	
lycopene	0.944	5.92	0.731	1.94	
firmness	0.724	1.89	0.638	1.65	
EC <sup>c</sup>	0.142	1.06	0.119	1.02	
SS <sup>d</sup> (surf)	0.002	1.01	0.001	0.99	
SS (extr)	0.010	1.00	0.126	1.05	
pH (surf)	0.304	1.08	0.389	1.25	
pH (extr)	0.438	1.27	0.326	1.18	
TA <sup>e</sup>	0.289	1.19	0.364	1.25	
SS (extr)/TA	0.285	1.19	0.435	1.34	

<sup>a</sup> SDR, standard deviation to RMSECV ratio. <sup>b</sup> TCI, tomato color index. <sup>c</sup> EC, electrical conductivity. <sup>d</sup> SS, soluble solids. <sup>e</sup> TA, titratable acidity.

predictions remain inadequate. Our results suggest that tomato fruit is better described by an averaged spectroscopic profile. Increasing the number of readings per fruit has been shown to better predict dry matter of tomato (41).

Wavelength Range Selection. Our results were obtained using a rather large range of wavelengths, from 400 to 1500 nm, using a scanning spectrometer. When we compared results from three different wavelength intervals, the 400-1000 nm region alone gave satisfactory results for most variables (Table 2), almost reaching the accuracy obtained using the whole 400-1500 nm spectrum (Table 1). On the other hand, computations using the 900–1500 nm range results in SDR values lower than 3.0 for all variables. Our results are in accordance with previous studies suggesting that the 360-750 nm range is suitable for measurement of lycopene content of tomato puree ( $r^2 = 0.97$ ) (42) and the 560-700 nm range ( $r^2 = 0.98$ ) for watermelon puree (10), in contrast with the 1000-2500 nm range recommended for homogenized and concentrated tomato products (12). In practice, for the design of rapid, low-cost, solid-state tools for measurement of large numbers of samples, either the visible-shortwave near-infrared region (400-1000 nm), measured by CCD array detectors, or the region between 1000 and 2500 nm, measured with InGaAs detectors, is available. The 400-1000 nm range is advantageous, because low-cost CCD detectors are readily available, whereas InGaAs detectors provide less resolution and necessitate cooling for optimal performance.

In conclusion, rapid and nondestructive quality measurement of whole tomato is possible using spectral reflectance data, although not all variables are predicted with the same accuracy. All surface color variables were expectedly easily measured. Rapid and accurate prediction of lycopene content is of particular interest, considering that reference methods are laborious, particularly the extraction procedure. Spectroscopy is thus a promising avenue for rapid analysis of other pigments of interest in fruits or vegetables, oftentimes linked to beneficial antioxidant properties. Tomato firmness measurement was less accurate, but still allows some practical uses such as detection of excess firmness or softness of some fruits. Improved predictions could be obtained if data sets included single cultivars with sufficient variability among samples. The visible and short-wave NIR region (400-1000 nm) is sufficient for the measurement of lycopene content and color variables. Hence, low-cost solid-state spectrometers could be promising instruments. Alternative optical configurations could improve results for internal measurements of soluble solids, pH, titratable acidity, and electrical conductivity. Use of an interactance probe will likely improve light penetration inside the fruit and its capture. A better

assessment of internal quality would allow prediction of variables linked to organoleptic quality.

#### LITERATURE CITED

- Chen, J. Y.; Zhang, H.; Miao, Y. L.; Matsunaga, R. NIR measurement of specific gravity of potato. *Food Sci. Technol. Res.* 2006, *11*, 26–31.
- (2) Clément, A.; Dorais, M.; Vernon, M. Multivariate approach to the measurement of tomato maturity and gustatory attributes and their rapid assessment by vis–NIR spectroscopy. J. Agric. Food Chem. 2008, 56, 1538–1544.
- (3) Shao, Y. N.; He, Y.; Gomez, A. H.; Pereir, A. G.; Qiu, Z. J.; Zhang, Y. Visible/near infrared spectrometric technique for nondestructive assessment of tomato 'Heatwave' (*Lycopersicum esculentum*) quality characteristics. J. Food Eng. 2007, 81, 672–678.
- (4) Slaughter, D. C.; Barrett, D.; Boersig, M. Nondestructive determination of soluble solids in tomatoes using near infrared spectroscopy. J. Food Sci. 1996, 61, 695–697.
- (5) Walsh, K. B.; Golic, M.; Greensill, C. V. Sorting of fruit using near infrared spectroscopy: application to a range of fruit and vegetables for soluble solids and dry matter content. *J. Near Infrared Spectrosc.* **2004**, *12*, 141–148.
- (6) Engelhard, Y. N.; Gazer, B.; Paran, E. Natural antioxidants from tomato extract reduce blood pressure in patients with grade-1 hypertension: a double-blind, placebo-controlled pilot study. *Am. Heart J.* 2006, *151*, 100.e1–100.e6.
- (7) Adetayo, O. O.; Rotimi, E. A. The anti-carcinogenic and antiatherogenic effects of lycopene: a review. *Trends Food Sci. Technol.* 2005, 16, 344–350.
- (8) Periago, M. J.; Rincón, F.; Agüera, M. D.; Ros, G. Mixture approach for optimizing lycopene extraction from tomato and tomato products. J. Agric. Food Chem. 2004, 52, 5796–5802.
- (9) Sadler, G.; Davis, J.; Dezman, D. Rapid extraction of lycopene and β-carotene from reconstitued tomato paste and pink grapefruit homogenates. J. Food Sci. 1990, 55, 1460–1461.
- (10) Davis, A. R.; Fish, W. W.; Perkins-Veazie, P. A rapid hexanefree method for analyzing lycopene content in watermelon. *J. Food Sci.* 2003, 68, 328–332.
- (11) Davis, A. R.; Fish, W. W.; Perkins-Veazie, P. A rapid spectrophotometric method for analyzing lycopene content in tomato and tomato products. *Postharvest Biol. Technol.* **2003**, *28*, 425–430.
- (12) Pedro, A. M.; Ferreira, M. M. Nondestructive determination of solids and carotenoids in tomato products by near-infrared spectroscopy and multivariate calibration. *Anal. Chem.* 2005, 77, 2505–2511.
- (13) Arias, R.; Lee, T.-C.; Logendra, L.; Janes, H. Correlation of lycopene measured by HPLC with the *L*\*, *a*\*, *b*\* color readings of a hydroponic tomato and the relationship of maturity with color and lycopene content. *J. Agric. Food Chem.* **2000**, *48*, 1697–1702.
- (14) USDA. U.S. Standards for Grades of Fresh Tomatoes; Washington, DC, 1991.
- (15) Batu, A. Determination of acceptable firmness and colour values of tomatoes. *J. Food Eng.* **2004**, *61*, 471–475.
- (16) Gomez, R.; Varon, R.; Amo, M.; Tardaguila, J.; Pardo, J. E. Differences in the rate of coloration in tomato fruit. *J. Food Qual.* **1998**, *21*, 329–339.
- (17) Hahn, F. Multi-spectral prediction of unripe tomatoes. *Biosyst. Eng.* **2002**, *81*, 147–155.
- (18) Barrett, D. M.; Garcia, E.; Wayne, J. E. Textural modification of processing tomatoes. *Crit. Rev. Food Sci. Nutr.* **1998**, *38*, 173–258.
- (19) Prasanna, V.; Prabha, T. N.; Tharanathan, R. N. Fruit ripening phenomena—an overview. *Crit. Rev. Food Sci. Nutr.* 2007, 47, 1–19.
- (20) Navas Moya, F. A.; Requena Rodriguez, A.; Tomas Balibrea, L. M. Non-destructive laser sorting of whole tomatoes. *Acta Hortic.* 2005, 674, 581–584.
- (21) Khuriyati, N.; Matsuoka, T. Near infrared transmittance method for nondestructive determination of soluble solids content in growing tomato fruits. *Environ. Control Biol.* **2004**, *42*, 217–223.
- (22) Fish, W. W.; Perkins-Veazie, P.; Collins, J. K. A quantitative assay for lycopene that utilizes reduced volumes of organic solvents. *J. Food Compos. Anal.* **2002**, *15*, 309–317.

- (23) Opiyo, A. M.; Ying, T.-J. The effects of 1-methylcyclopropene treatment on the shelf life and quality of cherry tomato (*Lycopersicon esculentum* var. *cerasiforme*) fruit. *Int. J. Food Sci. Technol.* 2005, 40, 665–673.
- (24) Sivakumar, D.; Korsten, L. Influence of modified atmosphere packaging and postharvest treatments on quality retention of litchi cv. Mauritius. *Postharvest Biol. Technol.* **2006**, *41*, 135–142.
- (25) Slaughter, D. C.; Thompson, J. F.; Tan, E. S. Nondestructive determination of total and soluble solids in fresh prune using near infrared spectroscopy. *Postharvest Biol. Technol.* 2003, 28, 437–444.
- (26) Bertrand, D. Une démarche générale pour l'établissement d'applications analytiques. In *La Spectroscopie Infrarouge et ses Applications Analytiques*; Bertrand, D., Dufour, E., Eds.; TEC & DOC: Paris, France, 2000; pp 381–388.
- (27) Bertrand, D. Spectroscopie de l'eau. In La Spectroscopie Infrarouge et ses Applications Analytiques; Bertrand, D., Dufour, É., Eds.; TEC & DOC: Paris, France, 2000; pp 93–105.
- (28) Lestander, T. A.; Geladi, P. NIR spectral information used to predict water content of pine seeds from multivariate calibration. *Can. J. For. Res.* 2005, *35*, 1139–1148.
- (29) Cozzolino, D.; Esler, M. B.; Dambergs, R. G.; Cynkar, W. U.; Boehm, D. R.; Francis, I. L.; Gishen, M. Prediction of colour and pH in grapes using a diode array spectrophotometer (400– 1100 nm). J. Near Infrared Spectrosc. 2004, 12, 105–111.
- (30) Polder, G.; van der Heijden, G. W. A. M.; van der Voet, H.; Young, I. T. Measuring surface distribution of carotenes and chlorophyll in ripening tomatoes using imaging spectrometry. *Postharvest Biol. Technol.* **2004**, *34*, 117–129.
- (31) Rodriguez-Amaya, D. B.; Kimura, M. General procedure for carotenoid analysis. In *HarvestPlus Handbook for Carotenoid Analysis*; HarvestPlus: Washington, DC, 2004; pp 8–20.
- (32) Fish, W. W. Interaction of sodium dodecyl sulfate with watermelon chromoplasts and examination of the organization of lycopene within the chromoplasts. *J. Agric. Food Chem.* **2006**, *54*, 8294–8300.
- (33) Anthon, G. E.; Barrett, D. M. Potential and limitations for determining lycopene in tomatoes by optical methods. *Acta Hortic.* 2006, 724, 243–248.
- (34) Hobson, G. E.; Adams, P.; Dixon, T. J. Assessing the color of tomato fruit during ripening. J. Sci. Food Agric. 1983, 34, 286–292.
- (35) Molyneux, S. L.; Lister, C. E.; Savage, G. P. An investigation of the antioxidant properties and colour of glasshouse grown tomatoes. *Int. J. Food Sci. Nutr.* 2004, 55, 537–545.
- (36) He, Y.; Zhang, Y.; Pereira, A. G.; Gomez, A. H.; Wang, J. Nondestructive determination of tomato fruit quality characteristics using vis/NIR spectroscopy technique. *Int. J. Inf. Technol.* 2005, *11*, 97–108.
- (37) Tu, K.; Jancsók, P.; Nicolai, B.; De Baerdemaeker, J. Use of laserscattering imaging to study tomato-fruit quality in relation to acoustic and compression measurements. *Int. J. Food Sci. Technol.* 2000, *35*, 503–510.
- (38) Lu, R. Assessing peach firmness by muti-spectral scattering. J. Near Infrared Spectrosc. 2005, 13, 27–35.
- (39) Peng, Y.; Lu, R. Modeling multispectral scattering profiles for prediction of apple fruit firmness. *Trans. ASAE* 2005, 48, 235–242.
- (40) Lammertyn, J.; Nicolai, B.; Ooms, K.; de Smedt, V.; de Baerdemaeker, J. Non-destructive measurement of acidity, soluble solids and firmness of Jonagold apples using NIR-spectroscopy. *Trans. ASAE* **1998**, *41*, 1089–1094.
- (41) Khuriyati, N.; Matsuoka, T.; Kawano, S. Precise near infrared spectral acquisition of intact tomatoes in interactance mode. J. *Near Infrared Spectrosc.* 2005, *12*, 391–395.
- (42) Davis, A.; Fish, W. W.; Perkins-Veazie, P. A rapid spectrophotometric method for analyzing lycopene content in tomato and tomato products. *Postharvest Biol. Technol.* **2003**, *28*, 425–430.

Received for review April 25, 2008. Revised manuscript received July 15, 2008. Accepted August 24, 2008.

JF801299R