

Detection of Sugar Adulterants in Apple Juice Using Fourier Transform Infrared Spectroscopy and Chemometrics

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Fourier transform infrared spectroscopy and attenuated total reflection sampling have been used to detect adulteration of single strength apple juice samples. The sample set comprised 224 authentic apple juices and 480 adulterated samples. Adulterants used included partially inverted cane syrup (PICS), beet sucrose (BS), high fructose corn syrup (HFCS), and a synthetic solution of fructose, glucose, and sucrose (FGS). Adulteration was carried out on individual apple juice samples at levels of 10, 20, 30, and 40% w/w. Spectral data were compressed by principal component analysis and analyzed using *k*-nearest neighbors and partial least squares regression techniques. Prediction results for the best classification models achieved an overall (authentic plus adulterated) correct classification rate of 96.5, 93.9, 92.2, and 82.4% for PICS, BS, HFCS, and FGS adulterants, respectively. This method shows promise as a rapid screening technique for the detection of a broad range of potential adulterants in apple juice.

KEYWORDS: Adulteration; ATR, authenticity; FTIR, apple juice; chemometrics

INTRODUCTION

Determining the authenticity of food is becoming more difficult. Criminal investigations of juice adulteration have shown that, as analytical capabilities have improved, adulteration practices have become more sophisticated (1, 2). It is possible for unethical firms to gain a market advantage over honest competitors and to defraud the consumer through the intentional adulteration of any juice drink. The primary advantage is the cost saving the manufacturer can realize by extending or replacing a product with ingredients of lesser value. The most common adulteration methods for fruit juice include dilution with water, addition of sugars [cane and beet sucrose (BS), invert or medium invert syrup, high fructose corn syrup (HFCS), and hydrolyzed inulin syrup], addition of pulpwash solids, or addition of a less expensive fruit juice (2). Adulteration of fruit juice is likely to remain a problem while the price of sugar and syrups is significantly cheaper than the juice itself. The consequences of misrepresentation and adulteration for financial gain cannot be ignored, as these practices may lead to the production of food that is harmful, with implications for nutrition and safety. An extreme instance of this was the Toxic Oil Syndrome epidemic in Spain in 1981, which arose following consumption of oil fraudulently sold as pure olive oil (3).

Detecting adulteration of foods rich in carbohydrates, such as apple juice, is particularly difficult because of the variety of commercial sweeteners available that match the concentration profiles of the major carbohydrates in those foods. A second significant challenge in the detection of adulterated apple juice

is the natural variation in authentic samples, a result of differences in species, maturity, climate, growing regions, seasons, processing, and storage conditions. Ranges in component compositions can be used to flag suspicious samples. Carbohydrates account for >98% of the total soluble solids in apple juice; fructose, glucose, and sucrose are the main carbohydrates with an approximate ratio of 6:3:2 and ranges from 5 to 8, 1 to 4, and 0 to 5% w/w, respectively (1). Three commercially available sweeteners that approximate the carbohydrate composition of apple juice are fully inverted beet/cane sugar, HFCS, and hydrolyzed inulin syrup.

Plants use either the Calvin (C₃) or the Hatch–Slack (C₄) pathway for photosynthetic CO₂ fixation. These separate pathways produce differences in the ¹³C/¹²C ratio of organic carbon in plants produced by one pathway over another. Thus, C₃-derived sugars in apple juice contain less of the ¹³C isotope than sugars from plants that follow the C₄ pathway, such as cane and corn sugars (4). Therefore, carbon isotope ratio analysis has been used to detect the addition of cane and corn sugars to fruit juices (5). However, 10–20% adulteration could be hidden within the wide natural range seen in the ¹³C ratios of apple juice sugars. The sensitivity of this approach can be improved by a factor of 2 by measuring the ¹³C isotope ratios of the individual sugars or of the pulp in cloudy juices (6). These values are then used as an internal standard to reduce the acceptable range of values for the juice. Sugars derived from C₃ plants, such as beet sugars and hydrolyzed inulin syrups, cannot be detected by this technique.

Chromatographic techniques, such as high-performance liquid chromatography (HPLC) and gas chromatography (GC), have been successfully used to determine authenticity in fruit juices by oligosaccharide profiling (7–11). This approach is based

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on the presence of fingerprint oligosaccharides in an adulterant that are either absent or present in very low concentrations in authentic samples. Methods have been developed for HFCS, invert syrups, and hydrolyzed inulin syrup with detection levels typically in the region of 5% w/w (10). However, as no single test on its own is sufficient to cover all types of misrepresentation, multiple tests are always recommended.

Spectroscopic approaches that consider the entire sample composition, for example, nuclear magnetic resonance (NMR) and infrared spectroscopy, have previously been applied to a range of authenticity problems and food composition profiling (12–15). Chemometric methods are applied to reduce the dimensionality of the resulting data collections and to extract useful quantitative information from the complex spectra. In contrast to the time-consuming chromatographic separation and carbon isotope ratio analysis techniques, these spectroscopic procedures can be performed quickly. Multiple spectra can be processed to reduce the signal-to-noise ratio, further improving the spectral information content.

Absorption bands in the midinfrared (MIR) spectrum are characteristic of the bonds and functional groups of a molecule. These bands involve many of the general stretching, bending, and wagging motions available to the molecule, and the overall spectrum may act as a fingerprint for a given compound or compounds. Thus, fingerprints of authentic juices may be considered to represent their overall chemical composition and therefore have the potential to detect adulteration. This method of detection possesses various benefits as an authenticity screening tool; it is extremely fast (tests can be carried out in 1–2 min), simple to use, and may be implemented by unskilled personnel. A large number of potential adulterants may be searched for in a single test; no sample preparation is required, and no waste material is produced during a test. From a regulatory perspective, it has the additional benefit of not destroying the sample under test.

In the work reported in this paper, the capabilities and limitations of MIR spectroscopy for detection of adulteration in single strength apple juice have been examined using a range of likely potential adulterants. These were HFCS, partially inverted cane syrup (PICS), BS, and a mixture of fructose, glucose, and sucrose in solution.

MATERIALS AND METHODS

Samples. Apples were gathered from orchards throughout the island of Ireland during the 2002 ($n = 69$) and 2003 ($n = 155$) harvest seasons (total $n = 224$). Nineteen apple varieties were included, i.e., Braeburn ($n = 2$), Bramley ($n = 50$), Cox ($n = 8$), Elstar ($n = 30$), Fiesta ($n = 11$), Gala ($n = 5$), Golden Delicious ($n = 20$), Granny Smith ($n = 1$), Howgate Wonder ($n = 1$), Idared ($n = 11$), Ingrid Marie ($n = 1$), Jonagold ($n = 32$), Jonagored ($n = 22$), Jupiter ($n = 3$), Karmijn de Sonne Ville ($n = 7$), Lord Lambourne ($n = 1$), Pinova ($n = 1$), Red Prince ($n = 3$), Redwood Elstar ($n = 1$), and unknown samples ($n = 14$). Apple juice was extracted from the fruit using a L'equip model 110.5 centrifugal juicer. Some randomly chosen whole fruit samples ($n = 142$) were held in cold storage (4 °C) for 3 months before juicing, and the remaining samples ($n = 82$) were juiced on arrival in the laboratory. A total of 224 unfiltered apple juice samples were thus produced and placed in frozen storage (−20 °C) on the day of juicing. Amylum UK provided HFCS (Isosweet 111). Fructose, glucose, and sucrose (Analar Grade) were obtained from Merck. PICS (Golden Syrup; Tate and Lyle plc) and BS (Irish Sugar plc) were purchased from local supermarkets. The ratios of fructose, glucose, and sucrose for each of the four adulterant solutions FGS, HFCS, PICS, and BS were 60:25:15, 45:55:0, 32:32:36, and 0:0:100, respectively. Before adulteration of authentic apple juice samples, each adulterant solution was diluted with distilled water to 12° Brix, i.e., a typical apple juice

soluble solids content. In the case of HFCS and sugar mixture adulterants (FGS), levels of 10, 20, 30, and 40% w/w adulteration were used. A total of 150 samples of authentic apple juice were adulterated, each at one level only. The total number of samples studied for each of these two adulterants was 374, i.e., 224 plus 150. In the case of the PICS and BS adulterants, 30 samples of authentic apple juice were adulterated at levels of 10, 20, and 30% w/w, thus producing 90 adulterated samples. Therefore, the total number of samples studied in the case of these two adulterants was 314, i.e., 224 plus 90. Brix values were measured by refractometry using an Abbé model 2WA benchtop refractometer; for the authentic apple juices, values ranged between 8 and 17°.

Instrumentation. MIR spectra were collected at room temperature on a BIO-RAD Excalibur series FTS 3000 spectrometer (Analytica Ltd., Dublin, Ireland); instrument control and spectral collection were performed using WIN-IR Pro (v 3.0) software supplied by the equipment manufacturer. Spectra were recorded on an in-compartment benchmark attenuated total reflectance (ATR) trough top plate using a 45° Ge crystal with 11 internal reflections. Twenty scans were coadded at a nominal resolution of 4 cm^{-1} . Single beam spectra of the samples were collected and ratioed against a background of air. Prior to data analysis, spectra were truncated to the useful range of the Ge ATR crystal (800–4000 cm^{-1}). Samples were applied to the ATR crystal to give total crystal coverage; the crystal was cleaned between samples with tepid water and dried with lens cleaning tissue. The spectral baseline recorded by the spectrometer was examined visually to ensure that no residue from the previous sample was retained on the crystal. All spectra were recorded in duplicate at room temperature (20–25 °C) without thermostatic control. All juice samples were defrosted and allowed to equilibrate to room temperature prior to analysis.

Data Processing. The means of duplicate spectra were used for statistical analysis. Spectra were exported from WIN-IR Pro as GRAMS files (ThermoGalactic, Salem, NH) and imported directly into The Unscrambler (v7.6; CAMO ASA, Norway). Models were developed using the spectral region between 880 and 1850 cm^{-1} , which is dominated by information on sugar composition. First, each spectrum was reduced to 16 score values to reduce the size of the data set and shorten analysis time. This was achieved by performing two independent principal component analyses (PCAs); the first was run on raw data using full cross-validation and variable weights of 1.0 while the second was run on first derivative spectra (seven points, Savitsky-Golay) using full cross-validation and variable weights of 1/standard deviation. Following examination of the residual variance after each PCA, components 1–8 were selected as the optimum to describe the data set variance in each case. Therefore, the first eight scores from each analysis were combined and used in all of the following discriminant and quantitative analyses.

Partial least squares (PLS) regression onto a dummy variable (discriminant PLS) was used for discrimination between the authentic and the adulterated apple juice samples; the dummy variable was assigned a value of −1 for an authentic apple juice and +1 for an adulterated juice. For each adulterant, samples were divided into two sets, A and B. Both sets contained the same number of authentic apple juices and an equal number of adulterated samples. Initially, a calibration was developed on set A and evaluated on set B. Afterward, a calibration was developed on set B and evaluated on set A. The results of each set were then combined. The analysis was carried out in this manner for all four adulterants. In this way, the number of prediction results obtained for authentic apple juice samples, apple juice samples adulterated with FGS, HFCS, PICS, and BS are 224, 150, 150, 90, and 90, respectively. A cutoff value equal to 0 was chosen to determine class identity in the discriminant PLS predictions.

For quantitative prediction of adulterant content, classical PLS regression was applied to the PCA scores using the same sample sets as before for each adulterant. Full cross-validation and variable weights of 1/standard deviation were used in model development. In all cases, only optimal models are discussed in this paper. These models were then used to classify the prediction sample set; samples with predicted adulterant contents greater than twice the standard error of prediction (SEP) were deemed to be adulterated.

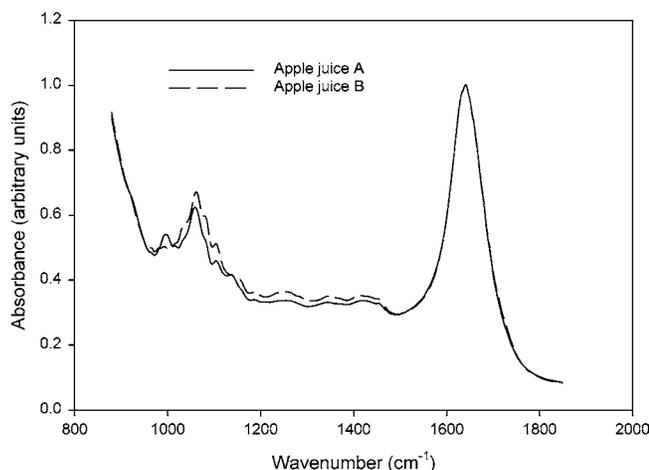


Figure 1. FTIR spectra of two randomly selected authentic apple juice samples.

Classification was also attempted by the *k*-nearest neighbor (*k*NN) method using Pirouette software (v3.10; Infometrix Inc., WA). This supervised classification method identifies an unknown sample on the basis of the identity of a predefined number of neighboring samples of known sample type, which were modeled in a calibration development step. The technique is based on the assumption that the closer samples lie in measurement space, the more likely they are to belong to the same category. The value of *k* is determined empirically during calibration, and a majority rule is applied in predictions: An unknown is classified in the group to which the majority of its *k* neighbors belong. *k*NN is well-suited to data sets with small sample numbers and can function even with only one calibration set sample per category. It is, however, sensitive to gross inequalities in the number of samples in each class (16) thereby necessitating equal sample numbers of authentic and adulterated juices during calibration. Samples were classified into two groups, authentic and adulterated, with calibration sample sets containing equal numbers of authentic and adulterated samples. Thus, 75 samples of each type (authentic and adulterated) were used in model development for the adulterants HFCS and FGS while 45 samples of each type were used in calibrations for the adulterants PICS and BS. Calibrations were developed on two sample sets A and B each containing different samples and structured as described in the preceding line; all of the samples not used in the calibration sample set were used in the prediction sample set. The results of the two prediction sets were then combined. In this manner, the total number of sample results for authentic juices and juices adulterated with FGS or HFCS is 298, 150, and 150, respectively, and for authentic juices and juices adulterated with PICS or BS, values of 358, 90, and 90, respectively, were achieved.

RESULTS AND DISCUSSION

Fourier transform infrared (FTIR) spectra of two randomly selected apple juice samples are shown in **Figure 1**. The spectrum of apple juice is dominated by water and sugar absorptions; bands appearing between 1150 and 1470 cm^{-1} are attributed to bending modes of C–C–H, C–O–H, and O–C–H groups (17), while more intense peaks in the region between 900 and 1150 cm^{-1} arise mainly from C–O and C–C stretching modes, with a peak around 1020–1060 cm^{-1} due to O–H vibrations (18). At lower energies, bands due to C–H and O–H bending vibrations are also useful for discrimination and quantification purposes. At 1725 cm^{-1} , absorption from organic acids (C=O stretch) appears as a shoulder on the large water absorption band at 1641 cm^{-1} .

The spectra shown in **Figure 1** reveal significant differences between the two juice samples. These are due to variations in the chemical composition between samples, particularly relating to water, fructose, glucose, and sucrose. The concentration of

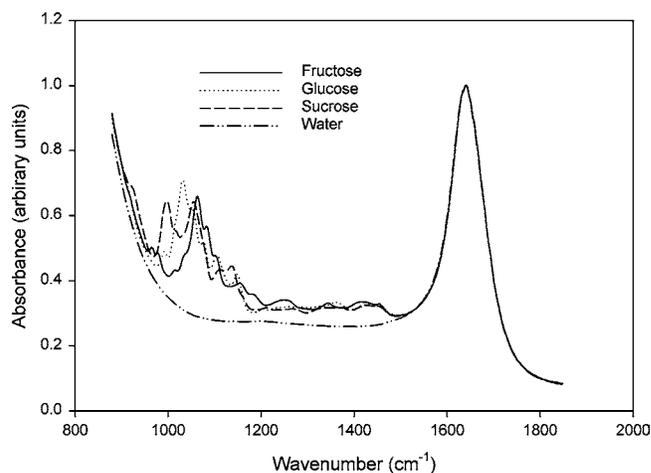


Figure 2. FTIR spectra of fructose, glucose, sucrose, and water.

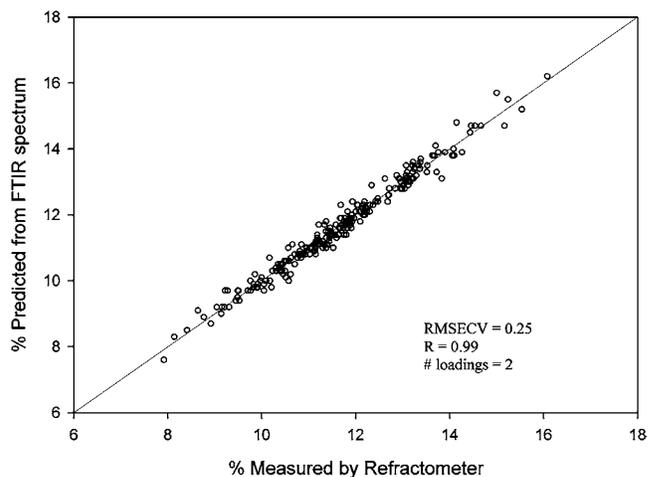


Figure 3. Regression plot of Brix values predicted by FTIR spectroscopy vs values measured by refractometry.

each of these components in the two juice samples was estimated from their spectra using predictive models developed from spectra of 64 synthetic sugar solutions comprising these four chemical species (water, fructose, glucose, and sucrose) in concentrations typical of those found in apple juice, i.e., water (8–16% w/w), fructose (4–10% w/w), glucose (1–5% w/w), and sucrose (0–5% w/w). Predicted values of 14.5, 9.5, 2.5, and 2.5% w/w and 12.5, 5.9, 0.7, and 5.9% w/w were obtained for water, fructose, glucose, and sucrose in juices A and B respectively, illustrating the large natural variability of these components in apple juice. Spectra of the major components of apple juice (water, fructose, glucose, and sucrose) are shown in **Figure 2**. Given the differences observed between these spectra, it is not surprising that FTIR spectroscopy can be used for accurate determination of the sugar and water composition of mixtures and syrups (19–21). For instance, in this study, the Brix values for all 224 authentic apple juice samples were predicted accurately (SEP = 0.25; range = 8–17°) from their MIR spectra by PLS regression. Reference values were measured by refractometry, and the linear regression of predicted vs measured Brix values is shown graphically in **Figure 3**.

Spectra of the adulterant solutions are shown in **Figure 4**. Because of the similarity of these spectra to those of authentic apple juices, chemometric techniques are required to distinguish between spectra of authentic juice samples and those of juices adulterated with these syrups.

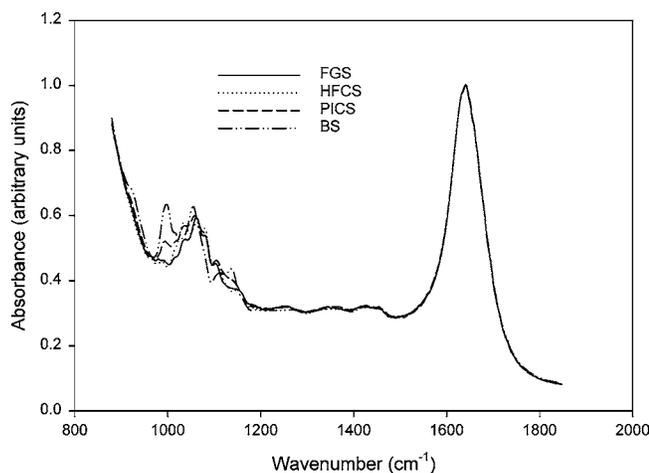


Figure 4. FTIR spectra of the four adulterant solutions used (FGS = fructose glucose sucrose mixture).

Table 1. Percentage Correct Classification of Prediction Samples Using Discriminant PLS and *k*NN Analysis to Detect PICS in Apple Juice

	PLS	<i>k</i> NN
authentic	96.0	95.3
adulterated	97.8	91.1
10% adulteration	93.3	76.7
20% adulteration	100	100
30% adulteration	100	96.7
overall	96.5	94.4

PICS. A summary of the prediction results obtained for authentic apple juice samples and samples adulterated with PICS is shown in **Table 1**. Results for the adulterated sample sets are further broken down in the table to show the percentage of correctly identified samples at each level of adulteration. The best results are obtained using PLS discrimination. An overall correct classification rate of 96.5% was achieved; 96% of the authentic juices and 97.8% of the adulterated samples were classified correctly. Those adulterated samples that were incorrectly classified were all adulterated at the lowest adulteration level, i.e., 10% w/w, although even at this level of adulteration, 93.3% of samples were classified correctly. The separation of samples in two dimensions following PLS modeling is shown in **Figure 5** in which a clear trend of increasing adulterant content is apparent in moving from the top right to the lower left regions of the plot. Examination of the regression coefficients in the PLS discriminant model revealed that the third and fifth variables are the most important in distinguishing between pure apple juice and those adulterated with PICS; these variables correspond to the third and fifth scores in the PCA of the raw spectral data. Some selected loadings from this PCA are shown in **Figure 6**. The third loading has troughs at 1723, 1300–1190, and 1064 cm^{-1} , which correspond to areas in the spectrum where organic acids and fructose absorb strongly. In the fifth loading, a large negative peak at 1064 cm^{-1} and a maximum at 1033 cm^{-1} correspond to the peak maxima of a fructose and a glucose spectrum, respectively. Therefore, discrimination in this case depends largely on changes in the concentration of acids and the ratio of fructose to glucose caused by the addition of PICS. Addition of PICS is expected to lower the acid concentration simply by dilution. A reduction in the ratio of fructose to glucose will also occur since the ratio in this adulterant is equal to 1.0 while apple juice samples have a value of at least 1.6 (*I*).

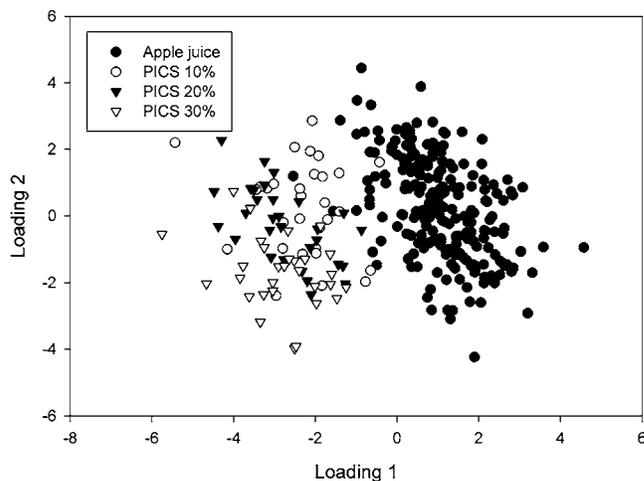


Figure 5. PLS scores plot of authentic apple juice and apple juice adulterated with PICS.

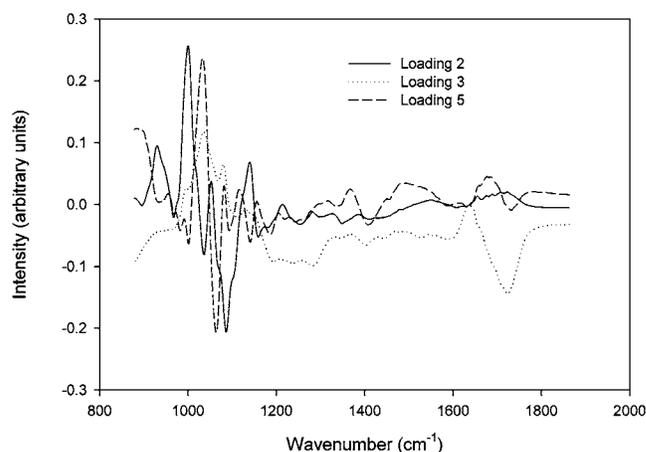


Figure 6. Selected loadings from a PCA of raw spectral data of authentic apple juice and apple juice adulterated at various levels with PICS.

Table 2. Percentage Correct Classification of Prediction Samples Using Discriminant PLS and *k*NN Analysis to Detect BS in Apple Juice

	PLS	<i>k</i> NN
authentic	94.6	91.6
adulterated	92.2	95.6
10% adulteration	80.0	86.7
20% adulteration	96.7	100
30% adulteration	100	100
overall	93.9	92.4

The application of *k*NN gave similar results, with an overall correct classification rate of 94.4% being achieved. Of the adulterated samples, 91.1% were classified correctly. As with the discriminant PLS model, the majority of misclassified samples arise from samples adulterated at a level of 10% w/w although this model identified these samples with less accuracy than the PLS technique (76.7 vs 93.3%).

BS. The addition of BS to apple juice samples was investigated using the same chemometric procedures as those reported above; the results are summarized in **Table 2**. Overall correct classification rates of 93.9 and 92.4% were achieved with PLS regression and *k*NN analysis, respectively. Differences observed between the results of these two procedures are due to the compromise between the number of false positive and false negative results, which is directly related to the choice of cut off point in the PLS analysis. Results for the adulterated sample

Table 3. Percentage Correct Classification of Prediction Samples Using Discriminant PLS and *k*NN Analysis to Detect HFCS in Apple Juice

	PLS	<i>k</i> NN
authentic	94.2	87.9
adulterated	89.3	84.7
10% adulteration	61.0	53.7
20% adulteration	100	88.2
30% adulteration	100	100
40% adulteration	100	100
overall	92.2	86.8

Table 4. Percentage Correct Classification of Prediction Samples Using Discriminant PLS and *k*NN Analysis to Detect a Fructose, Glucose, and Sucrose Solution in Apple Juice

	PLS	<i>k</i> NN
authentic	89.3	67.1
adulterated	72.0	87.3
10% adulteration	48.8	78.0
20% adulteration	47.1	76.5
30% adulteration	95.1	97.6
40% adulteration	97.1	97.1
overall	82.4	73.9

sets are further broken down in the table to show the percentage of correctly identified samples at each level of adulteration. The majority of misclassified adulterated samples involve adulteration at a level of 10% w/w. The most important variable in the PLS discriminant analysis corresponds to loading 2 in **Figure 6**. The four positively correlated peaks in this loading correspond to the four largest absorption bands in the sucrose spectrum at 8770, 9490, 10005, and 10750 cm^{-1} . Therefore, the concentration of sucrose in a sample is the most important discriminant variable for the detection of added BS. This result is not surprising as the adulterant is also sucrose.

HFCS. In the case of adulteration with HFCS, detection results are summarized in **Table 3**. This adulterant is expected to be more difficult to detect, as its chemical composition closely resembles that of a typical apple juice sample. However, because of the large range of naturally occurring concentrations of the major sugars in authentic apple juices, detection of BS or PICS is only slightly better. Discriminant PLS analysis again produces the better results, with an overall correct classification rate of 92.2 as compared to 86.8% for *k*NN analysis. Only samples adulterated at levels of 10% produce classification errors with PLS analysis. For quantitative prediction of HFCS content, the standard error of cross-validation (RMSECV) is 4.6%, producing a value of 9.1% for the 95% confidence band. The regression coefficients in the PLS analysis indicated that the fifth loading from the PCA on the raw data is important for separating authentic and adulterated samples. The trough at 1064 cm^{-1} and the peak at 1033 cm^{-1} correspond to the maximum absorbance of fructose and glucose, respectively. Therefore, this loading describes the fructose/glucose ratio and is also important for identifying the adulterant PICS. HFCS has a fructose/glucose ratio of 0.82, lower than that of a pure apple juice that typically has a value >1.6 (*I*).

Fructose, Glucose, and Sucrose Mixture. This completely synthetic mixture of sugars proved to be the most difficult adulterant to detect in apple juice using FTIR spectra and chemometrics. The results obtained are listed in **Table 4**. At all levels of adulteration, even as high as 40%, some adulterated samples were misclassified. Discriminant PLS analysis produced the better results, with an overall correct classification rate of

Table 5. Statistical Descriptors for Linear Regressions of Predicted vs Actual Sugar Adulterants in Apple Juice

adulterant	correlation coefficient	RMSECV ^a	slope of regression line	intercept of regression line
PICS	0.89	4.9	0.80	1.28
BS	0.90	4.6	0.80	1.13
HFCS	0.94	4.6	0.90	0.98
FGS	0.76	9.5	0.58	3.92

^a Root-mean-square error of cross-validation.

82.4%; 89.3% of the authentic apple juice samples and 72% of adulterated samples were identified correctly. The regression coefficients identified loadings 7 and 5 to be important. The seventh loading is presumably identifying minor components present in apple juices that are absent in the synthetic adulterant. The fifth loading is related to the fructose/glucose ratio with a large trough at 1064 cm^{-1} and a peak maximum at 1033 cm^{-1} . For the FGS adulterant, the fructose/glucose ratio is 2.4, which is an acceptable value for an apple juice. Therefore, as the results suggest, this loading is unlikely to discriminate between authentic and adulterated samples very well. The results from PLS and *k*NN analysis with FGS (**Table 4**) appear to produce similar or worse results for 20% as compared to 10% levels of adulteration and also for 40% as compared to 30% adulteration levels, although a gradual improvement with increased level of adulteration might be expected. This apparently anomalous result is due to the subsets used in the production of adulterated samples. Samples adulterated at levels of 10 and 30% w/w involved juices prepared from apples that had been stored for 3 months; samples adulterated at levels of 20 and 40% w/w were prepared from juices made from apples that had been juiced on arrival in the laboratory and also from apples that were stored for 3 months. This added variability in the samples adulterated at levels of 20 and 40% w/w has reduced the accuracy of predictions as compared to those of samples adulterated at levels of 10 and 30% w/w.

Prediction of Adulterant Content. Classical PLS regression analysis was applied to the 16 principal component scores calculated for each group of sample spectra to predict the percentage of each type of adulterant present. A summary of the results obtained is shown in **Table 5**. The model developed for PICS adulterant produced a root-mean-square error of cross-validation (RMSECV) value of 4.9% with a correlation coefficient equal to 0.89. The 95% confidence level for the prediction error associated with this model is $\pm 9.7\%$ adulteration (i.e., $\pm 1.98 \times \text{RMSECV}$). Similar prediction accuracies were obtained for BS and HFCS adulterants; this procedure was not able to effectively quantify adulteration by FGS solution as revealed by the values of the associated RMSECV, slope, and intercept (9.5, 0.58, and 3.92, respectively).

Conclusion. This work has shown that the application of MIR spectroscopy and chemometrics can be used to distinguish infrared spectra of regular apple juice samples from those of adulterated juices. The success of this technique depends largely on analysis of the concentrations and ratios of the major chemical components of the apple juice sample. Because of this, it is sensitive to a broad range of sugars and syrups and will complement more sensitive techniques that are used to identify specific adulterants.

ABBREVIATIONS USED

ATR, attenuated total reflectance; BS, beet sucrose; FTIR, Fourier transform infrared; GC, gas chromatography; HFCS,

high fructose corn syrup; HPLC, high-performance liquid chromatography; *k*NN, *k*-nearest neighbors; MIR, midinfrared; NMR, nuclear magnetic resonance; PCA, principal component analysis; PICS, partially inverted cane syrup; PLS, partial least squares; SEP, standard error of prediction.

ACKNOWLEDGMENT

We acknowledge local fruit producers for supplying apple samples.

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Received for review November 30, 2004. Revised manuscript received February 10, 2005. Accepted February 22, 2005. We acknowledge the Irish Department of Agriculture and Food (FIRM program) for financial support.

JF048000W