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Research Article

Use of Partial Least Square-Discriminant Analysis Combined with Mid Infrared Spectroscopy for Avocado Oil Authentication

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Abstract

The falsification of high price edible oils such as avocado oil become a serious problem in the oil trade. Simple and rapid methods for identifying and discriminating authentic Avocado Oil (AO) from its adulterants are increasing demand. This current work proposes the use of combination of mid infrared spectroscopy technique with Partial Least Square-Discriminant Analysis (PLS-DA) as direct and rapid tool to discriminate authentic AO from the adulterants of Soybean Oil (SO) and Grape Seed Oil (GSO) in binary and ternary mixture. Discrimination was carried out using the chemometrics approach, namely PLS-DA based on the infrared spectral data. The selected frequency used for authentication of AO was $1500-750\text{ cm}^{-1}$. Special spectral treatment of smoothing and offset correction was implemented to reduce the noise and background spectral. Furthermore, the high accuracy and clear discrimination were obtained with 100% correctness for binary mixture analysis and 93.3% for ternary mixture.

Key words: Mid infrared spectroscopy, avocado oil, soybean oil, grape seed oil, partial least square-discriminant analysis

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Data Availability: All relevant data are within the paper and its supporting information files.

INTRODUCTION

Avocado (*Persea americana* Mill.) is popular fruit in the world due to the pleasant flavor and good taste. The high contents of vitamins and other nutritious elements help in gaining health for people (Ashworth *et al.*, 2011; Flores *et al.*, 2006). The avocado pulp is buttery with high oil content. The concentration of oil varies which depends on the cultivar and the growth conditions (Takenaga *et al.*, 2008). Avocado Oil (AO) is suggested to be a part of daily diet, especially for cardiovascular disease since, it can lower the level of Low Density Lipoprotein (LDL) and triglyceride in blood (Requejo *et al.*, 2003).

The authentication of AO becomes very important, since the price of AO in the market of fats and oils is higher than that of common vegetable oils. The oil can be adulterated with cheaper oils such as grape seed oil, soybean oil, sunflower oil and others. The authenticity determination of the expensive vegetable oils is an interesting issue, since it is associated with the health and economic aspect of consumers (Nunes, 2014). Besides, the authenticity can be also related to the prohibition of certain religion like lard adulteration in vegetable oil (Rohman and Man, 2012). Therefore, the detection and quantification of oil adulterants in AO must be addressed to assure its quality and safety.

Several analytical methods have been suggested and developed for detection of adulterants in edible fats and oils such as Differential Scanning Calorimetry (DSC) (Chiavaro *et al.*, 2009; Marina *et al.*, 2009), chromatographic method (Lee *et al.*, 1998, 2001), Nuclear Magnetic Resonance (NMR) spectroscopy (Fang *et al.*, 2013), electronic tongue (Oliveri *et al.*, 2009) and electronic nose (Hai and Wang, 2006). However, these methods are wasting time, high-cost and involving difficulties in the operation of instruments. Very often, complex chemical treatment is required in sample preparation (Aparicio and Aparicio-Ruiz, 2000).

Mid-infrared spectroscopy has received great attention in the quantitative analysis of fats and oils over the years due to the simplicity with reduced or no-sample pre-treatment steps. It achieves high analysis speed with high sensitivity and good validity. This technique can also be considered as "Green analytical chemistry" because the use of solvent and chemical reagents is eliminated (Yan *et al.*, 2005). Fourier transform infrared (FTIR) spectroscopy techniques has been successfully used for authentication purposes such as analysis of black cumin oil in ternary mixture with corn and soybean oil (Rohman and Ariani, 2013), avocado oil in binary mixture with sesame oil (Lumaksoa *et al.*, 2015) and authentication of AO from canola oil (Quinones-Islas *et al.*, 2013), black cumin in

binary mixture with grape seed oil (Nurrulhidayah *et al.*, 2011), extra virgin oil adulterated with palm oil (Rohman and Man, 2010) and virgin coconut oil in binary mixture with sunflower and corn oil (Rohman and Man, 2011). However, there is no report associated with the authentication of AO using combination of FTIR spectroscopy and PLS-DA approach. Therefore, in this study, the method of FTIR spectroscopy is developed for rapid detection and discrimination of Soybean Oil (SO) and Grape Seed Oil (GSO) in binary and ternary mixture with AO by combining the FT-MIR spectroscopy and PLS-DA treatment.

MATERIALS AND METHODS

Avocado Oil (AO) was obtained by cold percolation technique with n-hexane as the solvent. The ratio of dried avocado pulp powder to the solvent is 1:10 (w/v). Grape Seed Oil (GSO) and Soybean Oil (SO) were purchased from the local market in Yogyakarta, Indonesia. These oils were well packaged in polyethylenephthalate (PET) bottles until being used for analysis. The quality grade of all samples was guaranteed by the supplier.

Preparation of oil samples: Calibration and validation samples composed of binary mixtures of AO-SO and AO-GSO and ternary mixtures of AO-SO-GSO were prepared accurately in the concentration ranges of 2.0-95.0% (v/v) using calibrated micropipette. The mixtures were shaken vigorously to ensure the total homogenization. Independent samples consist of pure AO and the adulterated AO with SO and GSO were prepared in order to evaluate the predictive ability of model.

Measurement of FTIR spectra: The FTIR spectra of samples were obtained using ABB 3000 FTIR-ATR spectrophotometer (Canada) with ATR crystal of ZnSe equipped with DTGS as element detector and potassium bromide (KBr) as beam splitter. The instrument was integrated with HorizonMB 3000 software for FTIR spectra processing. The measurements were directly carried out by introducing oil samples on ATR surface at controlled room temperature (25°C) in mid infrared (MIR) region (4000-650 cm^{-1}). These spectra were subtracted from reference spectrum of air, acquired by collecting a spectrum from the cleaned blank ATR crystal before the measurement of each oil sample replication. The sample spectra were collected in duplicate and displayed as the average spectra. At the end of every scan, the crystal was cleaned with hexane twice and dried with special soft tissue, cleaned with acetone and finally dried again with soft tissue following the collection of each spectrum.

Chemometrics analysis: Data analysis using PLS-DA was performed using the adds in XLSTAT2014 Addison integrated with Microsoft Excel 2007 software. Frequency regions selected are of in the fingerprint area ($1500-750\text{ cm}^{-1}$). Dataset was divided into 3 data i.e., training set (for calibration), validation set and test set. Pre-processing data including centering and reducing were implemented in order to reduce the abundant variables, decrease data complexity and to obtain the optimal amount of factors. The optimum factor number of PLS-DA was determined by cross-validation using N first row mode.

RESULTS AND DISCUSSION

FT-MIR spectral analysis: Each peak and shoulder in FTIR spectra in MIR region ($4000-650\text{ cm}^{-1}$) can be correlated to functional groups of edible fats and oils (Man and Rohman, 2013). The FTIR spectra of authentic AO, SO and CO at regions of $4000-650\text{ cm}^{-1}$ were shown in Fig. 1. The entire spectra look very similar and are dominated by FTIR spectra of triglycerides because of the main constituent (nearly 98%) of edible fats and oils are triglycerides (Giacomelli *et al.*, 2006). However, if one examines the spectra into detail, there are some differences in terms of peak intensities, which can be observed in the region around $1750-1700\text{ cm}^{-1}$ as well as at the fingerprint region, especially in $1085-1200\text{ cm}^{-1}$. Due to its property of FTIR spectra as the fingerprint technique, FTIR spectroscopy can be used to extract the differences among these oils (Rohman and Che Man, 2009).

No bands were observed for SO and GSO at 1713 cm^{-1} , while AO has absorption bands at 1713 cm^{-1} due to C = O stretching vibration of free fatty acid. Furthermore, AO revealed 2 peaks at 1099 and 1114 cm^{-1} , respectively. Both peaks originated from C-O stretching vibration. In AO spectra, the peaks at 1655 cm^{-1} due to C = C olefin stretching is absent. This informs that the degree of fatty acid unsaturation of AO is low (Rohman *et al.*, 2014; Alexa *et al.*, 2009). The differences of fatty acids composition of those oils contributed to the different peak intensities, especially at frequency of $1500-750\text{ cm}^{-1}$. These frequency regions can be exploited for the detection and discrimination purpose. The use of FTIR spectra at selected frequency regions can increase the accuracy and precision of analytical results (Rohman *et al.*, 2015; Vazquez *et al.*, 2000).

Discrimination of avocado oil from grapeseed oil and soybean oil:

The algorithm of PLS can be implemented to simplify the dimensionality of data, to find the relationship among the variables and the observations as well as to find the correlation between observation and variables in term of discriminating inter-objects (Vlachos *et al.*, 2006). The quality of classification model was visualized as graphic which contained cumulative value of Q^2 , R^2X and R^2Y . The cumulative value of Q^2 is the indicator of global goodness of fit and the predictive capability of model using certain amount of components. It is similar to R^2 from cross validation process (Barker and Rayens, 2003). The correlation between X and Y to the related components is performed by R^2X dan R^2Y value.

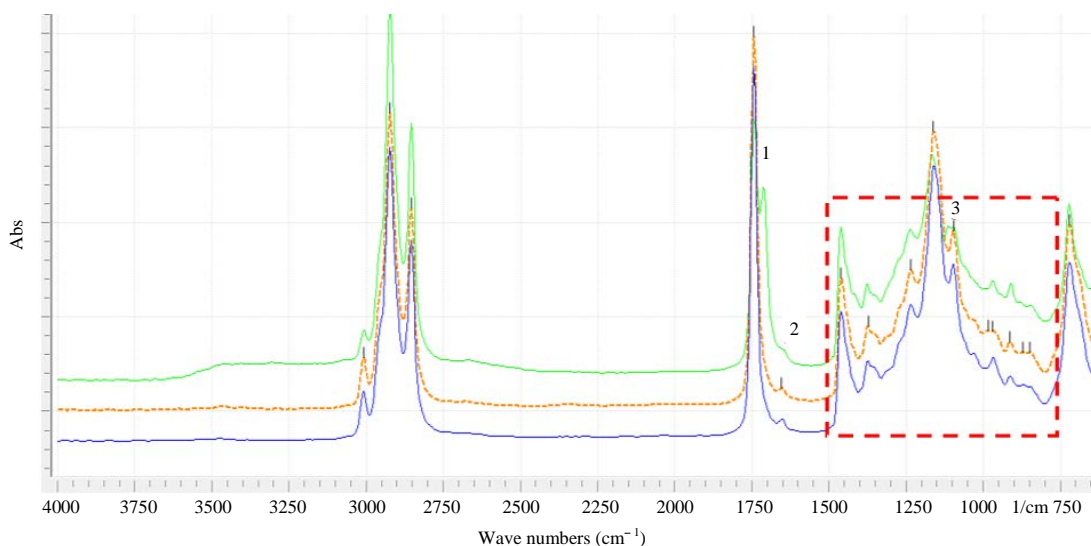


Fig. 1: FTIR spectra of avocado oil, soybean oil and corn oil scanned in mid infrared region ($4000-650\text{ cm}^{-1}$). The red dashed area confirms the fingerprint area for assessment, 1: 1715 cm^{-1} , 2: 1655 cm^{-1} , 3: 1099 cm^{-1} and 1114 cm^{-1}

Table 1: Confusion matrix of PLS-DA performances for discrimination of AO from SO and GSO in binary mixture with AO

From	To		Total	Correct (%)
	AO	Fake		
AO	1	0	1	100.00
Fake	0	14	14	100.00
Total	1	14	15	100.00

AO: Avocado oil, SO: Soyabean oil, GSO: Grape seed oil

The closer the cumulative to unity, the better the discrimination model obtained (Westerhuis *et al.*, 2008). Based on the calculation using PLS-DA algorithm, three factors are able to cover important information in X and Y variables. The factors can describe 94.00% variances which occurred in the spectral data with Q^2 , R^2X and R^2Y are 0.940, 0.967 and 0.981, respectively.

The uniqueness of PLS-DA is the capability to construct the classification function. Objects will be directed to certain class or group if the required passing grade of group is achieved. Thus, PLS-DA is belong to supervised pattern recognition rather than PCA which classify the objects based on the similarity of the Principle Component (PC) score and lead to unsupervised classification (Alexa *et al.*, 2009). It bears in our mind that the object will be included to be AO member if the obtained function value exceeding 1.000 and 0.576 in probability for AO criterion. Using this function, the membership of unknown object assessed can be estimated by PLS-DA model.

The performance of PLS-DA in discriminating the objects can be evaluated by confusion matrix as shown in Table 1. The value of percentage correctness of 100% indicate that overall of the objects are classified correctly to the appropriate group and separated to each other. The phenomenon called reclassification can occur if an object is removed from previous class to the new class which is more appropriate by the function. The oils (AO, SO and GSO) can be separated from each other just by involving 2 factors after extraction data by PLS-DA.

Discrimination of pure Avocado Oil (AO) from the adulterated AO in binary mixture: The PLS-DA was employed to discriminate pure AO from adulterated AO. The pure oil was labeled as AO, whereas, the adulterated oils was labeled as "Fake". Sample obtaining the highest membership value for AO will be considered as AO member. Meanwhile, the samples which cannot fulfil the requirement of membership value will be excluded from AO membership and will be recognized as fake oil. The inclusion of each object to the class is based on the function value. Theoretically, there are only two value, 1 (yes) and 0 (no). The value of 1 states that the object is

recognized as the class member and will be rejected from the class if the value is 0. However, since the chemical constituents of each sample variate, the value may be not 1 or 0 exactly (Broadhurst and Kell, 2006). In this case, the chemical composition variation is due to the mixing of the oils. The value of 0.50 can be assigned as the passing grade value or the threshold of acceptance. The negative value to 0.49 informs that the class reject the object to be the member as shown in Table 2.

By looking at the confusion matrix (Table 1), some more informative indices can be derived in order to synthesize this information. The simplest measure of the quality of a classification model and represents the percentage of correctly assigned objects is accuracy or non-error rate. The percentage of accuracy for discriminating AO from the binary is 100%. Based on Table 2, samples with 2% adulterants of SO and GSO can be assigned as fake. Therefore, those were rejected from AO class. The results in Table 1 show the good sensitivity and specificity of model. Sensitivity is associated to the capability of model to correctly recognize an object belonging to class x. It is stated as a ratio between the number of class x member recognized as the member of class x to total number of class x member. Meanwhile, the specificity characterizes the ability of class x to reject the objects of all the other classes (Aouidi *et al.*, 2012).

Discrimination of authentic Avocado Oil (AO) from adulterated AO in ternary mixture: For ternary analysis, the samples are divided to 3 classes/categories, namely AO, SO-GSO and fake AO. The correctness of discrimination during calibration step was 100% which indicates that overall samples are successfully classified into the correct class based on the acceptance criteria. Subsequently, the model was validated to prove the predictive ability. It can be shown that percentage correctness was 93.33%. The reclassification was occurred in sample with AO 97.5% from fake to AO. Table 3 contains validation result. The reclassification informs that there is similarity of spectra characteristic between pure AO and the fake oil.

It can be concluded that addition of 2.5% of adulterants to pure AO has not given yet the significant effects to the

Table 2: Discrimination validity of pure AO in binary mixture with SO and GSO using test set

Parameters	Class	Pred (class)	F (AO)	F (fake)	P (AO)	P (fake)
SO						
0	AO	AO	1.600*	-0.600	0.900	0.100
10	Fake	Fake	-0.941	1.941*	0.053	0.947
2	Fake	Fake	0.492	0.508*	0.496	0.504
50	Fake	Fake	0.435	0.565*	0.467	0.533
95	Fake	Fake	-0.428	1.428*	0.135	0.865
GSO						
0	AO	AO	0.946*	0.054	0.709	0.291
2	Fake	Fake	0.233	0.767*	0.369	0.631
5	Fake	Fake	0.417	0.583*	0.459	0.541
90	Fake	Fake	-0.190	1.190*	0.201	0.799
95	Fake	Fake	-0.140	1.140*	0.217	0.783

Pred: Predicted class, F: Function value, P: Membership probability, AO: Avocado oil, SO: Soyabean oil, GSO: Grape seed oil, *Value of function <0.50 indicate the unrecognized as a member of related class

Table 3: Validity of discrimination between pure AO from ternary mixture of SO and GSO using test set

AO (%)	Class	Pred	F (AO)	F (SO-GSO)	F (fake)	P (AO)	P (SO-GSO)	P (fake)
1	Fake	Fake	0.267	0.223	0.510	0.309	0.296	0.395
94.5	Fake	Fake	0.232	-0.047	0.815	0.282	0.213	0.505
97.5*	Fake	AO*	0.998*	-0.062*	0.064*	0.575*	0.199*	0.226*
100	AO	AO	1.000	0.000	0.000	0.576	0.212	0.212

AO: Avocado oil, SO: Soyabean oil, GSO: Grape seed oil, Pred: Predicted class, F: Function value, P: Membership probability, *Occurrence of reclassification

change of spectra absorbance of AO. The good separation of pure AO from adulterants (SO and GSO) in binary and ternary mixtures is shown in score plot of PLS-DA. The analysis rapidity and the technique feasibility allow the combination of FT-MIR and PLS-DA treatment to be a promising approach for discrimination of pure AO from the fake oils.

CONCLUSION

The discrimination between pure AO from the adulterants (SO and GSO) can be performed by a chemometrics approach of PLS-DA using FT-MIR spectral data at frequency region of 1500-750 cm^{-1} . Furthermore, FT-MIR spectroscopy combined with PLS-DA method presents high potential for differentiation and classification of AO and adulterated AO. Therefore, a simple, rapid and overall characterization of AO may be obtained at a low cost without complex preparation. The combination of FT-MIR and PLS-DA is necessary to be further developed for routine analysis in oil authentication.

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