

Rapid Determination of the Main Organic Acid Composition of Raw Japanese Apricot Fruit Juices Using Near-Infrared Spectroscopy

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The potential of near-infrared (NIR) spectroscopy to rapidly determine citric and malic acid contents of raw Japanese apricot (Japanese “ume”, also known as the Japanese plum) fruit juice was investigated. In total, 314 raw juice samples with different organic acid compositions were collected over a long growth period, and spectra (1100–1850 nm) of these samples were acquired using an NIR spectrophotometer with a 1-mm path length. Calibrations were performed using a partial least-squares regression method based on a calibration sample set (211 samples), while validations were performed based on a validation sample set (103 samples). The results revealed good agreement between NIR spectroscopy and capillary electrophoresis, including the correlation coefficient (r^2), standard error of prediction (SEP), and bias; no statistically ($p = 0.05$) significant differences were found for these parameters. Moreover, standard deviation ratios of reference data in the validation sample set to the SEP were higher than 3, indicating that NIR spectroscopy may represent an acceptable method for quantitative evaluation of citric and malic acids in raw Japanese apricot fruit juice.

KEYWORDS: Near-infrared spectroscopy; citric acid; malic acid; Japanese apricot fruit; Ume; juice; partial least-squares regression

INTRODUCTION

The Japanese apricot fruit (Ume, also known as the Japanese “plum,”) is a special fruit that is mainly produced in East Asia and contains large amounts of organic acids, mainly malic and citric acids. Although Ume fruit is unsuitable for consumption as a fresh food, consumption of its processed goods, such as Ume juice, Ume Sake (Japanese alcoholic beverage), and various pickled Ume products, has increased over recent years since they have health benefits and a sour taste, which Asian people enjoy. The taste and health benefits of the processed goods are influenced by variations in the main ingredients of Ume fruit, particularly the composition of the organic acids, which varies according to the harvesting season, cultivars, and production area. Therefore, determination of the organic acid composition of Ume fruit is very important for the production process to provide good quality products.

High-performance liquid chromatography (HPLC) (1–3) and capillary electrophoresis (4–8) techniques are usually used for determination of organic acids in biomaterials, but these methods are time-consuming and cost-intensive. Therefore, there is a demand for new and rapid analytical techniques for determining the organic acid compositions of raw biomaterials in the production field. Recently, near-infrared (NIR) spectroscopy has

become a well-accepted method for the determination of food constituents since it is fast, requires little or no sample preparation, and does not cause any environmental chemistry pollution. In the field of liquid agricultural materials, the NIR method has been used for determining the fat, lactose, and protein contents of raw milk (9–11) as well as the oleic or fatty acids and tocopherol in vegetable oils (12–14). The NIR technique was also shown to be effective for determining the sugar contents of honey (15–17) and fruit juice (18, 19). However, there have been few applications of the NIR technique for the determination of organic acids in fruit juices (20, 21). Moreover, the NIR technique has never been applied to fruit juices for simultaneous determination of malic and citric acids. Finally, the NIR technique has not yet been applied to Ume fruit.

In the present study, we applied the NIR technique to analyze the main organic acid compositions of raw Ume fruit juices. Specifically, the aim of our study was to investigate the potential of the NIR technique as a means for determining the citric and malic acid contents of raw Ume fruit juices containing very different compositions of organic acids.

MATERIALS AND METHODS

Sample Preparation. The Ume fruits of three cultivars, namely, Bungoume, Koshinoume, and Togoroume, were cultivated in Kotonooka-machi, Akita Prefecture, Japan, in 2004. To obtain a wide range

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Table 1. Mean and Range of the Malic and Citric Acid Contents of Raw Ume Fruit Juices Sampled in the Growth Process

variety	date (d-m-y)	no. of samples	malic acid (%)		citric acid (%)		
			mean	range	mean	range	
Koshinoume	01-Jun-04	5	3.31	3.16–3.53	0.25	0.00–0.5	
	04-Jun-04	5	3.54	3.39–3.67	1.20	0.81–1.45	
	07-Jun-04	5	3.39	3.06–3.61	1.29	0.89–1.66	
	11-Jun-04	5	3.41	3.24–3.58	1.62	1.05–2.00	
	14-Jun-04	5	3.49	3.40–3.58	2.14	1.72–2.69	
	17-Jun-04	5	3.45	3.29–3.70	2.38	2.14–2.91	
	21-Jun-04	5	2.86	2.80–2.92	2.93	2.76–3.21	
	25-Jun-04	5	2.68	2.39–2.87	3.59	3.27–4.11	
	28-Jun-04	5	2.59	2.50–2.73	4.17	4.02–4.67	
	30-Jun-04	5	2.23	2.07–2.50	3.89	3.46–4.41	
	06-Jul-04	5	2.19	2.01–2.37	4.81	4.32–5.17	
	09-Jul-04	7	2.17	2.01–2.34	5.16	4.71–5.45	
	12-Jul-04	7	2.00	1.61–2.40	5.26	4.22–6.08	
	15-Jul-04	10	1.88	1.52–2.17	5.41	5.09–6.06	
	20-Jul-04	10	1.54	1.15–1.90	5.57	4.80–6.06	
	23-Jul-04	5	1.38	1.05–1.79	5.53	4.73–6.57	
	Togoroume	01-Jun-04	5	3.85	3.37–4.32	0.00	0.00–0.00
		04-Jun-04	5	4.26	3.87–4.63	0.37	0.00–0.58
		07-Jun-04	5	4.11	3.92–4.56	0.58	0.34–0.74
		11-Jun-04	5	3.98	3.65–4.12	0.94	0.73–1.21
14-Jun-04		5	4.18	4.01–4.39	1.06	0.81–1.26	
17-Jun-04		5	4.58	4.19–4.89	1.26	0.74–1.71	
21-Jun-04		5	4.14	3.78–4.40	2.05	1.67–2.29	
25-Jun-04		5	3.30	2.93–3.69	2.44	1.95–2.85	
28-Jun-04		5	3.33	3.14–3.54	2.77	2.55–3.04	
30-Jun-04		5	3.09	2.91–3.45	3.01	2.73–3.24	
06-Jul-04		5	3.00	2.64–3.17	3.64	3.33–3.86	
09-Jul-04		7	2.77	2.36–3.38	3.84	3.52–4.18	
12-Jul-04		7	2.24	1.88–2.60	3.81	3.34–4.63	
15-Jul-04		10	2.04	1.32–2.43	4.04	3.47–4.75	
20-Jul-04		7	1.90	1.34–2.27	3.98	2.52–4.62	
Bungoume	01-Jun-04	5	3.45	3.10–3.69	0.06	0.00–0.29	
	04-Jun-04	5	4.21	3.81–4.63	0.00	0.00–0.00	
	07-Jun-04	5	3.98	3.74–4.11	0.19	0.00–0.52	
	11-Jun-04	5	4.15	3.91–4.28	0.05	0.00–0.27	
	14-Jun-04	5	4.07	3.80–4.41	0.20	0.00–0.65	
	17-Jun-04	5	4.27	3.80–4.68	0.40	0.00–0.68	
	21-Jun-04	5	3.82	3.73–4.04	1.50	1.08–1.79	
	25-Jun-04	5	3.38	3.31–3.44	1.94	1.78–2.12	
	28-Jun-04	5	3.16	3.02–3.32	2.22	2.10–2.56	
	30-Jun-04	5	2.66	2.49–3.00	2.21	2.00–2.43	
	06-Jul-04	5	2.23	1.95–2.42	3.17	2.73–3.78	
	09-Jul-04	7	1.89	1.65–2.45	3.62	3.07–4.52	
	12-Jul-04	7	1.43	1.00–1.90	4.15	3.86–4.49	
15-Jul-04	10	1.12	0.67–1.39	3.92	3.22–4.42		
20-Jul-04	10	0.86	0.66–1.12	3.62	3.19–4.04		
23-Jul-04	5	0.74	0.33–0.91	3.11	2.96–3.42		

of organic acid compositions, the Ume fruits were sampled twice a week for approximately 2 months during the growth period, and a total of 314 Ume fruits were collected. After harvesting, the flesh of the fruit samples was removed and the juice was squeezed out for use as the study samples. As shown in **Table 1**, the organic acid compositions of the Ume juice samples showed a very wide range, and the juice samples were considered to be suitable for investigating the potential of the NIR technique as a means of determining the citric and malic acid contents of raw Ume fruit juices.

Reference Analyses. The organic acid (citric and malic acids) components of the Ume fruit juice samples were analyzed by capillary electrophoresis using a UV detector (CAPI-3300; Ootukadenshi, Japan). Separations were performed in an uncoated fused-silica capillary with an effective length of 675 mm and an inner diameter of 75 μ m. An analytical migration liquid containing 20 mM quinolinic acid, 0.25 mM HDTMA, and Tris (pH 6.0) was used. The raw Ume fruit juice samples were centrifuged at 1000 rpm for 10 min, diluted 1:1000 by the addition of distilled water, and then passed through a 0.45- μ m porosity filter.

NIR Spectra. The transmittance (*T*) spectra of the Ume fruit juice samples were measured using a spectrophotometer (NIRSystems 6500; Foss NIRSystems Inc., Silver Spring, MD) and a 1-mm quartz cuvette.

The spectra were measured in the wavelength range from 1100 to 1850 nm at 2-nm intervals and the absorbances were recorded on a linked computer as $\log(1/T)$. The NIR spectrum of each sample was obtained by taking the average of 32 scans. All operations were performed at room temperature (20 °C). The second derivative spectra were obtained by performing a mathematical treatment with a subtraction gap size of 0 and a smoothing segment size of 20 using the NIR spectral analysis software (NSAS) program installed on the spectrophotometer.

Statistical Analysis. The 314 raw Ume juice samples were separated into two groups: 211 samples for calibration and 103 samples for validation. The significant organic acid (citric and malic acids) components of the Ume fruit juice samples selected for the calibration and validation sample sets are shown in **Table 2**. The calibration and validation sample sets showed similar means and standard deviations for the citric and malic acid contents. The Ume juice samples in the calibration set were used to establish the calibration models (multivariate equations) between the spectral data and laboratory reference values, while the Ume juice samples in the validation set were used to evaluate the calibrations.

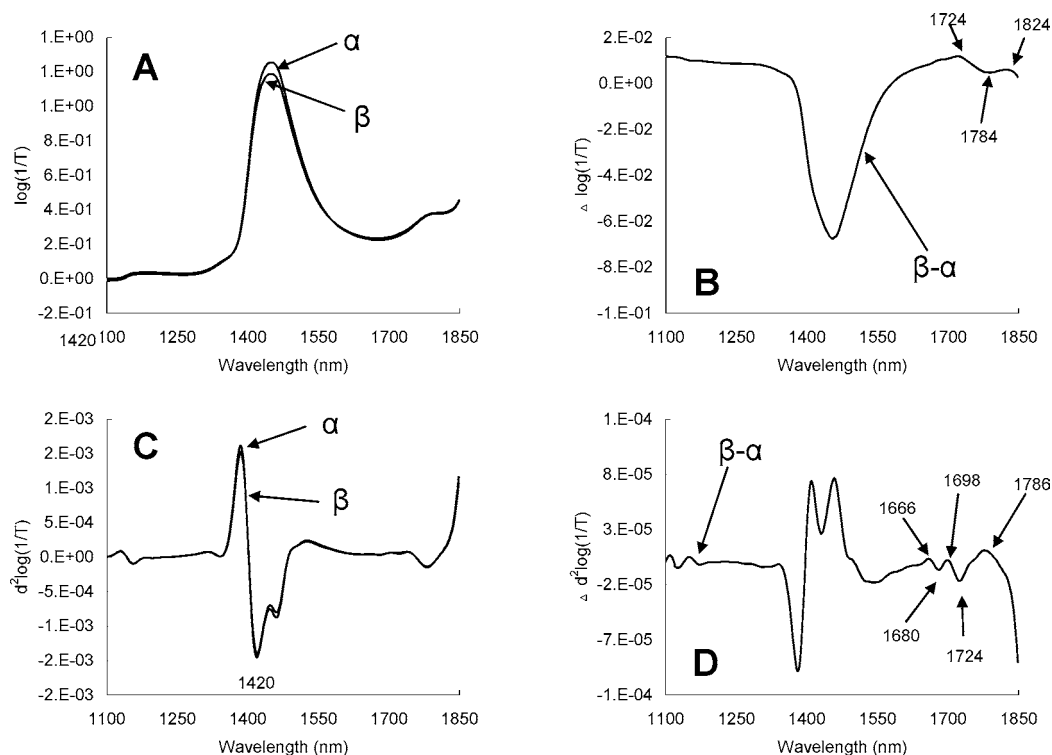


Figure 1. Original spectra and second derivative spectra of α and β samples and their difference spectra ($\beta-\alpha$). α : Raw Ume fruit juice sample containing 3.44% malic acid and 1.72% citric acid. β : Raw Ume fruit juice sample containing 2.00% malic acid and 6.06% citric acid.

Table 2. Mean, Range, and Standard Deviation (SD) of the Organic Acid Contents of the Ume Fruit Juice Samples in the Calibration and Validation Sample Sets

	calibration ($n = 211$)			validation ($n = 103$)		
	mean	range	SD	mean	range	SD
citric acid (%)	3.03	0.00–6.57	1.75	2.99	0.00–6.06	1.72
malic acid (%)	2.65	0.33–4.89	1.08	2.60	0.65–4.64	1.04

The partial least-square (PLS) regression method (22) was used to develop calibrations for determining the organic acid compositions of the raw Ume juice samples. The PLS calibrations were performed with the Unscrambler software (Version 7.6; CAMO AS, Trondheim, Norway), and both the spectral responses and respective reference data were used to determine the latent variables (PLS factors) in the calibration data set. The optimum number of factors for calibration—minimizing overfitting was based on the standard error of cross validation (SECV). The approach used was as follows: 90% of the samples from the calibration set was used for calibration, while the remaining 10% was used to calculate the standard error of prediction (SEP). This operation was carried out 10 times, using a different group for calibration and prediction each time. The SECV was calculated as the square root of the average of the squares of the 10 SEP values. The final calibration equation was developed with all the samples in the calibration set using the number of factors with the lowest SECV, and the standard error of calibration (SEC) was calculated.

The validation set (which did not include any samples from the calibration set) was used to check the performed calibration. The SEP and the correlation coefficient of the reference values versus the NIR values (r^2) were calculated.

RESULTS AND DISCUSSION

NIR Spectra. The original NIR spectra of two raw Ume fruit juice samples (α and β) containing very different organic acid compositions (α : 1.72% citric acid and 3.44% malic acid; β : 6.06% citric acid and 2.00% malic acid) are shown in **Figure 1A**. The two spectra were smooth in the wavelength region of

1100–1850 nm, and a broadband of water, the main component of raw Ume fruit juice, due to the first overtone of O–H stretching was observed around 1450 nm. Since the water band was very large, while the absorption peaks from other components were relatively weak and overlapped each other, spectral features based on the organic acid compositions could not easily be observed, although the two sample juices had very different organic acid compositions. Therefore, a difference spectrum ($\alpha-\beta$) (**Figure 1B**) was obtained to easily observe the spectral differences due to the organic acid compositions. Variation was observed in a wavelength range of 1600–1800 nm as well as around 1450 nm. The variation from 1600 to 1800 nm could be associated with the C–H stretching first overtone and may be related to the organic acid composition of the Ume fruit juice since citric and malic acids have C–H bonds in their chemical structures. These findings were confirmed by observing the second derivative spectra (**Figure 1C**) and their difference spectrum ($\alpha-\beta$) (**Figure 1D**). The bands around 1450 nm associated with the O–H stretching first overtone and the bands at 1660, 1685, 1695, 1725, and 1780 nm associated with the C–H stretching first overtone could be observed more clearly. Taken together, these observations suggest that the NIR spectra of raw Ume fruit juices can provide information about their organic acid compositions, particularly in the wavelength range of 1600–1800 nm.

Development of NIR Calibrations for the Citric and Malic Acid Contents. PLS regressions were performed based on the citric acid content or malic acid content and NIR second derivative spectra (1100–1850 nm) for the calibration sample sets. **Figure 2** shows the values indicating the performance of the calibration models, such as the SEC and SECV. As the number of factors included in the calibration model increased, the SEC decreased. Furthermore, the SECV decreased from an initial value of about 1.34% to about 0.30% with 10 factors and then either remained unchanged or increased very slowly. Therefore, the PLS calibration model with 10 factors was

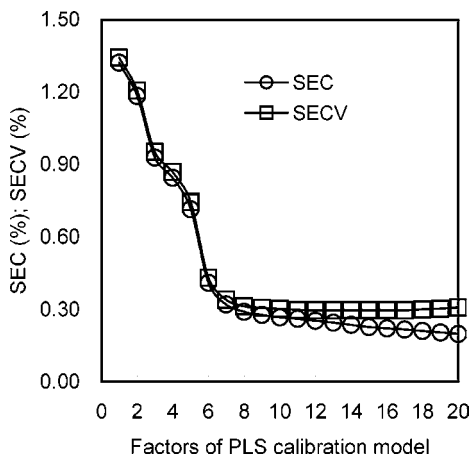


Figure 2. SEC and SECV of PLS regression for the citric acid contents of raw Ume fruit juices based on second derivative spectra (1100–1850 nm).

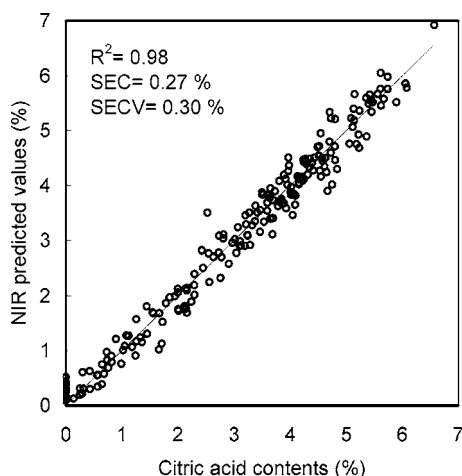


Figure 3. Scatter plots of citric acid contents versus the predicted values based on the calibration sample sets.

selected. The calibration results were represented graphically by plotting the reference citric acid contents versus the predicted values based on the NIR second derivative spectra (**Figure 3**). The plots showed a strong linearity. The obtained NIR calibration model showed a high degree of accuracy in predicting the citric acid contents of raw Ume fruit juices, with an R^2 of 0.98 and an SEC of 0.27%.

Figure 4 shows the performance (SEC and SECV) of the calibration model for the malic acid content. Similar to the case for the citric acid content, as the number of factors included in the calibration model increased, the SEC decreased, while the SECV decreased from an initial value of about 1.01% to about 0.24% with 11 factors and then remained unchanged or increased very slowly. Therefore, the PLS calibration model with 11 factors was selected. The calibration results are shown in **Figure 5**. Similar to the results for the citric acid content, the plots showed a strong linearity, as well as a high accuracy in predicting malic acid contents of raw Ume fruit juices, with an R^2 of 0.96 and an SEC of 0.21%.

Discussion of the NIR Calibration Models. Regression coefficients can be used to discuss the contributions of individual wavelengths to a PLS calibration model since a regression coefficient spectrum shows characteristic peaks and troughs that can indicate which wavelength range is important for the calibration model (22, 23).

Figures 6 and 7 show the regression coefficients of the PLS calibration models of the citric and malic acid contents,

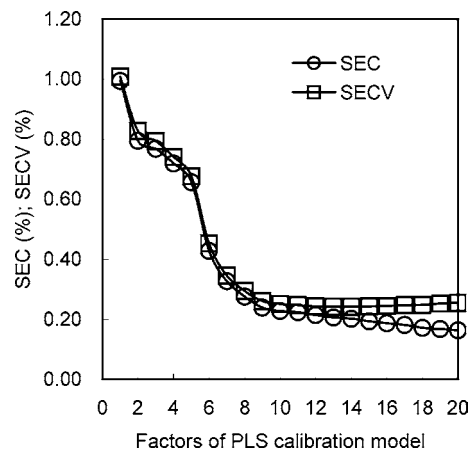


Figure 4. SEC and SECV of PLS regression for the malic acid contents of raw Ume fruit juices based on second derivative spectra (1100–1850 nm).

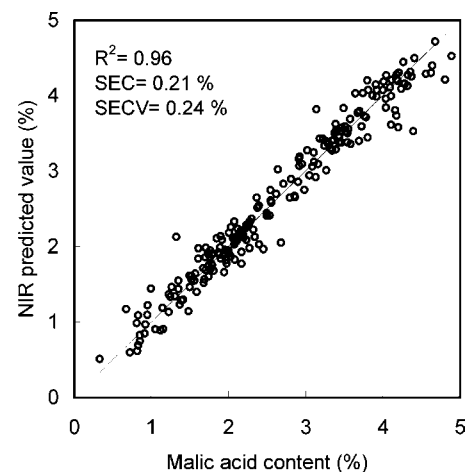


Figure 5. Scatter plots of malic acid contents versus the predicted values based on the calibration sample sets.

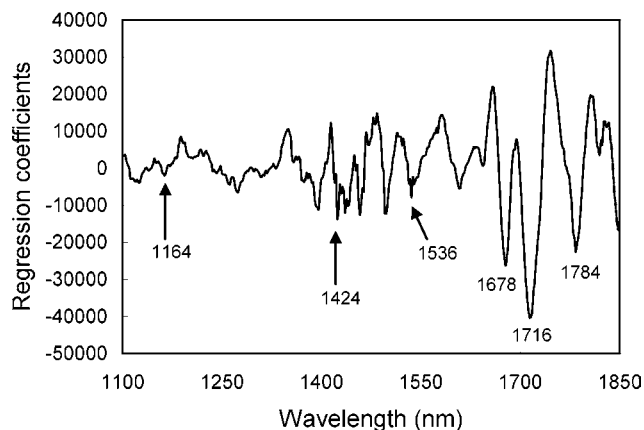


Figure 6. Regression coefficients in the PLS calibration model based on second derivative spectra (1100–1850 nm) for the citric acid contents of raw Ume fruit juices.

respectively. The regression coefficient spectra showed many remarkable peaks, especially in the wavelength range of 1600–1800 nm. However, before these peaks are examined for their contributions to the organic acid absorption, we should first discuss the absorption of aqueous citric acid and malic acid solutions.

Figure 8A shows the second derivative spectra of aqueous solutions of 16% citric acid or malic acid. Characteristic

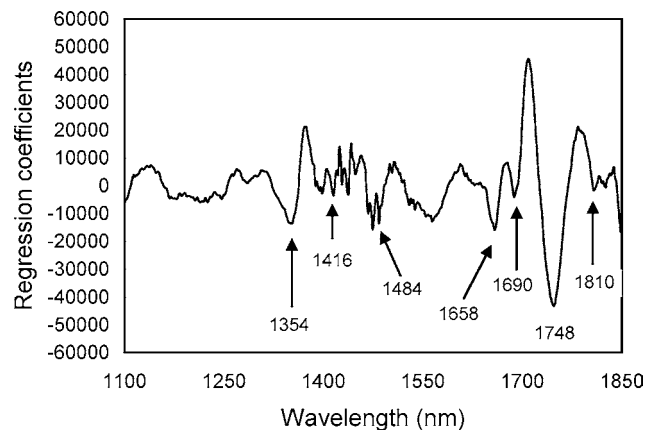


Figure 7. Regression coefficients in the PLS calibration model based on second derivative spectra (1100–1850 nm) for the malic acid contents of raw Ume fruit juices.

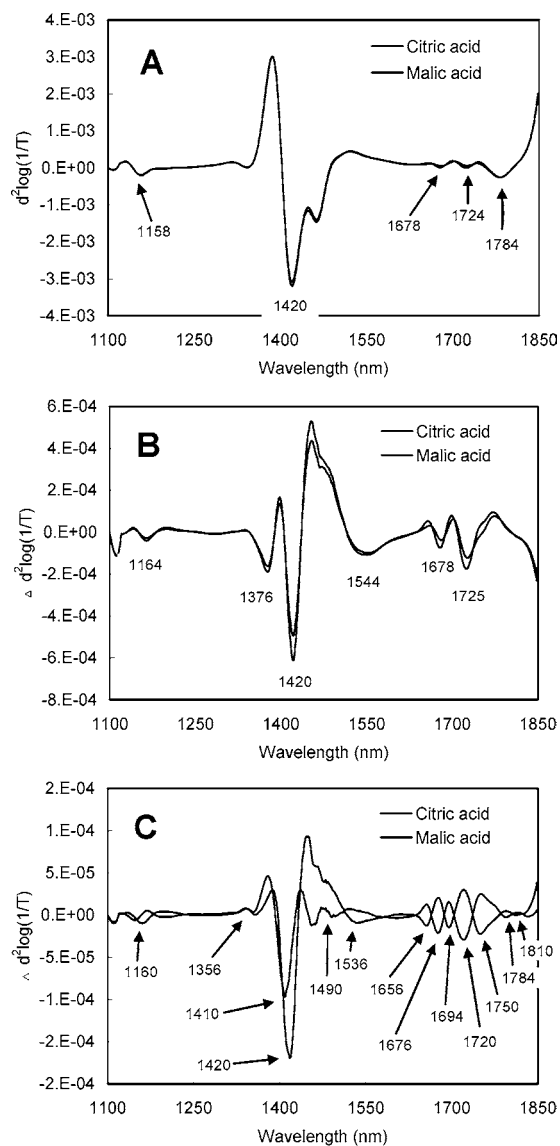


Figure 8. Second derivative spectra and difference spectra of aqueous solutions of standard citric and malic acid reagents. (A) Second derivative spectra (aqueous solutions of 16% citric acid or malic acid). (B) Difference spectra (aqueous solution of 16% citric acid or malic acid – distilled water). (C) Difference spectra (aqueous solution of 16% citric acid – aqueous solution of 8% citric acid and 8% malic acid, and aqueous solution of 16% malic acid – aqueous solution of 8% citric acid and 8% malic acid).

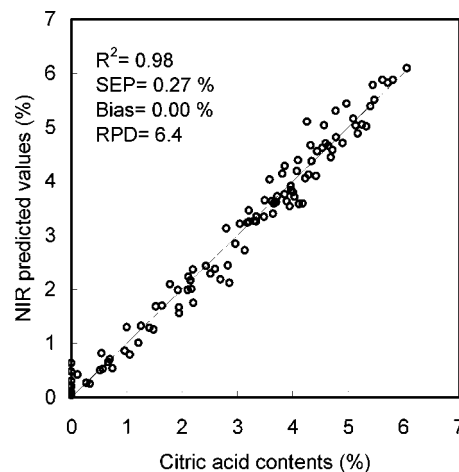


Figure 9. Scatter plots of citric acid contents versus the predicted values based on the validation sample sets.

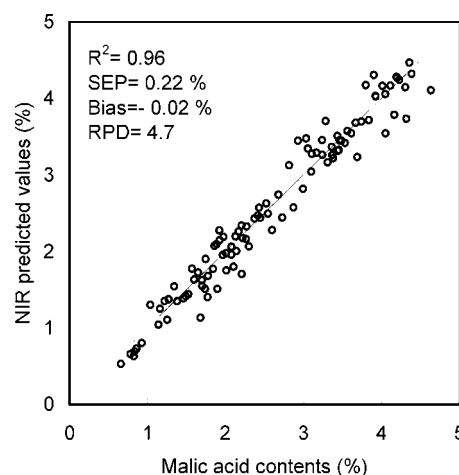


Figure 10. Scatter plots of malic acid contents versus the predicted values based on the validation sample sets.

absorption peaks at wavelengths of 1678 and 1724 nm for citric acid and malic acid were observed in comparison with the second derivative spectrum of water. These findings were clearly confirmed by observing the difference spectra based on water (**Figure 8B**). However, differences between citric acid and malic acid were difficult to observe. Therefore, difference spectra based on the aqueous citric and malic acid solutions (**Figure 8C**) were obtained. As a result, remarkable peaks at 1676, 1720, and 1784 nm were clearly observed for citric acid, while remarkable peaks at 1656, 1694, 1750, and 1810 nm were clearly observed for malic acid.

The remarkable peaks at 1678, 1716, and 1784 nm in the regression coefficient spectrum in **Figure 6** could be correlated to the absorption peaks of citric acid at 1676, 1720, and 1784 nm in **Figure 8C**, respectively, while the remarkable peaks at 1658, 1690, 1748, and 1810 nm in the regression coefficient spectrum in **Figure 7** could be correlated to the absorption peaks of malic acid at 1656, 1694, 1750, and 1810 nm in **Figure 8C**, respectively. Structural evaluations and infrared spectra suggested that these bands were likely to be due to C–H absorption with the stretching first overtone. Taken together, these results suggest that the PLS calibration models for the citric and malic acid contents of raw Ume fruit juices were established based on the absorptions of citric and malic acids.

NIR Validations. To test the validity of the calibration models, other independent validation samples (not included in

the calibration samples) were prepared as shown in **Table 2**. When the calibration models were used to predict the independent validation samples, good validation results were obtained. The validation results for the citric acid content are shown in **Figure 9**. An r^2 of 0.98 and SEV of 0.27%, very similar to the calibration results, were obtained under the condition of a very small bias (close to 0.00%). As result of a t-test, the bias was not thought to be significant ($p < 0.05$). As an index for judging the usefulness of the measurement accuracy of the calibration model, the ratio of the standard deviation of the reference data in the prediction sample set to the SEP (RPD) is usually utilized (24). An RPD value of 2.5–3.0 is regarded as adequate for rough screening, while a value above 3.0 is regarded as satisfactory for screening. In our case, an RPD value of 6.4 was obtained for the predication of the citric acid content, and the calibration model can therefore be considered to show suitable accuracy for measuring the citric acid contents of raw Ume fruit juices.

The validation results for the malic acid content are shown in **Figure 10**. An r^2 of 0.96, SEV of 0.22% and RPD of 4.7 were obtained under the condition of a small bias of 0.02%, which was not thought to be significant ($p < 0.05$). These results are very good, and the calibration model can therefore be considered to show suitable accuracy for measuring the malic acid contents of raw Ume fruit juices.

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Received for review May 24, 2006. Revised manuscript received November 1, 2006. Accepted November 5, 2006.

JF061461S