Quantification of carbohydrates in fruit juices using FTIR spectroscopy and multivariate analysis

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Abstract. A combination of Fourier-transform infrared spectroscopy (FTIR) and multivariate statistics was applied as screening tool for the quantitative determination of carbohydrates, such as glucose, fructose and sucrose, in 28 processed commercial fruit juices and 5 genuine juices obtained from squeezed fruits. A number of 13 mixtures of glucose, fructose and sucrose standard solutions were prepared at different concentrations, scanned by attenuated total reflectance (ATR) FTIR spectroscopy and analyzed in the 900 and 1400 cm⁻¹ spectral range. Principal component analysis (PCA) of the standard carbohydrate solutions enabled a better understanding of the main sources of variability affecting the FTIR spectra. Also, PCA enabled the grouping of apple, orange and peach juices. Calibration models for each carbohydrate, using partial least squares (PLS) regression were developed and used for prediction purposes. Cross-validation procedures indicated correlations of 0.88, 0.92 and 0.98 for glucose, fructose and sucrose, respectively, between HPLC measured values and FTIR first derivative spectra estimates. Carbohydrates in the expected concentration ranges were found for most of the pure fruit labelled juices. The samples with 4–50% pure fruit juice content showed discrepancies from average concentration values of authentic juices, mainly a high sucrose concentration can flag sucrose addition to maintain the juice sweetness intensity. The present results confirmed the efficiency of FTIR spectroscopy, in combination with multivariate statistics, as a rapid, reliable and cost-effective tool for routine monitoring of multiple constituents in fruit juices, as quality indicators.

Keywords: Glucose, fructose, sucrose, fruit juice, FTIR, PCA, PLS

1. Introduction

Evaluation of fruit juice quality and authenticity is an important applied research area, with relevant impact in industry, food science and consumer protection. Rapid and cost effective methods of carbohydrate determination in fruit juices are of high importance, since unscrupulous companies, manufacturers or traders seek substantial benefits using adulterated juices to gain market advantages over honest competitors, using cheaper ingredients (fruit juices, sugar and syrups) and/or false label indications for consumers.

Discrepancies in component ratios can be used to flag suspicious fruit juices, glucose, fructose and sucrose being main authenticity markers [13].

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In the case of commercial juices, some additives may significantly affect pH and total carbohydrate content, reducing the ability to obtain information on their quality (e.g., ripening stage of the source fruits). Often, pH regulators (e.g., citric acid), sucrose or other sweeteners are added so that pH and total carbohydrate content are no longer a reflection of the ripening stage of the source fruit. In these cases, evaluation of individual carbohydrate contents may still be used as an indicator of ripening stage [16].

Traditionally, carbohydrate content of foods (particularly in juices and beverages) are estimated based on refractive index measurements or volumetric procedures, which provide information about the total carbohydrate content. To quantify each carbohydrate, several methods can be employed, including enzymatic analysis and chromatographic methods [4,6,7].

However, chromatographic techniques (GC, HPLC), successfully used to evaluate fruit juice authenticity by oligosaccharide profiling [24], although accurate, are time consuming, expensive and difficult to implement in an *on-line* setting.

Other spectroscopic approaches, such as nuclear magnetic resonance (NMR) spectroscopy, considering the entire sample composition, may also be applied for authenticity studies and food composition profiling [19].

FTIR spectroscopy became an alternative technique for the analysis of carbohydrates in food samples, being cost-effective and potentially more rapid than the above mentioned methods. FTIR spectroscopy can potentially give information about the proportions of the three main carbohydrates (glucose, fructose and sucrose) and their variation with ripening. FTIR has been increasingly used, often coupled with chemometrics, to study a range of food samples [1,5,7,16,20,25,28] and particularly to study liquid foods such as juices and soft drinks [2,3,11,13,15,17,18,21,26]. For quantification of carbohydrates in several fruit juices and soft drinks, the use of a reduced calibration set, comprising only eight ternary mixtures of glucose, fructose, and sucrose at two concentration levels, has been previously proposed [11,26].

In a recent study we predicted the total antioxidant capacity of fruit juices by using FTIR-PLS, a correlation of 0.97 between measured and predicted values being found [23]. In the present study, FTIR spectroscopy, combined with PLS regression, as multicomponent analysis method, is used, in order to quantify simultaneously the glucose, fructose and sucrose content in 33 samples of pure, genuine and commercial juices, comparatively. Standardized mixtures of these three carbohydrates are used for calibration.

2. Materials and methods

2.1. Samples

A number of 28 soft drink juices were supplied from supermarkets. A number of 5 genuine (authentic) fruit juices (apple, peach, orange, pineapple and pear) were obtained by squeezing the corresponding fruits obtained from supermarkets. The 33 juice samples with pure fruit juice content between 4 and 100% are described in Table 1, according to the package label.

A total of 13 pure carbohydrate solutions (standard mixtures in double distilled water) with different concentrations of glucose (0.5–4.0 g/100 ml), fructose (0.5–14.0 g/100 ml) and sucrose (0.5–8.0 g/100 ml) were prepared, covering the concentration ranges representative for natural juice samples, and used for the development of the calibration models.

Table 1
Fruit juice samples notation and short description

No.	Sample	Description	No.	Sample	Description
1	Ap1_100%	Apple juice 100%	18	Or_G	Genuine orange juice (squeezed orange)
2	Ap2_100%	Apple juice 100%	19	Pc1_50%	Peach juice 50%
3	Ap3_100%	Apple juice 100%	20	Pc2_50%	Peach juice 50%
4	Ap4_100%	Apple juice 100%	21	Pc3_46%	Peach juice 46%
5	Ap5_40%	Green apple juice 40%	22	Pc4_45%	Peach juice 45%
6	Ap_G	Genuine apple juice (squeezed Jonagold apple)	23	Pc5_10%	Peach juice 10%
7	Ac_50%	Apricots juice 50%	24	Pc_G	Genuine peach juice (squeezed peach fruit)
8	Ch_15%	Cherry juice 15%	25	Pi1_100%	Pineapple juice 100%
9	Or1_100%	Orange juice 100%	26	Pi2_50%	Pineapple juice 50%
10	Or2_100%	Orange juice 100%	27	Pi_G	Genuine pineapple juice (squeezed pineapple)
11	Or3_100%	Orange juice 100%	28	Pr1_50%	Pear juice 50%
12	Or4_100%	Orange juice 100%	29	Pr2_50%	Pear juice 50%
13	Or5_100%	Orange juice 100%	30	Pr3_50%	Pear juice 50%
14	Or6_100%	Orange juice 100%	31	Pr4_30%	Pear juice 30%
15	Or7_100%	Orange juice 100%	32	Pr_G	Genuine pear juice (squeezed Packham pear)
16	Or8_100%	Orange juice 100%	33	To_100%	Tomato juice 100%
17	Or9_4%	Orange juice 4%			

2.2. FTIR spectroscopy

The mid-IR (MIR) absorbance spectra ($600\text{--}3500\text{ cm}^{-1}$) were recorded using a FTIR spectrometer (IR-Prestige, Shimadzu Europa GmbH, Duisburg, Germany) equipped with a deuterated L-alanine doped triglycene sulphate (DLATGS) detector working at room temperature. The spectral resolution was 4 cm^{-1} and 128 scans were accumulated for each spectrum. The sampling station was equipped with a horizontal attenuated total reflectance (ATR) accessory with multiple reflections (10 reflections) (PIKE Technologies, Madison, WI, USA). As reference, the background spectrum of air was collected. The juice samples were measured without any preparation, directly on the ZnSe ATR crystal. Between measurements the ATR crystal was carefully cleaned using distilled water and dried.

2.3. HPLC analysis

Carbohydrates were separated and quantified using a Shimadzu chromatograph, equipped with a binary pump delivery system, autosampler and refractive index detector RID-10A. The chromatographic separation of the compounds was achieved by using a C18 ($250 \times 4.6\text{ mm}$) Altima Amino modified column. Elution was performed by 30°C , with an isocratic solvent, acetonitrile: water (80:20, v/v) at a constant flow of 1.3 ml/min . Carbohydrates were identified by comparing the retention time with known standard solutions.

2.4. Principal components analysis (PCA) and partial least squares (PLS) regression

As described in the literature, PCA is used to find the main variability sources in a data set and the relationship between/within objects and variables [10,22]. PLS is used to model the relationship between a set of predictor variables X (n objects k variables) and a set of response variables Y (n objects m responses) [12]. In this study there is only one response (carbohydrate concentration), therefore Y has (n objects 1 response) dimensions. Based on the PLS model, the carbohydrate contents were predicted with prediction errors defined as root mean square error of prediction (RMSEP):

$$RMSEP = \sqrt{\frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{N}},$$

where N = number of samples, y_i = actual concentration and $\hat{y}_i$ = predicted concentration. *RMSEP* can be interpreted as the average prediction error, expressed in the same units as the original response values (g/100 ml in this study).

The Unscrambler software (CAMO, Norway) was used for multicomponent analysis by using the PCA and PLS routine analysis. Best RMSEP were obtained by using the first-derivative transformed spectra. The derivatives were calculated based on the Savitzky–Golay procedure, averaging left side and right side 4 points and using a 2nd degree polynomial.

Full cross validation was chosen in the model computation. With full cross validation, the same samples are used both for model estimation and testing. One sample is left out from the calibration data set and treated as an unknown sample, the model being calibrated on the remaining data points. Then the value for the left-out sample is predicted and the prediction residuals are computed. The process is repeated with another subset of the calibration set, and so on until every object has been left out once; then all prediction residuals are combined to compute the validation residual variance and RMSEP.

The calibration models were developed using the first-derivative spectra of the 13 pure standard solutions of glucose, fructose and sucrose. The carbohydrates fingerprint region in the spectral range 900–1400 cm^{-1} was used for calibration and prediction purposes. To avoid overfitting, the number of principal components (PCs) were correlated with the increasing of the explained validation variance.

3. Results and discussion

3.1. Spectral fingerprint of carbohydrates

In order to fingerprint the carbohydrate region, with specific glucose, fructose and sucrose absorptions, the ATR-FTIR absorption spectra of individual solutions of glucose (4 g/100 ml), fructose (14 g/100 ml) and sucrose (8 g/100 ml) were recorded, as presented in Fig. 1a. Glucose, fructose and sucrose show intense characteristic bands in the fingerprint region (900–1400 cm^{-1}) of the mid-infrared spectral range (Fig. 1a). It is clear from the plot that when the three carbohydrates are present in the same solution, strong band overlap occurs and seriously hinders individual carbohydrate quantification.

Several marker bands of glucose, fructose and sucrose were identified in the spectral range between 900 and 1400 cm^{-1} . The bands in the region 900–1153 cm^{-1} are assigned to C–O and C–C stretching modes, while those in the 1400–1199 cm^{-1} region are due to O–C–H, C–C–H and C–O–H bending vibrational modes of the carbohydrates [15].

Fig. 1. (a) FTIR spectra of glucose (4 g/100 ml), fructose (14 g/100 ml) and sucrose (8 g/100 ml) standards in parallel with apple, orange and peach commercial juices (samples Ap1, Or1 and Pc1 – described in Table 1) spectra. (b) First derivative FTIR spectra of glucose, fructose and sucrose standards presented above.

A higher sucrose level in the peach and orange juice as in the apple juice can be observed by visual inspection of the spectra in Fig. 1a, as revealed by the intense marker band of sucrose at 995 cm^{-1} . Direct quantification based on this band will be not accurate, due to overlapping bands from glucose and fructose in this region. Generally, an assessment of individual carbohydrates content in fruit juices, based on visual analysis of the FTIR spectra, is difficult or even speculative, considering the overlapping of several marker bands. Thus, multivariate statistical methods represent valuable tools for multicomponent analysis.

3.2. Principal component analysis (PCA)

For a better understanding of the main sources of variability affecting the FTIR spectra of the employed standard carbohydrate solutions (glucose, fructose and sucrose mixtures), PCA was performed on the corresponding first derivative spectra in the $900\text{--}1400\text{ cm}^{-1}$ region (Fig. 1b). Figure 2 shows the scores scatter plot of the first two principal components (PCs), which together account 93% of the total variability present in the spectra.

The obtained scores plot shows that the samples are distributed along concentration gradients, according to their carbohydrate composition, in the surface of a triangle. As expected, the three individual

Fig. 2. Scores scatter plot of the first two principal components, PC1 and PC2, obtained in the PCA analysis of the 13 standard carbohydrate solutions, using their first derivative FTIR spectra. The concentration (g/100 ml) of each carbohydrate is coded as $g \times f \times s$, where g, f and s are abbreviations for glucose, fructose and sucrose, respectively. (Colors are visible in the online version of the article; <http://dx.doi.org/10.3233/SPE-2011-0529>.)

(a)

Fig. 3. Loadings profiles of the first three principal components: PC1 (a), PC2 (b) and PC3 (c), obtained using the first derivative FTIR spectra of the set of 13 standard carbohydrate solutions. (Colors are visible in the online version of the article; <http://dx.doi.org/10.3233/SPE-2011-0529>.)

carbohydrate solutions at maximum concentration levels are located at the vertexes of the triangle: fructose is located in the positive side of PC1 axis, while sucrose and glucose are located in the negative side of PC1. This distinction can be further interpreted by inspecting the loadings corresponding to PC1 (Fig. 3a) [8]. It can be seen that the shape of PC1 (Fig. 3a) is very close to the first derivative spectrum of fructose (Fig. 1b).

(b)

(c)

Fig. 3. (Continued.)

Bands related to fructose are present at 960, 1007, 1028 and 1053 cm^{-1} in the positive PC1 loadings, and at 1070, 1091, 1111 cm^{-1} in the negative PC1 loadings. Comparison with the first derivative spectrum shown in Fig. 1b confirms that these are indeed the main characteristic bands of fructose. The contributions of glucose and sucrose to PC1 are much lower as the contribution of fructose.

The loadings plot along the PC2 axis (Fig. 3b) shows a high similitude to the first derivative spectrum of sucrose (Fig. 1b), but contributions from the first derivative glucose spectrum can be also observed. In the positive PC2 loadings region, bands of the first derivative spectrum of sucrose are observed at 985, 1045, 1099 and 1130 cm^{-1} , whereas the negative bands at 1007, 1022, 1072 and 1148 cm^{-1} contribute to the negative loadings. Fructose has a minor contribution to PC2, as also shown in Fig. 2, however, the contribution of glucose cannot be neglected, especially due to the bands at 1007, 1045, 1072 and 1085 cm^{-1} .

Fig. 4. Scores plot of the first two principal components, PC1 and PC2, obtained from the PCA of the apple, orange and peach juices (genuine and commercial). (Colors are visible in the online version of the article; <http://dx.doi.org/10.3233/SPE-2011-0529>.)

The loadings plot on the PC3 axis (Fig. 3c) shows that glucose has a major contribution to PC3. Glucose has negative contribution on the PC3 axis in the scores plot (not shown here). Thus, positive glucose bands from the first derivative spectrum (Fig. 1b) appear as negative loadings on PC3 (985, 1012, 1026 and 1074 cm^{-1}), whereas negative glucose bands appear as positive loadings (1043, 1058 and 1088 cm^{-1}).

The potential of FTIR spectroscopy combined with PCA to discriminate between different types of fruit juices is evaluated. Figure 4 shows the scores plot of PC1 and PC2 obtained after the PCA applied to the FTIR spectra of apple, orange and peach juices. The first two PCs of the PCA performed on the FTIR data explain 94% of the variance in the spectra.

Only the apple, orange and peach juice samples were introduced in the PCA shown in Fig. 4. A grouping of the pear and pineapple juices by PCA was unsuccessful, variations in pure fruit juice content having a high influence on the grouping. This influence can be also observed in the PCA of the juice samples in Fig. 4, e.g. the juice with 4% orange fruit content was positioned in the peach juice region, whereas the genuine peach juice appears as an outlier. However, a satisfactory grouping of most apple, orange and peach juices was achieved, in spite of variations in total pure fruit juice content.

3.3. Partial least squares (PLS) regression

In order to find the model with best predictive capacity, PLS regression was applied to the raw spectra, to the first derivative spectra, and to the second derivative spectra of the 13 carbohydrate standard mixtures. Table 2 shows the statistical parameters: number of used of principal components (PCs), root mean square error of prediction (RMSEP), root mean square error of calibration (RMSEC) and correlation.

The lower RMSEP values (Table 2) suggest that the best results are provided by the first derivative spectra. Also, first derivative spectra enhance the spectral differences between similar compounds and eliminate baseline drift effects [26]. Thus, the PLS-FTIR model using the first derivative spectra is able to predict carbohydrate contents in fruit juices with lowest prediction errors, as shown in Table 2.

Table 2

Statistical results (PCs, RMSEC, RMSEP and Correlation) of the application of PLS to the three sets of data: raw spectra, first derivative spectra and second derivative spectra of carbohydrate standard mixtures

Type of spectra	No. of PCs	RMSEC (g/100 ml)	RMSEP (g/100 ml)	Correlation (R)
<i>Raw spectra</i>				
Glucose	3	0.077	0.106	0.997084
Fructose	4	0.102	0.251	0.999643
Sucrose	3	0.057	0.080	0.999625
<i>First derivative spectra</i>				
Glucose	5	0.009	0.070	0.999956
Fructose	3	0.128	0.227	0.999436
Sucrose	3	0.062	0.089	0.999562
<i>Second derivative spectra</i>				
Glucose	5	0.011	0.248	0.999937
Fructose	3	0.103	0.245	0.999633
Sucrose	4	0.058	0.209	0.999620

To avoid overfitting, the number of principal components (PCs) is determined by the range in which the explained validation variance increases. Thus, the regression model with the best predictive capacity for glucose concentration used the first five PCs. The percentage of variance in glucose concentration explained by the model was 99.6%.

The regression model for fructose yielded satisfactory results. This model used only three, a lower number of PCs (Table 2), in order to obtain a minimum in the error of prediction (RMSEP). This model describes 99.7% of the variance in the fructose concentration.

Similarly, by using a model with three PCs the explained validation variance for sucrose was found to be 99.8%.

Thus, based on the optimized regression models described above, Table 3 shows the predicted concentrations for glucose, fructose and sucrose in the commercial and genuine fruit juices. The number of PCs used in the prediction was the same as that determined in the regression models (Table 2). A number of 12 juice samples were selected aleatory and analysed by HPLC, the obtained glucose, fructose and sucrose values being also shown in Table 3.

Comparing the values of the predicted and HPLC measured carbohydrate concentrations in the fruit juice samples, correlations of 0.88, 0.92 and 0.98 were found for glucose, fructose and sucrose, respectively.

The 100% fruit labelled apple juice samples show expected values of glucose, fructose and sucrose. For authentic apple juice, an approximate ratio between glucose, fructose and sucrose of 3:6:2 is reported, whereas carbohydrates range from 1–4 (glucose), 5–8 (fructose) and 0 to 5 g/100 ml (sucrose) [15].

Raw oranges have a medium glucose, fructose and sucrose content of 2.2–2.4, 2.5–3 and 4–4.8 g/100 ml, respectively [9,27]. It can be seen that the predicted values (2.44, 2.49, 4.01 g/100 ml) for the genuine, squeezed orange juice are in good concordance with the above mentioned medium ranges. The samples, Or8_100% and Or9_4% show considerable deviations from the mean values. It can be also seen in the PCA analysis that the Or8_100% sample (positioned in Figure 4 at negative PC2 values) shows a considerable deviation from the other orange juice samples. The orange juice labelled 4% fruit (Or9_4%) shows a sucrose concentration (7.90 g/100 ml) of almost two times higher compared

Table 3

Predicted (FTIR) and measured (HPLC) glucose, fructose and sucrose concentrations (g/100 ml) in commercial and genuine fruit juices

No.	Sample	Glucose		Fructose		Sucrose	
		FTIR	HPLC	FTIR	HPLC	FTIR	HPLC
1	Ap1_100%	3.28	3.1	6.9	6.8	1.15	1.47
2	Ap2_100%	3.99	–	9.92	–	1.52	–
3	Ap3_100%	3.62	–	9.33	–	2.44	–
4	Ap4_100%	3.23	–	7.62	–	1.28	–
5	Ap5_40%	4.91	–	6.32	–	1.21	–
6	Ap_G	2.72	3.01	8.4	8.8	1.71	2.1
7	Ac_50%	3.96	2.85	3.08	4.42	8.88	8.84
8	Ch_15%	8.30	6.01	7.67	10.01	2.51	2.35
9	Or1_100%	2.91	3.01	3.03	3.52	4.1	4.36
10	Or2_100%	3.84	–	3.95	–	3.83	–
11	Or3_100%	3.18	–	3.32	–	3.31	–
12	Or4_100%	3.62	–	3.84	–	4.96	–
13	Or5_100%	3.78	–	3.97	–	4.49	–
14	Or6_100%	3.65	–	3.83	–	3.57	–
15	Or7_100%	3.72	–	3.87	–	4.43	–
16	Or8_100%	5.08	–	5.14	–	6.05	–
17	Or9_4%	2.35	–	2.3	–	8.12	–
18	Or_G	2.44	2.19	2.49	2.21	4.01	4.47
19	Pc1_50%	3.50	–	3.07	–	10.28	–
20	Pc2_50%	4.48	–	4	–	9.34	–
21	Pc3_46%	2.49	–	2.4	–	8.32	–
22	Pc4_45%	3.02	2.1	2.64	3.7	8.28	8.21
23	Pc5_10%	2.88	–	2.89	–	7.09	–
24	Pc_G	0.66	0.75	0.71	1	3.4	3.6
25	Pi1_100%	5.20	3.21	4.6	5.89	6.61	6.01
26	Pi2_50%	4.93	–	4.6	–	3.74	–
27	Pi_G	2.33	2.4	2.51	2.6	5.45	5.33
28	Pr1_50%	2.48	1.88	3.85	3.98	7.71	8.45
29	Pr2_50%	2.71	–	4.34	–	4.31	–
30	Pr3_50%	2.86	–	4.87	–	8.35	–
31	Pr4_30%	2.26	–	7.95	–	6.52	–
32	Pr_G	3.19	2.63	9.49	8.82	1.18	1.44
33	To_100%	1.98	–	1.78	–	0.15	–

to the other orange juices, probably due to the addition of supplementary sucrose, necessary to maintain the sweetness intensity.

Pure peach juice is characterized by a high sucrose content of approximate 5.5 g/100 ml and lower glucose and fructose contents, of 1.1 and 1.3 g/100 ml, respectively [9,27]. Glucose and fructose concentrations below the above mentioned values were predicted for the genuine peach juice. The lower values can be due to a harvest at a different ripening stage as the fruits processed to commercial juices.

Ripe mature pineapple flesh juice contains about 7 g/100 ml sucrose and 3 g/100 ml each of glucose and fructose [14]. An expected sucrose content was predicted for the genuine pineapple and Pi1_100% juice samples, whereas the 50% fruit pineapple juice shows only 3.74 g/100 ml sucrose.

Authentic pear juice is characterized by a high fructose and low sucrose content [9,27]. The genuine pear juice shows concentrations of 9.49 and 1.18 g/100 ml for fructose and sucrose, respectively. Therefore, due to the high sucrose content (4.31–8.35 g/100 ml) predicted for the commercial pear juice samples, the addition of sweeteners is supposed.

Finally, a 100% tomatoes vegetable juice was also analyzed. The predicted values of glucose and sucrose are in good concordance with literature values [9,27], the lack of sucrose in tomatoes is shown also by the predicted value. Also, a total predicted carbohydrate content of 3.76 g/100 ml is in good agreement with the labelled value of 3.5 g/100 ml.

4. Conclusions

FTIR spectroscopy and multivariate statistics (PCA and PLS) enabled reliable evaluation of fruit juice quality. The first derivative FTIR spectra were found to exhibit the best predictive capacity, due to low RMSEP values. PCA analysis of the standard carbohydrate solutions enabled a better understanding of the main sources of variability affecting the FTIR spectra, whereas PCA of the fruit juices FTIR spectra enabled the grouping of apple, orange and peach juices. A satisfactory correlation between carbohydrate predicted data, using FTIR spectroscopy, and HPLC reference values was found. Overall, the present results suggest that FTIR spectroscopy, in combination with multivariate statistics, represents a rapid, reliable and cost-effective tool for routine monitoring of multiple constituents in fruit juices, as quality indicators.

Acknowledgements

Financial support from the EU-FP6-Project COLL-CT-2005-012461, Quali juice, is highly acknowledged. Support from CNCS-UEFISCDI, project number PN II-RU TE_323/2010 is highly acknowledged by N. Leopold.

References

- [1] V. Bellon-Maurel, C. Vallat and D. Goffinet, *Appl. Spectrosc.* **49** (1995), 556.
- [2] F. Cadet, *Talanta* **48** (1999), 867.
- [3] F. Cadet and B. Offmann, *J. Agric. Food Chem.* **45** (1997), 166.
- [4] T.R.I. Cataldi, G. Margiotta and C.G. Zambonin, *Food Chem.* **62** (1998), 109.
- [5] M.A. Coimbra, A. Barros, D.N. Rutledge and I. Delgadillo, *Carbohydr. Res.* **317** (1999), 145.
- [6] C. Corradini, G. Canali and I. Nicoletti, *Semin. Food Anal.* **2** (1997), 99.
- [7] M. Defernez and R.H. Wilson, *J. Sci. Food Agric.* **67** (1995), 461.
- [8] I.F. Duarte, A. Barros, I. Delgadillo, C. Almeida and A.M. Gil, *J. Agric. Food Chem.* **50** (2002), 3104.
- [9] M.E. Ensminger and A.H. Ensminger, *Foods and Nutrition Encyclopedia*, CRC Press, Boca Raton, FL, 1997.
- [10] K.H. Esbensen, D. Guyot, F. Westad and L.P. Houmøller, *Multivariate Data Analysis: In Practice*, Camo Process AS, Oslo, 2002.
- [11] S. Garrigues, F.J. Rambla and M. De La Guardia, *Fresenius J. Anal. Chem.* **362** (1998), 137.
- [12] P. Geladi and B.R. Kowalski, *Anal. Chim. Acta* **185** (1986), 1.
- [13] J. He, L.E. Rodriguez-Saona and M.M. Giusti, *J. Agric. Food Chem.* **55** (2007), 4443.
- [14] Y.H. Hui, *Handbook of Food Products Manufacturing*, Wiley, Hoboken, NJ, 2007.
- [15] J. Irudayaraj and J. Tewari, *Appl. Spectrosc.* **57** (2003), 1599.
- [16] M. Kačuráková and R.H. Wilson, *Carbohydr. Polym.* **44** (2001), 291.
- [17] R. Kellner, B. Lendl, I. Wells and P.J. Worsfold, *Appl. Spectrosc.* **51** (1997), 227.

- [18] J.F.D. Kelly and G. Downey, *J. Agric. Food Chem.* **53** (2005), 3281–3286.
- [19] J.F.D. Kelly, G. Downey and V. Fouratier, *J. Agric. Food Chem.* **52** (2004), 33.
- [20] E.K. Kemsley, J.K. Holland, M. Defernez and R.H. Wilson, *J. Agric. Food Chem.* **44** (1996), 3864.
- [21] E.K. Kemsley, R.H. Wilson, G. Poulter and L.L. Day, *Appl. Spectrosc.* **47** (1993), 1651.
- [22] W. Kessler, *Multivariate Datenanalyse für die Pharma-, Bio- und Prozessanalytik*, Wiley, Weinheim, 2006.
- [23] L.F. Leopold, N. Leopold, H.A. Diehl and C. Socaciu, *J. Food Anal. Methods* (2011), 1–3, available at: <http://www.springerlink.com/content/e22618762443k212/>, <http://dx.doi.org/10.1007/s12161-011-9251-z> (published Online First™, 6 June 2011).
- [24] G.G. Pan, P.A. Kilmartin, B.G. Smith and L.D. Melton, *J. Sci. Food Agric.* **82** (2002), 421.
- [25] M.D. Queji, G. Wosiacki, G.A. Cordeiro, P.G. Peralta-Zamora and N. Nagata, *Int. J. Food Sci. Tech.* **45** (2010), 602.
- [26] F.J. Rambla, S. Garrigues, N. Ferrer and M. De La Guardia, *Analyst* **123** (1998), 277.
- [27] US Department of Agriculture, Agricultural Research Service, USDA National Nutrient Database for Standard Reference, Release 22, Nutrient Data Laboratory Home Page, 2009, available at: <http://www.ars.usda.gov/ba/bhnrc/ndl>.
- [28] R.H. Wilson and H.S. Tapp, *Trends Anal. Chem.* **18** (1999), 85.