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ORIGINAL PAPER

Use of the SAW Sensor Electronic Nose for Detecting the Adulteration of Virgin Coconut Oil with RBD Palm Kernel Olein

A. M. Marina · Y. B. Che Man · I. Amin

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Abstract An electronic nose (zNose^{TM}) was applied to the detection of adulteration of virgin coconut oil. The system, which is based on a surface acoustic wave sensor was used to generate a pattern of volatile compounds present in the samples. Virgin coconut oil was mixed with refined, bleached and deodorized palm kernel olein at a level of adulteration from 1 to 20% (wt/wt). Adulterant peaks were identified from the chromatogram profile and fitted to a curve using linear regression. The best relationship ($R^2 = 0.91$) was obtained between the peak tentatively identified as methyl dodecanoate and the percentage of palm kernel olein added. Pearson's correlation coefficients (r) of 0.92 and 0.89 were obtained between adulterant peak methyl dodecanoate and of the iodine and peroxide values, respectively. Principal component analysis (PCA) was used to differentiate between pure and adulterated samples. The PCA provided good differentiation of samples with 74% of the variation accounted for by PC 1 and 17% accounted for by PC 2. Pure samples formed a separate cluster from all of the adulterated samples.

Keywords Adulteration · Electronic nose · Palm kernel olein · Principal component analysis · Virgin coconut oil

A. M. Marina · Y. B. Che Man
Department of Food Technology, Faculty of Food Science and Technology, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor D.E., Malaysia
e-mail: marina_manaf@yahoo.com

Y. B. Che Man (✉) · I. Amin
Halal Products Research Institute, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor D.E., Malaysia
e-mail: yaakobcm@gmail.com

I. Amin
Department of Nutrition and Dietetics, Faculty of Medicine and Health Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor D.E., Malaysia

A. M. Marina
School of Health Sciences, Universiti Sains Malaysia, 16150 Kubang Kerian, Kelantan, Malaysia

Introduction

Coconut oil is extensively used for edible and industrial purposes. The oil is rich in medium chain fatty acids and exhibits good digestibility [1]. Various methods have been developed to extract coconut oil, either through dry or wet processing. Dry processing is the most widely used form of extraction. Virgin coconut oil is coconut oil that is obtained through wet processing. Unlike commercial coconut oil, virgin coconut oil is unrefined and does not undergo the deodorizing and bleaching processes, which preserves its natural volatile and chemical components. The mild processing of virgin coconut oil, ensures that it retains its pleasant and rather delicate flavor. Virgin coconut oil currently commands a higher price than refined coconut oil. Moreover, virgin coconut oil has been proven to give beneficial effect to health such as preventing the oxidation of low density lipoprotein lipid [2], increasing the antioxidant enzymes [3] and reducing the cholesterol and triglyceride level [4]. All the beneficial findings further emphasize the therapeutic value of virgin coconut oil. Because of its value, virgin coconut oil is prone to be adulterated by oils of less value. Thus, a rapid and efficient method for the detection of adulteration needs to be developed for virgin coconut oil. Methods for monitoring adulteration in virgin coconut oil using Fourier transform

infrared (FTIR) spectroscopy [5] and differential scanning calorimetry (DSC) [6] have been developed recently.

The analysis of volatile components is increasingly being used in the characterization of food products. The analytical methods employed usually involve a series of extractions and chromatographic separations, which demands a lot of time and results in destruction of the sample. Since the profile of volatile compounds in a sample is unique and can be easily destroyed by simple processes, there is an increasing interest in developing efficient analytical techniques for the monitoring of volatile compounds or flavor components in food products. An electronic nose can provide a good alternative for analyzing volatile compounds. It works in a way analogous to the way a human nose functions and does not require prior separation of individual volatile components.

The use of electronic noses in the food industry is now much more common than it was several years ago. The ability of an electronic nose to assess food quality, especially in sensory analysis, has broadened its usage in the analysis of various food products. Electronic noses have been used to analyze food products such as green tea [7], cheddar cheese [8], wine [9], honey [10] and orange juice [11]. Electronic nose technology has also been used to monitor the quality of peaches [12], pears [13] and tomatoes [14].

The fat and oil industries have made use of electronic noses for various purposes. Characterization of vegetable oils by an electronic nose was studied by Gan et al. [15] and Martin et al. [16]. Oxidation of olive, sunflower [17] and corn oil [18] has also been studied using an electronic nose. The classification of animal (pig) fats using an electronic nose was studied by Carrapiso et al. [19]. Electronic noses have also been used in studies on the storage of oil. Cosio et al. [20] found that electronic nose was able to explain the different storage conditions of olive oil. Gan et al. [21] utilized the surface acoustic wave (SAW) sensor-based electronic nose to monitor storage stability of refined, bleached and deodorized (RBD) palm olein and Shen et al. [22] studied the relationship between electronic nose analysis and sensory evaluation of vegetable oils during storage. The use of electronic noses in the analysis of adulteration in vegetable oils has been explored by Mildner-Szkudlarz and Jelen [23] in olive oil, by Hai and Wang [24] in sesame oil and by Che Man et al. [25] in RBD palm olein. The present study was conducted to determine if adulteration of virgin coconut oil by palm kernel olein could be detected using SAW sensor-based electronic nose.

Materials and Methods

Sample Preparation

Virgin coconut oil was produced according to method by Nevin and Rajamohan [2]. The endosperm of mature coconut milk was grated and made into a viscous slurry and then squeezed through cheese cloth to obtain coconut milk. The coconut milk was refrigerated for 48 h and then subjected to mild heating (50 °C) in a thermostat oven. Virgin coconut oil was obtained by filtering the heated coconut milk through cheese cloth. RBD palm kernel olein was obtained from the Malaysian Palm Oil Board (Selangor, Malaysia). All chemicals and solvents used were of analytical grade.

Blend Preparation

Virgin coconut oil and RBD palm kernel olein were mixed in proportions ranging from 1 to 10% RBD palm kernel olein, in 1% increments (w/w), and from 10 to 20% RBD palm kernel olein, in 5% increment (w/w). Each blend was prepared in triplicate.

Fatty Acid Analysis

Fatty acid methyl esters (FAMEs) were prepared according to the method of Cocks and Van Rede [26] by dissolving oil samples (50 mg) in hexane (0.8 ml) and sodium methoxide (1 M, 0.2 ml), followed by subsequent analysis using a gas chromatograph (Agilent Technologies model 6890 N, Santa Clara, CA) fitted with an FID detector. A RESTEX 2330 polar capillary column (0.25 mm internal diameter, 30 m length and 0.2 μm film thickness; Restek Corp, Bellefonte, PA, USA) was used at a column pressure of 1.03×10^5 Pa. The initial column temperature was 50 °C (held for 2 min). The temperature was then increased to 180 °C at a rate of 5 °C/min, held for 2 min at 180 °C, increased at a rate of 8 °C/min to 200 °C and held for 5 min at 200 °C. Standard methyl esters of fatty acids were used as authentic samples and peak identification was done by comparing relative retention times.

Operational System for zNose™

The zNose™ quantifies the olfactory response by simulating hundreds of chemical sensors spanning a continuous range (chromatogram) of retention time. Input vapors enter the system through a temperature-controlled inlet and are preconcentrated for a carefully measured period of time. The concentrated vapors are injected as a short pulse into a temperature programmed capillary column. The dispersed column effluent then passes to a SAW integrating detector, which records the time and amount of each chemical response [21].

The zNose™ uses a two-steps process to analyze vapors. The first step samples ambient inlet vapors and concentrates them in a Tenax trap. Sample preconcentration is carefully controlled to produce a repeatable and

accurate collection of ambient vapors for analysis in the second step. In the second step, the trap is rapidly heated and release vapors are re-focused on the head of the relatively low temperature (40 °C) capillary column. Then the column temperature is programmed to follow a linear rise to its maximum temperature causing the different chemical species in the sample to be released, travel through the column and collect on the surface of a temperature controlled SAW crystal [15].

Electronic Nose Analysis

Fast/GC SAW electronic nose (zNose^{TM}) Model 7100 (Electronic Sensor Technology, Newbury Park, CA, USA) was used to analyze samples in this study. An aliquots of 5 g of samples were weighed into septa-sealed screw cap vials. The samples were equilibrated in a water bath at 60 °C for 10 min. To analyze each sample, the sample's vapor was introduced into the electronic nose. The electronic nose was programmed according to the following operation conditions: injection time of 5 s, inlet temperature of 200 °C, valve temperature of 160 °C, detector temperature of 40 °C, ramp from 40 to 160 °C at 10 °C/s, helium flow rate of 2.9 ml/s and data acquisition time of 12 s. MicroSense version 5.29 software (New Bury Park, CA, USA) was used for data collection for the electronic nose.

Chemical Analyses

The iodine value (Cd 1d-92) and the peroxide value (Cd 8-53) were determined according to AOCS methods [27].

Statistical Analyses

All measurements were conducted in triplicate and averaged using Microsoft Excel software. Trend line equations were further developed from the frequency data of electronic nose. Data from chemical and electronic nose analyses were subjected to analysis by Duncan's multiple range test using SAS Statistical Computer Package version 6.12 (SAS Cary, NC, USA) to identify differences among means. The statistical significance was declared at $P < 0.05$. Principal component analysis (PCA) was carried out using the Unscrambler software version 9.7 (CAMO AS, Trondheim, Norway) to classify the samples into pure and adulterated samples. Partial least squares (PLS) were generated using Minitab software, Release 14 (Minitab Inc, PA, USA).

Results and Discussion

Fatty Acid Composition

The fatty acid composition of virgin coconut oil adulterated with different percentage of RBD palm kernel olein is shown in Table 1. Virgin coconut oil contains predominantly saturated fatty acids, with lauric acid (C12) being the most abundant fatty acid. Virgin coconut oil is also rich in medium chain fatty acids. Generally, the fatty acid content of RBD palm kernel olein does not vary much from that of virgin coconut oil. RBD palm kernel olein also contains more lauric acid than any other fatty acid and contains high amount of medium chain fatty acids, but to a

Table 1 Fatty acid composition of virgin coconut oil adulterated with different levels of RBD palm kernel olein

RBD palm kernel olein (%)	Fatty acid (%)									
	C6:0	C8:0	C10:0	C12:0	C14:0	C16:0	C18:0	C18:1	C18:2	C18:3
0	0.49^{a}	7.02^{a}	6.24^{a}	47.76 ^{g}	19.49^{a}	7.23^{i}	3.64^{d}	6.02^{l}	1.20^{m}	0.10^{bc}
1	0.46^{e}	6.71^{c}	6.01^{b}	48.69^{a}	19.08^{b}	7.95^{h}	3.65^{cd}	6.13^{k}	1.21^{l}	0.10^{bc}
2	0.46^{e}	6.69^{d}	5.96^{c}	48.25^{b}	18.79^{c}	8.94^{bcd}	3.56^{e}	6.13^{k}	1.21^{k}	0.01^{b}
3	0.48^{b}	6.79^{b}	5.97^{c}	48.10^{c}	18.60^{d}	8.87^{g}	3.41^{h}	6.42^{j}	1.25^{j}	0.10^{bc}
4	0.47^{c}	6.68^{e}	5.88^{d}	47.85^{e}	18.53^{f}	8.95^{b}	3.58^{e}	6.66^{i}	1.30^{i}	0.10^{bc}
5	0.46^{e}	6.58^{g}	5.84^{f}	47.81^{f}	18.53^{f}	8.97^{b}	3.50^{f}	6.90^{h}	1.32^{h}	0.10^{bc}
6	0.48^{b}	6.79^{b}	5.97^{c}	48.10^{c}	18.60^{d}	8.89^{fg}	3.41^{h}	6.43^{j}	1.24^{j}	0.10^{bc}
7	0.47^{d}	6.64^{f}	5.85^{e}	48.00^{d}	18.56^{e}	8.90^{ef}	3.46^{g}	7.03^{g}	1.37^{g}	0.10^{bc}
8	0.46^{e}	6.52^{i}	5.77^{g}	47.57^{h}	18.38^{g}	8.92^{de}	3.53^{f}	7.30^{f}	1.38^{f}	0.10^{bc}
9	0.46^{e}	6.56^{h}	5.77^{h}	47.50^{i}	18.28^{h}	8.93^{cde}	3.58^{e}	7.37^{e}	1.41^{e}	0.10^{bc}
10	0.45^{f}	6.44^{j}	5.72^{i}	47.54^{j}	18.29^{i}	8.94^{bcd}	3.68^{c}	7.43^{d}	1.43^{d}	0.10^{bc}
15	0.44^{g}	6.31^{k}	5.6^{j}	47.17^{k}	17.97^{j}	8.95^{bc}	6.06^{b}	8.84^{c}	1.55^{c}	0.10^{bc}
20	0.44^{g}	6.21^{l}	5.46^{k}	46.72^{l}	17.66^{k}	8.96^{b}	6.09^{b}	9.09^{b}	1.67^{b}	0.11^{b}
100	0.23^{h}	3.56^{m}	3.22^{l}	42.38^{m}	13.08^{l}	9.13^{a}	7.95^{a}	20.14^{a}	2.16^{a}	0.14^{a}

Means within each column with different letters are significantly different at $P < 0.05$

lesser degree than virgin coconut oil. This makes the detection of adulteration of virgin coconut oil by RBD palm kernel olein quite difficult to detect especially at adulteration levels below 10%. However, RBD palm kernel olein contains a much higher percentage of oleic acid (C18:1) than virgin coconut oil. Thus, as the percentage of adulteration increases, there is gradual increase in the percentage of oleic acid. The increase in the percentage of oleic acid could therefore serve as a marker for adulteration and could allow detection of adulteration using chromatographic techniques. However, relying primarily on the fatty acid profile for the detection of adulteration is not sufficiently accurate as there are large natural variations in the levels of some fatty acids.

Electronic Nose Analysis

The changes that occurred as palm kernel olein was slowly added to virgin coconut oil were able to be monitored qualitatively by the VaporPrint™ image (Fig. 1). This image can be interpreted as the chemical signature of a substance's smell. The image also represents the graphical display of the SAW detector sensor converted into a polar format, using the retention time as the angular variable and the SAW detector response as the radial variable. The VaporPrint™ image was very useful for a quick qualitative identification of volatile compounds. Figure 1 shows that as virgin coconut oil was slowly adulterated by RBD palm kernel olein, the VaporPrint™ image changed accordingly with the aroma pattern slowly becoming more like the VaporPrint™ of the adulterant as the percentage of adulteration increased. The number on the polar plot in Fig. 1 represents the retention time of the peaks, which was measured in seconds. The unique feature of the VaporPrint™ was its ability to provide visual evidence that the sample was not pure even before the data were analyzed.

The zNose™ operates based on a gas chromatography principles. The frequency profile from the SAW sensor was translated into its first derivative by the instrument software which yielded chromatogram similar to a gas chromatogram. Each peak corresponds to a specific volatile aroma compound. The area under each peak was correlated with the corresponding compound's concentration and was measured in counts. Table 2 shows the electronic nose data for virgin coconut oil adulterated with different percentages of RBD palm kernel olein. The electronic nose data (peaks A–H) were obtained from the sensor signal values (expressed as frequency counts), which represented the concentration of specific chemical compounds. Peaks that changed according to the changes in the adulterant concentration were selected and considered to be adulterant peaks. As shown in Table 2, there were significant differences ($P < 0.05$) between the peak areas for adulterant concentration of 0 and 1% for most of the compounds. This indicates that the presence of the adulterant was sensed even at 1%, which also explains the differences in the fatty acid composition in Table 1.

Table 3 shows the volatile compounds corresponding to peaks A–H and their odor descriptions. The identification of these peaks was tentatively based on a database of Kovats indices stored in the substance library of the Microsense software using *n*-alkanes as the standard. Some of the volatile compounds found in this study, such as octane and lactones, were also identified in coconut oil by Pai et al. [28] and Jayalekshmy et al. [29] and in roasted palm kernels as reported by Jayalekshmy et al. [30]. Lactones were the main components giving the characteristic mild, sweet and pleasant coconut flavor [31]. It was not the focus of this study to determine the exact identity of each volatile compound in virgin coconut oil, but it is interesting to note that the substance library database in the software accompanying he zNose™ does provide useful guidance on the properties of the volatile compounds studied.

To demonstrate the relationship between the sensor signal values and the percentage of adulteration, the compounds' concentrations were plotted versus the percentage

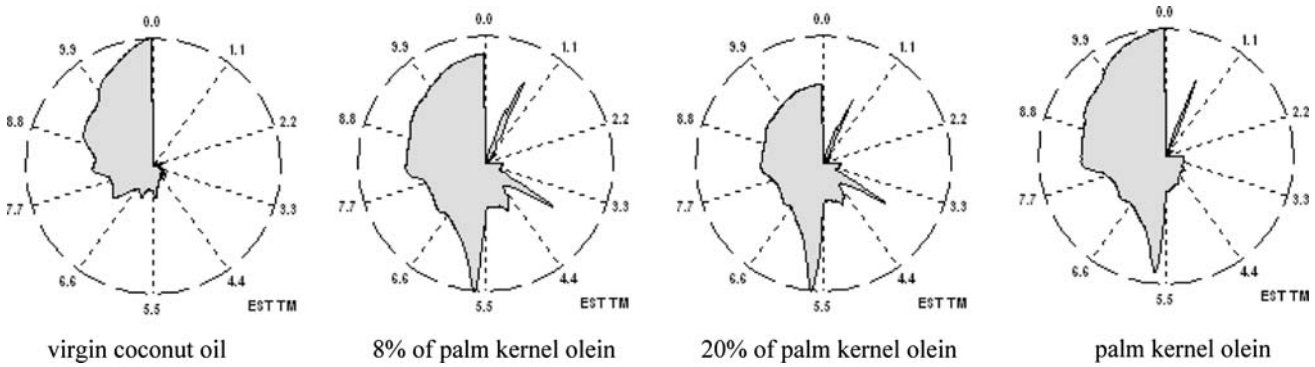

Fig. 1 VaporPrint™ of virgin coconut oil adulterated with different percentage of RBD palm kernel olein (*numbers* on the plot represent retention time, measured in seconds)

Table 2 The electronic nose data of virgin coconut oil adulterated with different percentages of RBD palm kernel olein

RBD palm kernel olein (%)	Peak A	Peak B	Peak C	Peak D	Peak E	Peak F	Peak G	Peak H
0	410.67^{i}	244.33^{a}	1,854.33^{a}	2,595.30^{a}	409.67^{cd}	2,272.70^{g}	3,059.00^{a}	68.67^{d}
1	588.67^{h}	59.67^{de}	118.00^{e}	228.00^{c}	283.33^{d}	2,455.70^{g}	1,020.70^{b}	41.33^{e}
2	1,767.00^{d}	122.00^{bc}	386.00^{cd}	1,686.30^{b}	286.33^{d}	3,356.30^{f}	371.30^{c}	54.33^{de}
3	1,334.00^{f}	115.00^{bc}	439.33^{bc}	1,295.00^{b}	436.67^{bc}	3,193.70^{f}	528.00^{c}	64.33^{d}
4	1,780.33^{e}	128.00^{bc}	375.33^{cd}	1,450.30^{b}	420.33^{bc}	4,847.30^{d}	535.00^{c}	98.33^{bc}
5	2,801.67^{a}	27.00^{e}	133.00^{e}	1,074.30^{b}	409.67^{cd}	3,573.30^{f}	222.00^{c}	55.33^{de}
6	1,612.67^{e}	59.00^{de}	73.33^{e}	1,574.30^{b}	349.33^{cd}	3,637.70^{ef}	191.50^{c}	100.67^{bc}
7	1,853.00^{d}	137.67^{b}	266.00^{d}	1,301.70^{b}	82.33^{e}	3,841.00^{ef}	501.00^{c}	88.00^{c}
8	1,090.00^{g}	121.67^{bc}	375.33^{cd}	1,304.67^{b}	364.33^{cd}	4,283.70^{de}	462.30^{c}	65.67^{d}
9	2,175.33^{c}	90.67^{cd}	134.33^{e}	1,489.00^{b}	483.67^{bc}	3,444.70^{f}	259.70^{c}	91.67^{c}
10	1,745.00^{d}	129.00^{bc}	481.33^{bc}	1,178.00^{b}	543.76^{b}	5,582.70^{c}	570.00^{c}	98.00^{bc}
15	2,310.00^{b}	140.57^{b}	489.67^{bc}	1,473.00^{b}	979.67^{a}	7,433.30^{b}	535.30^{c}	112.33^{b}
20	2,863.00^{a}	148.00^{b}	559.00^{b}	1,597.70^{b}	1,005.33^{a}	9,749.70^{a}	500.30^{c}	190.67^{a}

Means within each column with different superscripts are significantly different at $P < 0.05$

Table 3 Tentative identification of volatile compounds from the electronic nose profile

Peak	Kovats indices	Substance	Odor description
A	800	3-Hexenal	Green, fruity, leaf-like
B	1000	Trimethyl pyrazine	Roasted
C	1155	Citronellal	Fatty
D	1263	Decanol	Fat
E	1350	2-Undecenal	Sweet
F	1447	Methyl dodecanoate	Fatty
G	1525	Delta-decalactone	Coconut
H	1672	Butyl laurate	Oil

of adulteration. Figure 2 displays the compounds with the highest coefficient of determination (R^2). Adulterant peaks F and H with R^2 values of 0.91 and 0.81, respectively, appeared to be the best predictors for quantitative determination of the level adulteration as the size of these peaks correlated well with the increasing level of adulteration. The relationship was found to follow a second order polynomial. A relationship of the same order was reported by Che Man et al. [25] for the adulteration of RBD palm olein by lard. Biswas et al. [17] who conducted a study on sunflower and olive oil, also discovered a curvilinear relationship between surface acoustic sensing device reading and oxidation time.

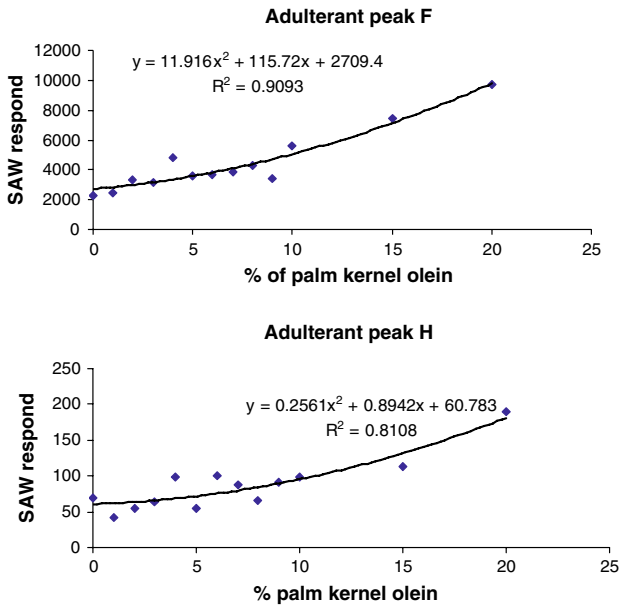

Fig. 2 Compound's concentration versus percentage of adulteration for adulterant peak *F* and *H*, which had the highest coefficients of determination (R^2)

Chemical Analyses

Chemical tests namely for iodine and peroxide values were also conducted to complement the electronic nose data (Table 4). The iodine value is a measure of the degree of unsaturation of fats and oils and peroxide value is a measure of oxidation or rancidity. The chemical data show that both peroxide and iodine values increased with the increased of adulteration level. This was expected as RBD palm kernel olein contains more unsaturated fatty acids and thus, has higher iodine value than coconut oil. Since RBD palm kernel olein is more unsaturated, it is more sensitive to oxidation, which explains the increase in the peroxide value that was observed as the level of adulteration increased.

To investigate the relationship between the chemical data and the electronic nose data, Pearson's correlation

Table 4 Chemical test values of the virgin coconut oil blended with RBD palm kernel olein

Palm kernel olein (%)	Peroxide value	Iodine value
0	0.49^{e}	5.58^{h}
1	1.48^{e}	5.71^{gh}
2	1.86^{de}	6.47^{fg}
3	1.61^{de}	6.73^{fg}
4	1.82^{cd}	8.76^{fg}
5	2.22^{bc}	9.26^{efg}
6	2.62^{bc}	9.90^{def}
7	3.19^{bc}	10.03^{cde}
8	3.09^{bc}	10.91^{cde}
9	3.36^{bc}	11.04^{cd}
10	3.83^{b}	11.55^{c}
15	4.87^{a}	13.96^{b}
20	7.34^{a}	15.10^{a}

Means within each column with different superscripts are significantly different at $P < 0.05$

Table 5 Pearson's correlation coefficients between chemical tests and adulterant peaks

	Adulterant peaks		
	E	H	F
Peroxide value	0.77	0.87	0.92
Iodine value	0.73	0.81	0.89

coefficients were determined. A high correlation was observed between the iodine value and each of the adulterant peaks E, F and H with correlation coefficients (r) ranging from 0.73 to 0.89 (Table 5). The peroxide value also correlated strongly with the adulterant peaks, with correlation coefficient (r) of 0.77, 0.87 and 0.92 for adulterant peaks E, H and F, respectively.

Principal Component Analysis

Principal component analysis was completed based on the electronic nose data in Table 2. PCA is a well known pattern recognition technique that projects the data into a reduced hyperspace defined by the principal components (PC). Figure 3 illustrates the PCA score plot of virgin coconut oil adulterated with RBD palm kernel olein. The score plot better illustrates the electronic nose data in Table 2. It represents the projection of samples defined by PC 1 and 2. The first PC described 74% of the variation while PC 2 accounted for 17% of the variation; thus, 91% of the variance was explained by the first two PCs. The numbers on the plot represent the percentage of adulteration. It is clear that the 0% (pure virgin coconut oil) samples, which formed one cluster, were well separated from

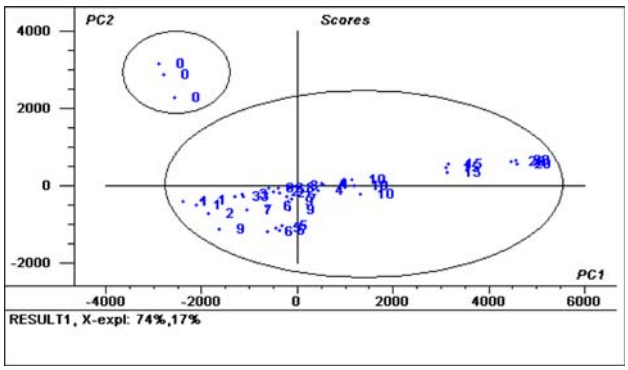

Fig. 3 PCA score plot of virgin coconut oil adulterated with different levels of RBD palm kernel olein

the other samples, which were the samples with adulterant levels from 1 to 20%. Within the adulterant sample group, the percentage of adulteration was generally organized from left to right with respect to increasing amounts of adulteration. The separation improved as the level of adulteration increased.

To determine which variables influenced the separation of the samples, a loading plot was analyzed. The PCA loading plot (Fig. 4) represents the projection of variables in the same plane as the score plot. The absolute value of the loading in a component describes the importance of the contribution of the component. Thus, the farther a variable is far away from the origin, the greater the contribution of that variable to the model. According to Fig. 4, the main compound that caused the separation of the samples based on PC 1 was component F (methyl dodecanoate), followed by component A (3-hexenal). The concentrations of these two compounds were highest in the 20% adulteration sample, indicating that these compounds were dominant in the palm kernel olein. The loading plot also revealed that on the PC 2 plane, compound G, C and D (delta-decalactone, citronellal, and decanol, respectively) were responsible for the separation of samples. These compounds were

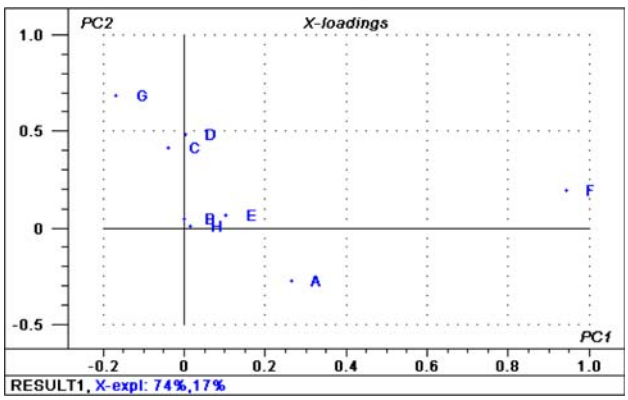

Fig. 4 PCA loading plot of virgin coconut oil adulterated with different levels of RBD palm kernel olein

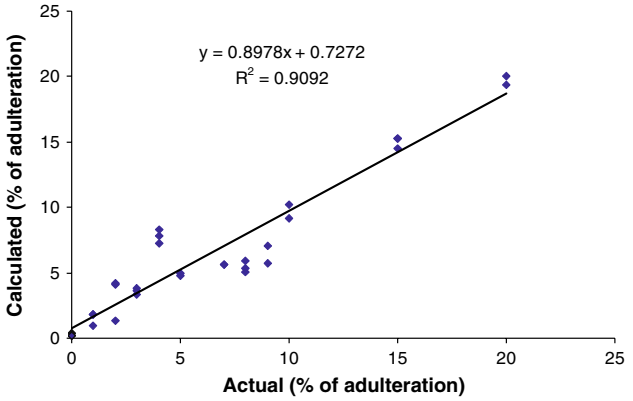

Fig. 5 Partial least square model of actual versus calculated values of RBD palm kernel olein in virgin coconut oil

found mainly in the pure virgin coconut oil. Thus, PCA separated the samples into two PCs, the first PC according to compounds contained mostly in palm kernel olein and the second PC according to compounds contained mostly in virgin coconut oil.

Partial Least Squares Analysis

After classification of the pure and adulterated samples, the adulterant concentration was quantified using PLS analysis (Fig. 5). The signals for the electronic nose values as demonstrated in Table 2 (peak A–H) were used for the PLS analysis. A cross validation was performed by removing one sample at a time. Linear regression of the actual and calculated percentages of adulteration gave the equation of $y = 0.8978x + 0.7272$. The coefficient of determination (R^2) for the model was 0.91, indicating that the model fit the data very well. This study has demonstrated the prospect of using zNose™ electronic nose as a tool to detect adulteration of virgin coconut oil. Excellent results were obtained for the differentiation between pure and adulterated samples down to the 1% detection limit. This technique has the potential to be implemented in routine quality control because it allows rapid sample differentiation without having to acquire detailed knowledge on the compositions of the headspace of the analyzed samples. Moreover, the method is convenient, nondestructive and requires no usage of toxic chemicals.

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