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Measurement of Conjugated Linoleic Acid (CLA) in CLA-Rich Potato Chips by ATR-FTIR Spectroscopy

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ABSTRACT: A conjugated linoleic acid (CLA)-rich soy oil has been produced by photoisomerization of soy oil linoleic acid. Nutritional studies have shown that CLA possesses health benefits in terms of reducing certain heart disease and diabetes risk factors. Potato chips are snacks that are readily produced in the CLA-rich soy oil containing CLA levels similar to those of the oil used for frying. The objective of this study was to develop an FTIR method to rapidly determine the CLA content of oil in potato chips. Photoirradiated soy oil samples with ~25% total CLA were mixed with control soy oil, and 100 soy oil samples with total CLA levels ranging from 0.89 to 24.4% were made. Potato chips were fried using each of these 300 g CLA rich soy oil mixtures at 175 °C for approximately 3 min. Duplicate GC-FID fatty acid analyses were conducted on oil extracted from each batch of potato chips. The chip samples were ground and then scanned using ATR-FTIR spectroscopy with the aid of a high-pressure clamp, and duplicate spectra of each sample were averaged to obtain an average spectrum. Calibration models were developed using PLS regression analysis. These correlated the CLA isomer concentrations of potato chips obtained by GC-FID fatty acid analysis with their corresponding FTIR spectral features. The calibration models were fully cross validated and tested using samples that were not used in the calibration sample set. Calibrations for total CLA, *trans,trans* CLA, *trans*-10,*cis*-12 CLA, *trans*-9,*cis*-11 CLA, *cis*-10,*trans*-12 CLA, and *cis*-9,*trans*-11 CLA had coefficients of determinations (R^2_v) between 0.91 and 0.96 and corresponding root-mean-square error of prediction (RMSEP) ranging from 0.005 to 1.44. The ATR-FTIR technique showed potential as a method for the determination of the CLA levels in unknown potato chip samples.

KEYWORDS: conjugated linoleic acid (CLA), GC-FID, ATR-FTIR, photoisomerization, potato chips

■ INTRODUCTION

Conjugated linoleic acid (CLA) is a collective term used for the geometric and positional conjugated isomers of linoleic acid.[1] *cis*-9,*trans*-11 CLA and *trans*-10,*cis*-12 CLA are the common naturally occurring isomers of CLA from ruminant and dairy sources.[2] The level of CLA in animal fat typically ranges between 0.3 and 0.8% CLA/g of fat.[3] Biomedical animal studies concluded that CLA has potent beneficial health benefits including anticarcinogenic[4,5] and antiatherosclerotic effects[6,7] and reducing adiposity.[8,9] The conventional dietary sources do not provide sufficient CLA to produce a clinical effect without increase in dietary saturated fat. Therefore, there is an interest in greater nutritional sources of CLA low in saturated fat.

Jain and Proctor[10] developed a method for the production of CLA-rich soy oil by the photoisomerization of linoleic acid to CLA by UV radiation. This photoisomerized oil contained 23% CLA, with 17.5% being the *trans,trans* CLA isomers and the remaining consisting of various *cis,trans* CLA isomers.[10] A recent nutritional study[11] showed that 0.5% dietary CLA-rich soy oil reduced total serum cholesterol and LDL cholesterol by 41 and 50%, respectively. Furthermore, liver weight and liver lipids were also reduced by 35 and 39%, respectively, and hemoglobin glycosylation, a diabetes indicator, was significantly reduced.

The CLA-rich soy oil has been used as a frying medium for the production of CLA-rich potato chips as a dietary CLA-rich oil source.[12] The potato chips contained ~40% oil, with CLA levels in the oil similar to that found in the oil before frying. The determination of the CLA levels in the oil in the potato chips utilized Soxhlet extraction of the oil from the potato chips followed by the GC-FID FAME analysis of the extracted oil.

However, this multistep method requires the use and disposal of chemical reagents and is expensive and time-consuming. Therefore, development of a rapid ATR-FTIR method for CLA fatty acid analysis in situ in a food matrix, without solvent extraction or chemical reagents, could be of great value.

ATR-FTIR spectroscopy has been used for the quantification of CLA fatty acids in CLA rich oil.[13] Kadamne et al.[13] developed PLS regression models for the prediction of CLA in CLA-rich soy oil by ATR-FTIR spectroscopy. The method provided rapid CLA fatty acid analysis of the CLA-rich soy oil with high accuracy. The CLA fatty acid isomers have a "fingerprint" absorption pattern in the mid-infrared spectrum with the *trans*, *trans* CLA isomers producing a peak at 988 cm^{-1} and the *cis,trans* CLA isomers producing two peaks at 981 and 947 cm^{-1}, respectively.[14] The advantages of FTIR over the conventional CLA measurement by GC-FID FAME analysis are rapid analysis time, high accuracy, ease of sample handling, nondestructive methods, and no use of chemicals. FTIR techniques coupled with chemometrics are emerging tools for rapid quantitative lipid analysis in food systems.[15]

Sivakesava and Irudayaraj[16] used FTIR-PAS technology to study the oxidation behavior of potato chips. Shiroma and Rodriguez-Saona[17] used FTIR spectroscopy along with PLS regression analysis to monitor potato chip quality. They scanned ground potato chips by mid-infrared spectroscopy using a high-
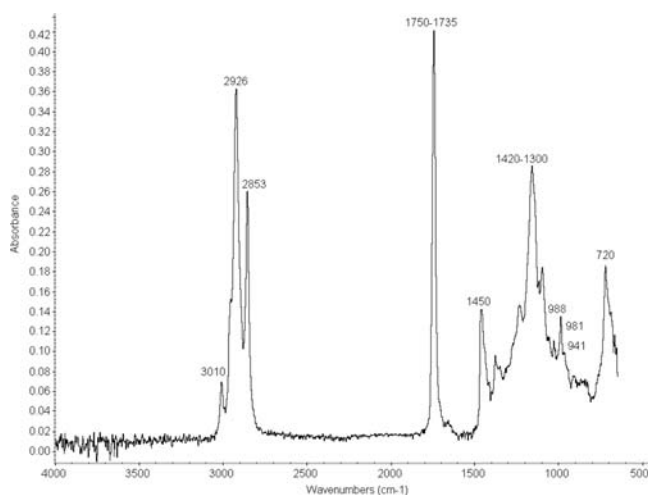
Table 1. Correlation Coefficients for the Different Isomers of CLA at 1% Level of Probability[1]

	trans,trans CLA	trans-10,cis-12 CLA	trans-9,cis-11 CLA and cis-10,trans-12 CLA	cis-9,trans-11 CLA
total CLA	0.98	0.97	0.77	0.99
trans,trans CLA		0.96	0.67	0.98
trans-10,cis-12 CLA			0.79	0.98
trans-9,cis-11 CLA and cis-10,trans-12 CLA				0.73

Figure 1. ATR-FTIR spectrum in the mid-infrared region ($4000-650$ cm^{-1}) of potato chips fried in CLA-rich soy oil.
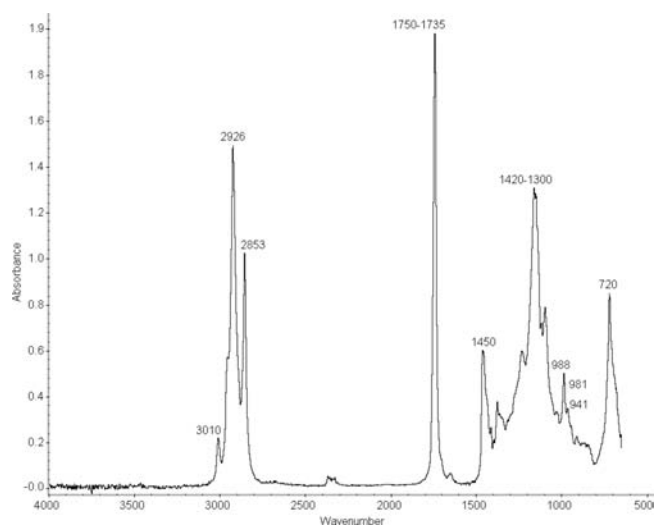
Figure 2. ATR-FTIR spectra in the mid-infrared region of CLA-rich soy oil.

pressure clamp, which enabled increased contact of the oil from the potato chips with the crystal. The spectra of the potato chip and the oil extracted from the potato chips were similar and indicated that ATR-FTIR spectra of the potato chips were oil related.

Conventional CLA analysis by GC-FID FAME analysis requires $2-3$ h, including a preliminary oil extraction by the Soxhlet method, prior to chromatographic analysis. Therefore, the method is unsuitable for rapid analysis of large numbers of potato chip samples.

The objective of this study was to develop an ATR-FTIR method for determination of total CLA, trans,trans CLA, cis-9, trans-11 CLA, trans-9,cis-11 CLA, cis-10,trans-12 CLA, and trans-10,cis-12 CLA of the oil in potato chips prepared with CLA-rich oil, without oil extraction.

■ MATERIALS AND METHODS

Materials. Refined, bleached, and deodorized (RBD) soy oil (Wesson, ConAgra, Irvine, CA) containing 52% linoleic acid and 6% linolenic acid, as measured, and Russet potatoes were obtained from a local grocery store (Fayetteville, AR) and stored at 4 °C. Sodium methoxide and anhydrous sodium sulfate (EMD Chemicals, Darmstadt, Germany) were used for methyl ester preparation. Heptadecanoic acid methyl ester (17:0; Sigma-Aldrich, St. Louis, MO) was used as a standard for GC.

Preparation of CLA-Rich Soy Oil. The photoirradiation process described by Jain and Proctor[10] was used to synthesize CLA-rich oil by isomerizing linoleic acid in the presence of UV light. Sixteen 1 L batches of CLA-rich soy oil were synthesized. This oil was diluted using RBD soy oil, and 100 CLA-rich soy oil dilutions (300 g) were prepared containing CLA levels ranging from 0 to 25%.
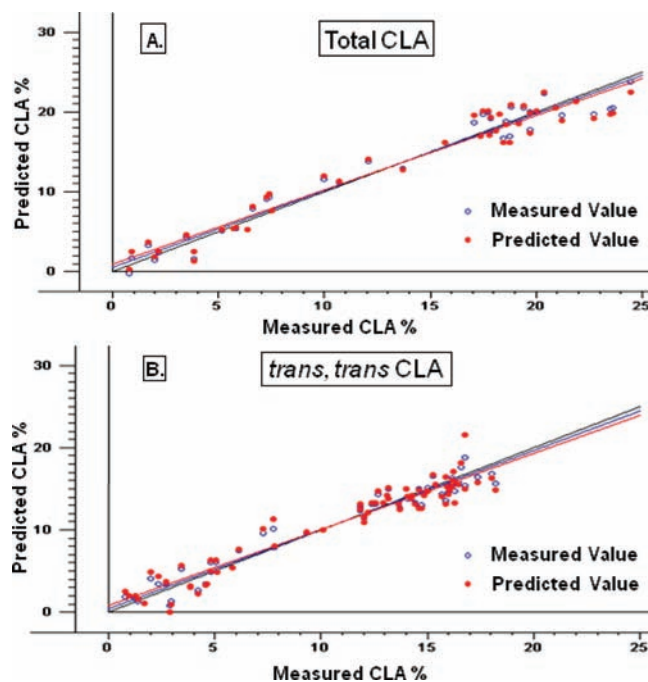
Figure 3. Calibration and validation plots for the models of (A) total CLA and (B) trans,trans CLA.

Potato Chip Preparation. Russet potatoes were peeled, washed, and sliced to $^{1}/_{32}-^{2}/_{32}$ in. using a rotary slicer.[12] These slices were washed with distilled water for about 5 min and dried using paper toweling. The chips were prepared by frying 10 potato slices in 2 batches

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Table 2. Model Statistics for the Prediction of CLA Isomers in Photoisomerized CLA-Rich Soy Oil

parameter[b]	models[a]				
	total CLA	*trans, trans* CLA	*trans*-10,*cis* 12-CLA	*trans*-9, *cis*-11 CLA and *cis*-10, *trans*-12 CLA	*cis*-9, *trans*-11 CLA
calibration					
min value	0.78	0.75	0.08	0.03	0.07
max value	24.48	18.22	1.68	0.14	2.30
R^2_c	0.96	0.96	0.91	0.95	0.960
RMSEC	1.44	1.12	0.13	0.005	0.13
SEC	1.46	1.13	0.13	0.006	0.13
bias	-3.45×10^{-7}	-2.64×10^{-7}	3.82×10^{-8}	-2.04×10^{-9}	-2.12×10^{-9}
SD_c	7.47	5.48	0.43	0.03	0.65
validation					
R^2_v	0.95	0.92	0.88	0.91	0.94
RMSEV	1.77	1.55	0.15	0.01	0.16
SEV	1.79	1.56	0.15	0.01	0.16
bias	-4×10^{-3}	-1.01×10^{-2}	-1.1×10^{-3}	3.05×10^{-5}	-1×10^{-3}
RPD	4.17	3.15	2.87	3.00	4.06

[a] Models comprising 85 samples. [b] R^2_c, coefficient of determination of calibration; RMSEC, root-mean-square error of calibration; SEC, standard error of calibration; SD_c, standard deviation in the values of calibration set data obtained by GC-FID analysis; R^2_v, coefficient of determination of validation; RMSEV, root-mean-square error of validation; SEV, standard error of validation; RPD, relative predictive determinant (= SD_c/SEV).

of 5 slices each in a Presto FryBaby (National Presto 96 Industries Ltd., Eau Claire, WI) each using 300 g of CLA-rich soybean oil dilutions at 175 °C for approximately 3 min. The potato chips were placed in plastic bags, flushed with nitrogen, and stored at −4 °C.

Oil Extraction and GC-FID Analysis. The oil from 2 g of potato chips was extracted in duplicate by 30 mL of petroleum ether followed by vortexing for 2 min and later centrifuging for 5 min.[18] The solvent was evaporated using a Rotavapor R-114 (Buchi, Switzerland) to recover the oil. Fatty acid methyl esters were prepared from each extracted oil sample.[19] The methyl esters were analyzed by GC-FID for CLA fatty acid content by duplicate analysis.[20]

Collection of ATR-FTIR Spectra. An ATR-FTIR spectrum of the potato chip samples was collected using the OMNIC software on an Impact 410 instrument (Nicolet, Madison, WI) in the absorption mode. The instrument was equipped with an interferometer and a DTGS-KBr detector operating at a resolution of 4 cm^{-1}. The potato chips were ground using a pestle and mortar and were pressed onto the ZnSe plate using a high-pressure clamp (Spectra-Tech, Stamford, CT) with a sufficient pressure the crystal can withstand. The spectra were scanned in duplicate over the wavenumber interval of 4000−650 cm^{-1} averaging 128 scans with a data spacing of 1.928 cm^{-1}. The duplicate spectra of each sample were averaged to obtain an average spectrum. The background sample was collected under the same instrumental conditions every 120 min. The sample holder was rinsed with methanol and then water between runs.

Statistical Analysis. Chemometric models were developed using PLS regression analysis to characterize the potato chip ATR-FTIR spectral data to relate them to the levels of total CLA, *trans,trans* CLA, *trans*-10,*cis*-12 CLA, *trans*-9,*cis*-11 CLA, *cis*-10,*trans*-12 CLA, and *cis*-9, *trans*-11 CLA as measured by GC-FID analysis of the extracted oil.

Calibration Model Development and Data Analysis. The spectra were analyzed using a multivariate regression software Unscrambler v9.8 (Camo, Oslo, Norway). The FTIR spectra (dependent variable) were imported as Omnic (.spa) into Unscrambler v9.8 as numerical data. The levels of total CLA, *trans,trans* CLA, *trans*-10,*cis*-12 CLA, *trans*-9,*cis*-11 CLA, *cis*-10,*trans*-12 CLA, and *cis*-9,*trans*-11 CLA were used as independent variables. The calibration set consisted of 85 randomly selected samples with total CLA levels ranging from 0.89 to 24.48% CLA. The spectral data were pretreated by mean centering,

weighing by their standard deviations, linear baseline correction, and baseline offset. The spectra were analyzed by partial least-squares regression technique (PLS-1). A full cross-validation technique was used to examine the prediction ability of the calibration models. In this technique, each sample in the calibration set is used to test the model derived from the set of remaining samples. The prediction residual for each excluded sample was calculated. This process is repeated until each sample in the calibration set is excluded once and a root-mean-square error value (RMSE) of the cross-validation is calculated. The Martens' uncertainty test, which is based on the jack-knifing technique, is performed during the validation step that assesses the stability of the regression results, identifies the perturbing samples or variables, and selects the significant *x*-variables shown in the weighted regression coefficients plot. The outlier samples in the validated plot and the nonsignificant *x*-variables in the model were identified by Unscrambler, and the model was recalculated excluding the outliers and the nonsignificant *x*-variables.

Validation of the Calibration Models. The performance of the calibration models was evaluated by using a test set of approximately 15 potato chip spectra that were not included in the calibration set. The samples in the test set were preanalyzed for their CLA isomer concentrations using GC-FID.[19,20] The levels of total CLA and its individual isomers in the test set were predicted using the developed models using the prediction option in the Unscrambler software. A JMP 7.0.2 data sheet (SAS Institute, Inc., Cary, NC) was used to correlate the predicted and actual concentrations. The adequacy of prediction was assessed by the accuracy of the prediction values (based on the equation of plot) and coefficients of determination of prediction (R^2_p). The evaluation of the calibration models was done by the coefficient of determination of calibration (R^2_c), root-mean-square error of calibration (RMSEC), and standard error of calibration (SEC). The validated models were evaluated in terms of the coefficient of determination of validation (R^2_v), root-mean-square error of validation (RMSEV), standard error of validation (SEV), and relative predictive determinant (RPD), also known as the discrimination index.

■ RESULTS AND DISCUSSION

Correlation Coefficients. The correlation coefficients summarizing the strength of linear relationships between the CLA
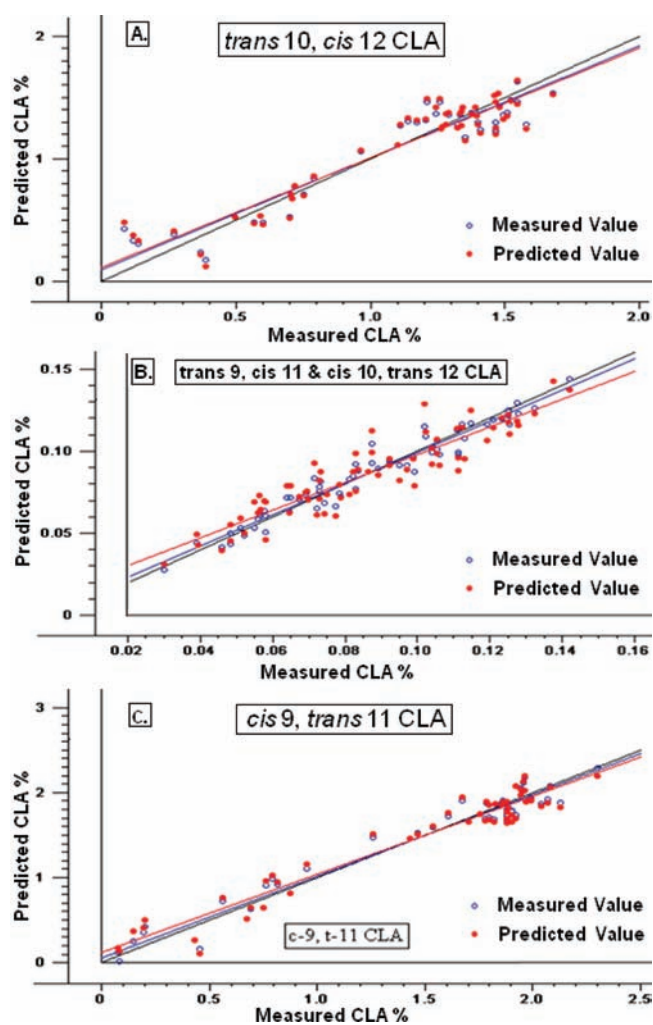
Figure 4. Calibration and validation plots for the models of (A) *trans*-10,*cis*-12 CLA, (B) *trans*-9,*cis*-11 and *cis*-10,*trans*-12 CLA, and (C) *cis*9, *trans*-11 CLA.

Figure 5. Weighted regression coefficients for the fully cross-validated models of (A) total CLA and (B) *trans,trans* CLA.

isomer levels, as measured by GC-FID FAME analysis in the extracted oil samples from potato chips, are presented in Table 1. The data show that all of the isomers of CLA were significantly correlated with each other. Among all of the correlations, total CLA, *trans,trans* CLA, *cis*-9,*trans*-11 CLA, and *trans*-10,*cis*-12 CLA had high positive correlations. *trans*-9,*cis*-11 CLA and *cis*-10, *trans*-12 CLA had correlations between 0.67 and 0.77 with the other CLA isomers.

ATR-FTIR Spectra. Figure 1 shows a typical ATR-FTIR spectrum of potato chips prepared with CLA-rich soy oil. The wavenumbers of the peaks in the potato chip spectrum were identical to those in the spectrum of the CLA-rich soy oil obtained by Kadamne et al.[13] This indicates that only the oil component contributes to the potato chip spectra. The common bands in the spectrum are seen in Figure 1 and were at 2926 cm^{-1} (asymmetric $-CH_2$ stretch), 2853 cm^{-1} (symmetric $-CH_2$ stretch), 1450 cm^{-1} (asymmetric $-CH_3$ bending), 1465 cm^{-1} ($-CH_3$ symmetric scissoring), and 720 cm^{-1} ($-CH_2$ rocking vibration).[21] The small peak at 3010 cm^{-1} represents the *cis* double bond stretching of the unsaturated fatty acid.[21] The highest absorbance in the spectra was produced by the stretching of the ester carbonyl between 1750 and 1735 cm^{-1}.[21] The ester carbonyl also produces a peak between 1300 and 1100 cm^{-1} due
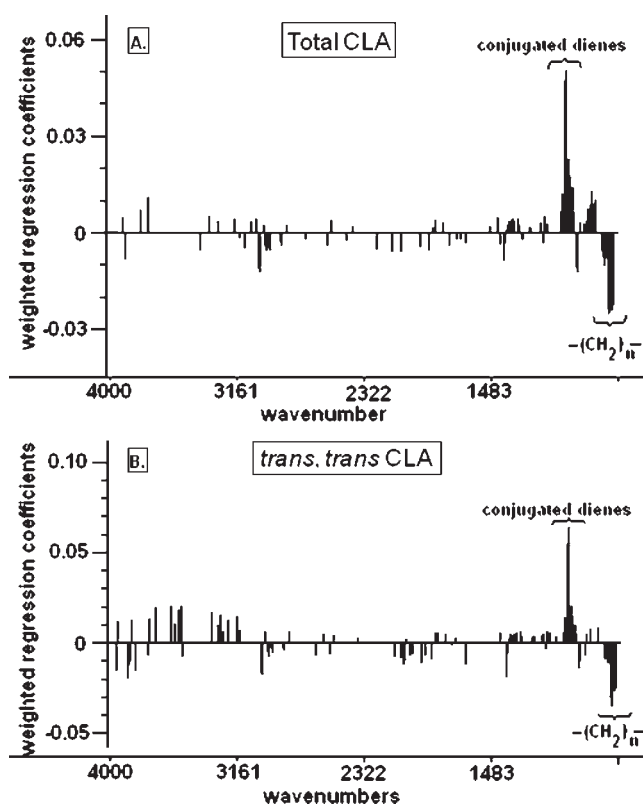
to the coupling of the C=O and C=C stretches, and the peak between 1420 and 1300 cm^{-1} indicates carboxylate ions.[21] The *trans,trans* conjugated dienes produce a peak at 988 cm^{-1}, whereas the peaks at 981 and 947 cm^{-1} are characteristic of the *cis,trans* conjugated dienes.[14]

Figure 2 shows a typical ATR-FTIR spectrum of CLA-rich oil extracted from potato chips. Although the wavenumbers of the peaks in the potato chip and the oil spectrum were identical, the absorbance intensities of the peaks at each wavenumber in the oil spectrum were higher than those in the potato chip spectrum. High oil absorbance intensities were also observed in the CLA-rich oil spectrum reported by Kadamne et al.[13] The reduced intensity of absorption in the food matrix (Figure 1) relative to the oil (Figure 2) is probably due to less oil per unit volume in the food matrix. The food matrix contains only ~35% oil[10] relative to the oil matrix, which is 100%. The absorbance of the spectral features from the matrix may be due to the surface oil that would reduce the penetration of the non-oil matrix. Furthermore, —OH and other groups will be involved in hydrogen bonding with lipid C=O, which may reduce stretching. The spectra did not indicate that any other chip matrix components were extracted with the oil.

Calibration Models. Figures 3 and 4 represent the calibration and validation models developed in this study using PLS regression analysis. The statistics for these models are given in Table 2. The statistics show that all of the developed models had a high correlation between the FTIR and the GC-FID FAME results indicated by the R^2_c and the R^2_v values. The R^2_c value for all of the calibration models ranged from 0.91 to 0.96, and for the validation models R^2_v values ranged from 0.88 to 0.95. The RMSE value, which is based on the size of the residuals, signifies
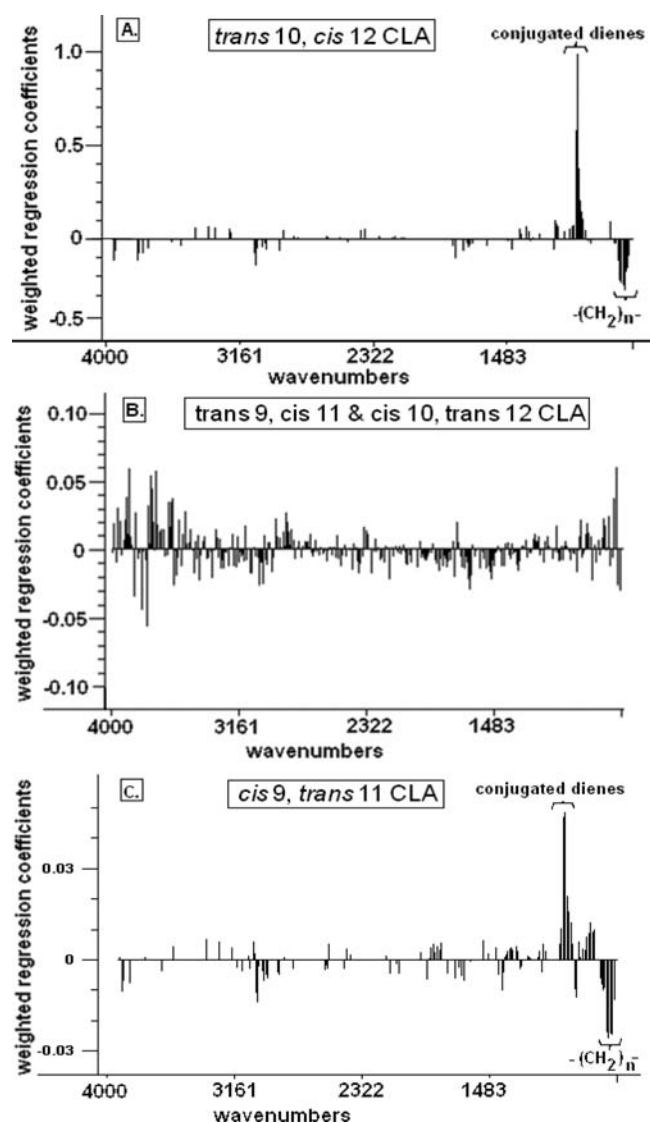
Figure 6. Weighted regression coefficients for the fully cross-validated models of (A) *trans*-10,*cis*-12 CLA, (B) *trans*-9,*cis*-11 CLA and *cis*-10, *trans*-12 CLA, and (C) *cis*-9,*trans*-11 CLA.
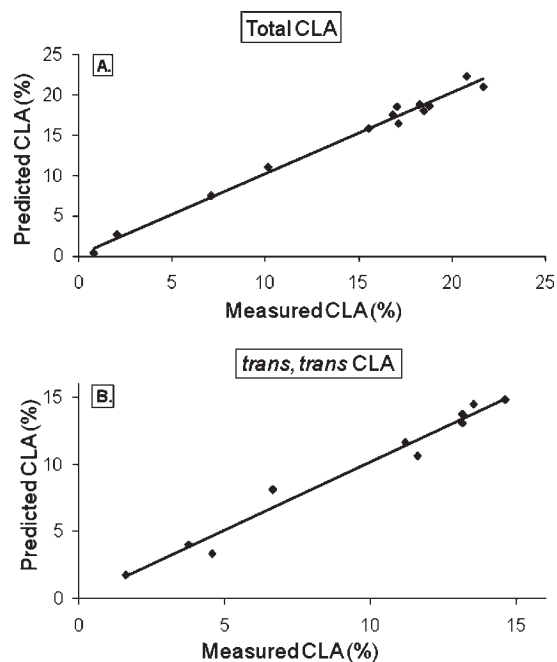

Figure 7. Linear plots for the measured and predicted values of (A) total CLA and (B) *trans,trans* CLA in the CLA-rich soy oil by the developed models.

the accuracy of the model. Table 2 also shows the RMSE values for both the calibration and validation sets are dependent on the relative concentration of the CLA fatty acid in the sample, which is low for isomers present at relatively lower concentrations. For example, the RMSEC and RMSEV for *cis*-9,*trans*-11 CLA were 0.13 and 0.16% CLA when present at concentrations between 0.07 and 2.3% CLA, whereas for *trans*, *trans* CLA these values were 1.12 and 1.54% CLA when present at 0.74−18.21% CLA concentration. The RPD ($=SD_c/SEC$) values for all of the models are also listed in Table 2. Higher RPD (>2) values are usually preferred as they indicate that the range of variation in the values of the CLA isomers is higher than the prediction error.[22] The RPD values for all of the models developed in this study were with the range of 3.0−4.17. These results indicate the models were sufficient for screening the levels of CLA in potato chip samples. The statistical regression analysis and the parameters reported in Table 2 are similar to those reported by Kadamne et al. on CLA-rich oil alone.[13] However, the models presented

by Kadamne et al.[13] were stronger than those presented here in terms of the R^2 and RPD values. This could be because the present study deals with estimation of CLA levels of oil embedded in a food matrix, whereas the previous study measured CLA levels in oil directly. Also, the technique used for the collection of the FTIR spectra involved grinding of potato chips followed by precise arrangement on ZnSe and collection of the spectrum using a high-pressure clamp arrangement. Slight variations in any of the steps may have resulted in variations in the ATR spectra. In contrast, in the previous study[13] the oil spectra were collected by placing oil directly on the ZnSe crystal.

Weighted Regression Coefficients. The regression coefficients assist in identifying the significant *x*-variable in a relationship to a given response variable (% CLA). The predictors with large regression coefficients play an important role in the regression model, whereas the predictors with the small weighted coefficients are negligible.

The weighted regression coefficients are assigned by the PLS regression to the models for the prediction of total CLA presented in Figure 5A and ranged from 0.05 to −0.02. The plot showed that the model was highly specific and positively correlated for the wavenumbers between 1000 and 950 cm^{-1}, which corresponds to conjugated dienes found in CLA. Vibrations in the range of 723−698 cm^{-1} correlated negatively with total CLA prediction. These bands are most likely due to $(CH_2-)_n$ alkyl chains, but single *cis* double bonds may also contribute in this range. Both of these functional groups would be more prevalent in the absence of *trans,trans* CLA, which is the major CLA isomer in CLA-rich oil.

The regression coefficient plot for the model of *trans,trans* CLA isomer in Figure 5B was similar to that of total CLA, and the size of the regression coefficients, 0.07 to −0.02, was also almost similar. This is not surprising because *trans,trans* CLA comprises most of the total CLA.

The weighted regression coefficients of *trans*-10,*cis*-12 CLA (Figure 6A) ranged from 1.0 to 0.02 and had the largest regression coefficients in the conjugated dienes range (1000–950 cm^{-1}) of all the models developed. However, the main features of the regression plot were similar to those discussed above, with absorption at 723–698 cm^{-1} correlating negatively with a correlation coefficient of −0.02.

The plot for the weighted regression coefficient of the *trans*-9,*cis*-11 CLA and *cis*-10,*trans*-12 CLA is shown in Figure 6B with a range of 0.07 to −0.06. The weighted regression coefficients for the model were not specific for CLA isomers. They showed strong positive correlation in the region of 4000–3500 cm^{-1}, but there are no CLA-specific functional groups present in this spectral region. However, the model did have adequate statistical parameters including R^2 and RPD of 0.95 and 3.0, respectively.

Figure 6C shows the weighted regression coefficients for the model of *cis*-9,*trans*-11 CLA. The significant regression coefficients and their size for this model were similar to those of the model for total CLA.

Interestingly, an additional positive correlation for the −CH stretch α to the double bond of the esterified unsaturated fatty acids was reported by Kadamne et al.[13] for CLA-rich soy oil models. This correlation was not observed for any of the CLA-rich potato chip models developed in this study.

Validation of the Calibration Set. All of the developed models were successful in predicting CLA levels, as demonstrated by plotting the predicted results obtained using models developed against the measured CLA levels by GC-FID FAME analysis. These plots are shown in Figures 7 and 8, and the statistics of the plot are given in Table 3. These plots had R^2_P values ranging from 0.95 to 0.99 and RMSEP values between 0.01 and 0.85% CLA. The equations for the linear fit of the data showed that total CLA and *trans,trans* CLA had gradients of almost 1 and intercepts close to 0. This indicates that the predicted value and the measured value were close. The suitability of the developed calibrations for the prediction of CLA levels provided the levels of CLA in the unknown samples and was within the CLA levels listed in Table 2.

The equations for the plot of the other individual CLA isomers had slopes of <1 (0.72312, 0.85501, and 0.85891), indicating that the models slightly underpredicted the CLA levels. However, addition of more sample points to the calibration model may make the models more robust.

This study demonstrates a rapid method for the measurement of CLA content in a food system, potato chips, directly from the product without oil extraction or chemical modification. An ATR-FTIR calibration model was developed on the basis of chemometric analysis of the ATR-FTIR absorptions and CLA fatty acid levels obtained by GC. Individual models for the measurement of total CLA, *trans,trans* CLA, *cis*-9,*trans*-11 CLA, *trans*-9,*cis*-11 CLA, *cis*-10,*trans*-12 CLA, and *trans*-10,*cis*-12 CLA were developed. The results show that the method was rapid, comprehensive, and accurate. The regression coefficients for the models show that the spectral wavelengths characteristic for the CLA were highly significant in the models. The current method is highly specific only for the matrix of potato chips fried in CLA-rich soy oils and cannot be applied to other food systems. However, it does demonstrate CLA analysis directly from a food matrix and provide justification for investigating the development of further models of CLA quantification as more foods are developed that include CLA-rich oil. The method developed minimizes the time, labor, and use of chemicals and costs involved in CLA fatty acid analysis relative to GC analysis.
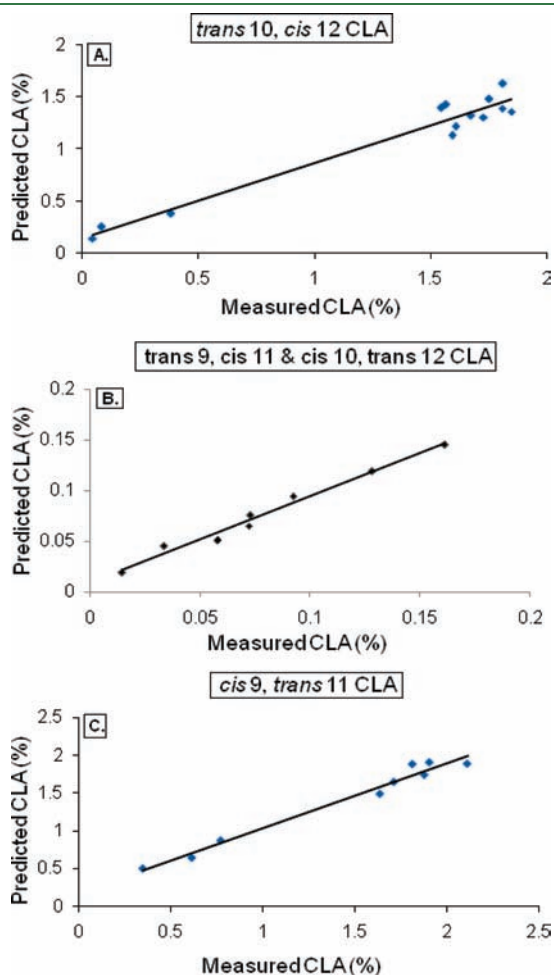

Figure 8. Linear plots for the measured and predicted values of (A) *trans*-10,*cis*-12 CLA, (B) *trans*-9,*cis*-11 and *cis*-10,*trans*-12 CLA, and (C) *cis*-9,*trans*-11 CLA in the CLA-rich soy oil by the developed models.

Table 3. Statistics of the Linear Plot of the Measured versus Predicted Values of the CLA Isomers Based on the Developed Models

model[a]	R^2_P [b]	line eq	RMSEP[c]
total CLA	0.99	$y = 1.01223x + 0.08362$	0.77
trans,trans CLA	0.97	$y = 1.02164x - 0.02213$	0.85
trans-10,*cis*-12 CLA	0.95	$y = 0.72312x + 0.13976$	0.11
trans-9,*cis*-11 CLA and *cis*-10,*trans*-12 CLA	0.98	$y = 0.85501x + 0.00894$	0.01
cis-9,*trans*-11 CLA	0.98	$y = 0.85891x + 0.17190$	0.09

[a] Models presented in Table 2. [b] R^2_P, coefficient of determination of prediction. [c] RMSEP, root mean square error of prediction.

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■ ABBREVIATIONS USED

CLA, conjugated linoleic acid; ATR-FTIR, attenuated total reflectance—Fourier transform infrared; GC, gas chromatography; FID, flame ionization detector; PLS, partial least-squares; RMSEC, root-mean-square error of calibration; RMSEP, root-mean-square error of prediction; SEP, standard error of prediction; SDc, standard error of calibration.

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