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# Investigation of fatty acid composition and *trans* fatty acid formation in extracted oils from French-fried potatoes and classification of samples using chemometric approaches

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**Abstract:** The present study investigates fatty acid composition and trans fatty acid formation in oils extracted from French-fried potatoes, which were produced in the laboratory and collected from different restaurants. Potatoes were fried at 180 °C at different frying periods (1, 7, 13, 19, 25, and 31 min) and the fatty acid composition of the extracted oils was determined. Principal component analysis and hierarchical cluster analysis were used to characterize and classify the samples. Four major fatty acids were identified in the samples, namely palmitic acid, stearic acid, oleic acid, and linoleic acid. Linolelaidic acid (C18:2 *trans*) was detected in the oil samples extracted from potatoes fried in margarine. Three principal components (PCs) and 4 main clusters were obtained from the chemometric analysis, which characterized the samples. Three PCs were found to be explanatory of more than 84.96% of the total variability in the data set.

**Key words:** Fatty acid composition, French-fried potatoes, *trans* configuration, principal component analysis, hierarchical cluster analysis

## 1. Introduction

Frying is a process of immersing food in hot oil at temperatures between 150 °C and 190 °C. It is used in food preparation and is commonly practiced to produce various foods that have unique sensory characteristics with regard to color, taste, crispness, and palatability. Fried foods are highly appreciated by consumers (Dobarganes et al., 2000; Boskou et al., 2006). French-fried potatoes are consumed throughout the world by consumers of all ages (Choe and Min, 2007; Sahin and Sumnu, 2009). Despite present dietary guidelines that suggest a decrease in the consumption level of fat in our daily diet, fried foods, and especially French fries, are widely consumed and are among the most popular snack foods. Frying is a complex process during which heat and mass are transferred simultaneously. During the frying process, heat transfer occurs in terms of convection between the oil and the surface of the food, while conduction occurs in the structure of the food. When the food is immersed into the heated frying oil, the water evaporates because of the high temperature and is transferred through the surface of the food due to high pressure. At the end of the frying process, the desired texture is formed (Dobarganes et al., 2000; Sahin and Sumnu, 2009). During the frying process, oils are repeatedly used at elevated temperatures under the atmospheric oxygen and receive maximum oxidative and thermal abuse. Many chemical reactions, such as hydrolysis and oxidative or thermal degradation, occur in the structure of the oil. Because of some physicochemical changes, new compounds, such as volatile chain-scission products, nonvolatile oxidized derivatives, and dimeric, polymeric, or cyclic substances occur in the oil depending on the frying conditions. Fried foods absorb these compounds during the frying process (Chang et al., 1978; Dobarganes et al., 2000; Gertz, 2000; Karn et al. 2014). Choe and Min (2007) reported that deep-fat frying causes a decrease in the unsaturated fatty acid concentration of oil and an increase in foaming, color, viscosity, density, specific heat, free fatty acid content, polar materials, and polymeric compound levels. In general, frying might be a reason for the formation of *trans* polyunsaturated fatty acids (Sebedio et al., 1987; Karn et al., 2014). Pozo Diez (1995) reported that the percentage of elaidic acid, a *trans* form of oleic acid, increased in olive oil and sunflower oil, the latter of which shows high oleic acid content during potato frying. As is known, *trans* fatty acid is an

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unsaturated fatty acid that has at least a double bond in the *trans* configuration. The double-bond angle of the *trans* fatty acids is smaller than that of the *cis* isomeric configuration, and the acyl chain is more linear compared to the *cis* configuration. Therefore, the *trans* configuration is a more rigid molecule with different physical properties, such as a higher melting point and greater thermodynamic stability (Taşan and Dağlıoğlu, 2005). Kinsella et al. (1981) reported that there are some concerns related to possible adverse physiological effects of *trans* fatty acids, since their structure is similar to that of saturated ones. Mensink and Katan (1990) and Brühl (2014) reported that the replacement of oleic acid with *trans* unsaturated fatty acid isomers caused an increase in low-density lipoprotein and decrease in high-density lipoprotein levels. In addition, the intake of *trans* fatty acids caused an increase in plasma concentration of lipoprotein, which is a risk factor for coronary artery disease (Mensink et al., 1992; Nestel et al., 1992; Nestel, 2014). It was reported that colon and breast cancers are positively associated with the intake of *trans* fatty acid (Bakker et al., 1997; Bougnoux et al., 2010).

The chemometric method is a classification technique that combines mathematical, statistical, and other logic-based methodologies to effectively manage and interpret experimental data (Haswell, 1992). Principal component analysis (PCA) and hierarchical cluster analysis (HCA) are rather popular chemometric techniques among the multivariate exploratory methodologies that are widely used for food quality evaluation and the differentiation or classification of food samples (Lima et al., 2010; Kermanshahi et al., 2010). Many studies in the literature reported the effective application of chemometric methods such as PCA or HCA (Sato, 1994; García-López et al., 1996; Martín-Carratalá et al., 1998; Brodnjak-Vončina et al., 2005; Matos et al., 2007; Kadegowda et al., 2008; Sathe et al., 2008; Toker et al., 2013; Dogan and Toker, 2014).

The aims of the present study are: 1) to determine the fatty acid composition and *trans* fatty acid formation in French-fried potatoes depending on the frying period at constant temperature, 2) to observe the change in fatty acid composition and *trans* fatty acid presence in French-fried potatoes collected from 13 different restaurants at 2 different times, and 3) to characterize and classify the samples according to their fatty acid composition by using PCA and HCA.

## 2. Materials and methods

### 2.1. Materials

Three different commercially available frying oils, margarine (C14:0 (1.05%), C16:0 (39.7%), C18:0 (4.3%), C18:1 (40.99%), and C18:2 (11.5%)), sunflower oil (C14:0 (0.2%), C16:0 (9.8%), C18:0 (3.86%), C18:1 (28.0%), and C18:2 (55.9%)), and mixed frying oil (C14:0 (0.4%), C16:0 (18.9%), C18:0 (3.85%), C18:1 (23.3%), and C18:2 (47.3%)), were purchased from local markets in Kayseri, Turkey. Sliced potatoes were provided from SuperFresh (Kerevitaş Food Co., Bursa, Turkey). Standard fatty acid methyl esters were purchased from ACCU Standard Inc. (New Haven, CT, USA).

### 2.2. Frying process of potato slices

For the frying process, the different frying oils (margarine, sunflower oil, and mixed frying oil) were placed in the fryer separately and heated to a constant frying temperature (180 °C). Subsequently, potato slices (100 g) were placed into the fryer together with 2 L of frying oil, and the frying process was started immediately. Potatoes were fried separately for different time periods (1, 7, 13, 19, 25, or 31 min) (Table 1). The frying times were selected according to the literature (Krokida et al., 2000). Additionally, the times were slightly modified in order to observe whether frying time affects the *trans* fatty acid formation. The samples were consumable after frying and their sensory aspects were suitable for analysis. A batch of 100 g of sliced potatoes was fried separately during each frying process for different time periods. After frying, the potatoes were removed from the fryer and placed on a tray to cool. The cooled potatoes were then subjected to oil extraction by using petroleum ether in a Soxhlet extractor system (BÜCHİ, B-811, Germany). The oils extracted from the fried potatoes were placed into Eppendorf tubes and stored in a deep freezer (–24 °C, Uğur, Turkey) until analysis. Each extraction treatment was performed in duplicate with 2 repetitions.

### 2.3. Collection of fried potato slices from local restaurants

Fried potato samples were collected from 13 different restaurants in Kayseri (1A–13A, Table 1). One week later, the collection of samples was repeated (1B–13B, Table 1). Afterwards, all samples were subjected to an oil extraction process with petroleum ether using a Soxhlet extraction system (BÜCHİ, B-811, Germany). Extracted oils were placed into the Eppendorf tubes and stored in a deep freezer (–24 °C, Uğur) until analysis. Extraction treatment was performed in duplicate with 2 repetitions.

### 2.4. Determination of fatty acid composition and *trans* fatty acid content of oils

The fatty acid composition of the samples was determined according to the method described in the Agilent application catalog (Agilent, 2008) with some modifications. All samples were subjected to analysis of fatty acid composition in a single batch. For the methylation of fatty acids, 100 mg of oil sample was saponified with 100 µL of 2 M KOH (prepared with methanol), and 3 mL of *n*-hexane was added to the mixture. The mixture was vigorously shaken with a vortex (Nüve NM 110, Turkey) for 1 min and was then centrifuged at 2516 × *g* for 5 min at 25 °C (Nüve, NF 800R, Turkey). One milliliter of solution

**Table 1.** Sample codes used for HCA and PCA analysis.

| Samples collected from restaurants | | | |
|---|---|---|---|
| Sample no. | Sample code | Location | |
| 1 | 1A | Restaurant A | |
| 2 | 2A | Restaurant B | |
| 3 | 3A | Restaurant C | |
| 4 | 4A | Restaurant D | |
| 5 | 5A | Restaurant E | |
| 6 | 6A | Restaurant F | |
| 7 | 7A | Restaurant G | First week |
| 8 | 8A | Restaurant H | |
| 9 | 9A | Restaurant K | |
| 10 | 10A | Restaurant L | |
| 11 | 11A | Restaurant M | |
| 12 | 12A | Restaurant N | |
| 13 | 13A | Restaurant O | |
| 14 | 1B | Restaurant A | |
| 15 | 2B | Restaurant B | |
| 16 | 3B | Restaurant C | |
| 17 | 4B | Restaurant D | |
| 18 | 5B | Restaurant E | |
| 19 | 6B | Restaurant F | |
| 20 | 7B | Restaurant G | Second week |
| 21 | 8B | Restaurant H | |
| 22 | 9B | Restaurant K | |
| 23 | 10B | Restaurant L | |
| 24 | 11B | Restaurant M | |
| 25 | 12B | Restaurant N | |
| 26 | 13B | Restaurant O | |
| Samples produced in the laboratory | | | |
| 27 | M1M | Frying with margarine for 1 min | |
| 28 | M7M | Frying with margarine for 7 min | |
| 29 | M13M | Frying with margarine for 13 min | |
| 30 | M19M | Frying with margarine for 19 min | |
| 31 | M25M | Frying with margarine for 25 min | |
| 32 | M31M | Frying with margarine for 31 min | |
| 33 | MIX1M | Frying with mixed oil for 1 min | |
| 34 | MIX7M | Frying with mixed oil for 7 min | |
| 35 | MIX13M | Frying with mixed oil for 13 min | |
| 36 | MIX19M | Frying with mixed oil for 19 min | |
| 37 | MIX25M | Frying with mixed oil for 25 min | |
| 38 | MIX31M | Frying with mixed oil for 31 min | |
| 39 | S1M | Frying with sunflower oil for 1 min | |
| 40 | S7M | Frying with sunflower oil for 7 min | |
| 41 | S13M | Frying with sunflower oil for 13 min | |
| 42 | S19M | Frying with sunflower oil for 19 min | |
| 43 | S25M | Frying with sunflower oil for 25 min | |
| 44 | S31M | Frying with sunflower oil for 31 min | |

was put into vials and 1 µL of sample injection was started immediately in a gas chromatography system (Agilent 6890, USA), equipped with a flame ionization detector and HP-88 column (100 m × 0.25 mm ID). Injection block temperature was set at 250 °C. The oven temperature was kept at 103 °C for 1 min and then increased from 103 °C to 170 °C at 6.5 °C/min, increased from 170 °C to 215 °C for 12 min at 2.75 °C /min, and finally set to 230 °C for 5 min. Helium was used as carrier gas with a flow rate of 2 mL/min and the split rate was 1/50. Two replications were conducted for the determination of the fatty acid composition of the oil samples. Fatty acid compositions were expressed as % in total triglyceride.

### 2.5. PCA and HCA

Classification of extracted oils depending on fatty acid composition was achieved by PCA and HCA using 2008 XLSTAT Software (XLSTAT, USA). In addition, correlations among the fatty acids were determined using Pearson correlations with XLSTAT Software. PCA is a multivariate statistical technique that generates a set of new orthogonal axes or variables known as principal components (PCs) depending on the original variables. In HCA, Euclidean distance as a dissimilarity distance was utilized, and Ward's methodology was used as the grouping technique (Ward, 1963; Sneath and Sokal, 1973).

## 3. Results and discussion

### 3.1. Fatty acid composition of the oils extracted from fried potatoes

#### 3.1.1. Effect of frying time

Three different oils (margarine, mixed oil, and sunflower oil) were used for frying. The effect of different frying times (1, 7, 13, 19, 25, and 31 min) on the fatty acid composition of the oils extracted from the fried potato samples was investigated. The fatty acid composition of samples is shown in Table 2. Major fatty acids present in the samples fried in margarine were palmitic acid (C16:0), oleic acid (C18:1 *cis*), and linoleic acid (C18:2 *cis*). The fatty acid composition of the samples was in accordance with previous studies, except for *trans* fatty acid composition (Tsanev et al., 1998; Jiri and Jan, 2000; Matsuzaki et al., 2002; Triantafillou et al., 2003; Karabulut and Turan, 2006; Kandhro et al., 2008). However, the fatty acid composition results were compatible with several margarine samples studied by Aro et al. (1998) and Karabulut and Turan (2006). A slight difference between the fatty acid compositions of the samples may be due to the use of different oils to formulate margarines. There was no clear trend between the fatty acid profile and frying time. However, while the C18:2 content of the samples decreased ($P < 0.05$) at the end of the frying process (31 min), there was no significant change in C16:0 and C18:1 *cis* content ($P > 0.05$). It is known that C18:2 is beneficial for the regulation of lipid levels (Mori et al., 2000), reduced risk of cardiovascular problems (Kris-Etherton et al., 2002), and improvement of immune functions (Hwang, 2000). C18:2 *trans* fatty acid was observed in a very small quantity in the oils extracted from the samples fried in margarine, while frying time was found to have no effect on its amount ($P > 0.05$).

As seen in Table 2, the most prevalent fatty acid in mixed oil was linoleic acid (C18:2 *cis*). Palmitic acid (C16:0) and oleic acid (C18:1) were also prevalent. The results revealed that the contents of C16:0 and C18:2 did not change significantly with the increase in frying time ($P > 0.05$). On the other hand, C18:1 decreased with increasing frying time ($P < 0.05$). The *trans* fatty acid was not observed in the oil extracted from the samples fried in mixed oil during the frying process ($P > 0.05$). This result was expected because it is known that the main sources of *trans* fatty acid are hydrogenated oils (Tsuzuki et al., 2010). Tsuzuki et al. (2010) reported that the concentration of *trans* fatty acid did not increase after the tenth frying process at 160 °C, 180 °C, or 200 °C.

Linoleic acid, oleic acid, and palmitic acid accounted for approximately 94% of fatty acids of the oil samples extracted from potatoes fried in sunflower oil. These results are in accordance with previous studies (Kim et al., 2010; Yalcin et al., 2012). There were no significant differences between fatty acid levels at the beginning (first minute) and the end (31st minute) of the frying process ($P > 0.05$). Similar to the samples fried in mixed oil, *trans* fatty acid was not observed in the samples fried in sunflower oil.

Although there was no *trans* fatty acid in the sample fried in the mixed and sunflower oil, its formation during frying could be anticipated. Bansal et al. (2009) reported a linear relationship between the formation of *trans* 18:1 fatty acids and heating time in several vegetable oils. In addition, Tsuzuki et al. (2010) found that the amount of *trans* C18:1 acid increased in rice bran oil, safflower oil, and sesame oil during the heating period of 4 h at 180 °C. In the present study, although there were minute changes in the concentration of *trans* fatty acids as a result of utilizing the potato frying oil for 31 min, statistical analysis revealed that those changes were not significant ($P > 0.05$). According to the results, mixed and sunflower oils could be recommended for frying French fries instead of margarine oil, considering the *trans* fatty acid content of the fried product.

#### 3.1.2. Fatty acid composition of samples collected from restaurants

Earlier in this study potato samples were fried in the laboratory for different time periods using 3 different frying oils. In this section, fried potato samples were collected from local restaurants and their fatty acid composition was determined after the extraction of their oils. Table 1 shows the samples (sample code, collection period).

**Table 2.** Fatty acid composition (%) of oils extracted from fried potato samples.

| Samples | C12:0 | C14:0 | C16:0 | C16:1 | C18:0 | C18:1 *trans* | C18:1 *cis* | C18:2 *trans* | C18:2 *cis* | C20:1 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.33 | 0.94 | 26.46 | 0.12 | 4.31 | 4.37 | 49.41 | 0.08 | 8.99 | 0.41 |
| 2 | 0.47 | 0.99 | 35.29 | 0.09 | 4.47 | 0.00 | 39.83 | 0.00 | 17.55 | 0.17 |
| 3 | 0.60 | 1.26 | 39.89 | 0.18 | 4.74 | 0.00 | 39.19 | 0.00 | 13.28 | 0.07 |
| 4 | 0.55 | 1.11 | 39.57 | 0.10 | 3.69 | 0.00 | 40.86 | 0.00 | 12.17 | 0.15 |
| 5 | 0.38 | 1.06 | 39.30 | 0.19 | 4.39 | 0.00 | 42.20 | 0.00 | 11.14 | 0.16 |
| 6 | 0.42 | 1.16 | 41.87 | 0.22 | 4.62 | 0.00 | 41.11 | 0.00 | 9.31 | 0.15 |
| 7 | 0.39 | 1.13 | 43.01 | 0.18 | 4.80 | 0.00 | 39.35 | 0.00 | 10.17 | 0.14 |
| 8 | 0.18 | 1.09 | 42.57 | 0.19 | 4.74 | 0.00 | 39.45 | 0.00 | 10.67 | 0.14 |
| 9 | 0.35 | 0.55 | 41.03 | 0.19 | 4.64 | 0.00 | 39.96 | 0.00 | 11.82 | 0.15 |
| 10 | 0.13 | 0.47 | 18.94 | 0.14 | 4.87 | 0.00 | 32.02 | 0.00 | 42.13 | 0.13 |
| 11 | 0.43 | 1.05 | 38.02 | 0.18 | 4.52 | 0.00 | 40.34 | 0.00 | 14.42 | 0.15 |
| 12 | 0.40 | 1.11 | 40.44 | 0.18 | 4.54 | 0.00 | 41.16 | 0.00 | 11.12 | 0.14 |
| 13 | 0.53 | 1.27 | 38.89 | 0.18 | 4.80 | 0.00 | 39.47 | 0.00 | 13.47 | 0.14 |
| 14 | 0.27 | 0.56 | 22.08 | 0.19 | 3.85 | 7.19 | 53.88 | 0.00 | 10.20 | 0.74 |
| 15 | 0.28 | 0.82 | 31.80 | 0.16 | 4.30 | 0.00 | 37.11 | 0.00 | 24.74 | 0.07 |
| 16 | 0.38 | 0.96 | 34.25 | 0.18 | 4.40 | 1.44 | 42.39 | 0.00 | 14.79 | 0.25 |
| 17 | 0.37 | 0.95 | 33.49 | 0.18 | 4.38 | 1.72 | 42.80 | 0.00 | 14.86 | 0.27 |
| 18 | 0.37 | 0.91 | 32.10 | 0.18 | 4.34 | 2.07 | 43.13 | 0.00 | 15.61 | 0.29 |
| 19 | 0.33 | 0.84 | 30.74 | 0.18 | 4.25 | 2.48 | 43.86 | 0.00 | 16.04 | 0.33 |
| 20 | 0.35 | 0.90 | 32.48 | 0.17 | 4.33 | 1.54 | 41.86 | 0.00 | 17.21 | 0.24 |
| 21 | 0.36 | 0.91 | 32.61 | 0.18 | 4.34 | 1.85 | 42.81 | 0.00 | 15.70 | 0.28 |
| 22 | 0.36 | 0.90 | 32.28 | 0.18 | 4.33 | 1.93 | 42.89 | 0.00 | 15.89 | 0.28 |
| 23 | 0.35 | 0.89 | 32.04 | 0.18 | 4.32 | 1.98 | 42.91 | 0.00 | 16.09 | 0.28 |
| 24 | 0.35 | 0.89 | 32.03 | 0.18 | 4.32 | 1.96 | 42.87 | 0.00 | 16.19 | 0.28 |
| 25 | 0.35 | 0.90 | 32.29 | 0.18 | 4.33 | 1.85 | 42.67 | 0.00 | 16.22 | 0.27 |
| 26 | 0.35 | 0.90 | 32.25 | 0.18 | 4.33 | 1.91 | 42.83 | 0.00 | 16.02 | 0.28 |
| 27 | 0.26 | 1.01 | 39.22 | 0.17 | 4.27 | 0.00 | 40.59 | 0.78 | 12.25 | 0.15 |
| 28 | 0.26 | 1.01 | 39.47 | 0.17 | 4.30 | 0.00 | 40.98 | 0.76 | 11.94 | 0.15 |
| 29 | 0.27 | 1.02 | 39.64 | 0.17 | 4.32 | 0.00 | 40.70 | 0.77 | 11.87 | 0.14 |
| 30 | 0.26 | 1.02 | 39.83 | 0.17 | 4.31 | 0.00 | 41.09 | 0.78 | 11.60 | 0.14 |
| 31 | 0.26 | 1.01 | 39.74 | 0.17 | 4.31 | 0.00 | 40.88 | 0.77 | 11.55 | 0.14 |
| 32 | 0.26 | 1.03 | 39.71 | 0.18 | 4.35 | 0.00 | 40.83 | 0.77 | 11.50 | 0.14 |
| 33 | 0.06 | 0.46 | 19.56 | 0.23 | 3.84 | 0.00 | 24.25 | 0.00 | 46.27 | 3.16 |
| 34 | 0.06 | 0.43 | 18.19 | 0.24 | 3.82 | 0.00 | 23.06 | 0.00 | 48.50 | 3.35 |
| 35 | 0.05 | 0.41 | 17.79 | 0.24 | 3.82 | 0.00 | 22.54 | 0.00 | 49.40 | 3.46 |
| 36 | 0.02 | 0.40 | 17.60 | 0.24 | 3.79 | 0.00 | 22.34 | 0.00 | 49.55 | 3.49 |
| 37 | 0.05 | 0.42 | 18.66 | 0.24 | 3.82 | 0.00 | 23.32 | 0.00 | 47.84 | 3.34 |
| 38 | 0.05 | 0.44 | 18.89 | 0.24 | 3.85 | 0.00 | 23.41 | 0.00 | 47.36 | 3.29 |
| 39 | 0.00 | 0.17 | 9.13 | 0.10 | 3.84 | 0.00 | 27.78 | 0.00 | 57.01 | 0.16 |
| 40 | 0.00 | 0.19 | 9.93 | 0.10 | 3.85 | 0.00 | 28.04 | 0.00 | 55.92 | 0.16 |
| 41 | 0.05 | 0.19 | 9.65 | 0.10 | 3.80 | 0.00 | 27.98 | 0.00 | 56.11 | 0.16 |
| 42 | 0.05 | 0.21 | 10.78 | 0.10 | 3.87 | 0.00 | 28.39 | 0.00 | 54.48 | 0.16 |
| 43 | 0.03 | 0.22 | 9.77 | 0.11 | 3.91 | 0.00 | 28.22 | 0.00 | 56.24 | 0.16 |
| 44 | 0.04 | 0.17 | 9.80 | 0.10 | 3.86 | 0.00 | 28.03 | 0.00 | 55.85 | 0.15 |

It was found that the amount of palmitic acid (C16:0) ranged from 18.94% to 43.01% while oleic acid (C18:1) and linoleic acid (C18:2) ranged from 32.02% to 53.88% and 8.99% to 42.13%, respectively (Table 2). According to the fatty acid profiles, it can be concluded that most oil samples used in the different restaurants had similar fatty acid compositions. Except for sample 1A, there was no *trans* fatty acid formation in the samples collected in the first week. However, *trans* C18:1 was detected in the samples collected in second week, except for sample 2. When the samples collected in the first and second week were compared, the *trans* C18:1 contents of the samples of the second week were higher than those of the first week. This finding might be due to the fact that the oil used in the frying process may not have been changed during the collection time interval. The same oil might have been used in the restaurants to fry the potatoes repeatedly, and repeated frying may have caused the formation of the *trans* fatty acids. Repeated use of the same oil is a potential health risk due to the possible formation of toxic compounds such as acrylamide or *trans* fatty acids. Among the samples collected in the first week, only one sample contained *trans* fatty acids. However, in the second week, 12 samples had *trans* fatty acids (approximately 92% of the oil samples analyzed). This rate was considered to be very high. Therefore, restaurants should avoid repeated use of frying oils, and oils should be examined for the inclusion of *trans* fatty acids. Consumers should take *trans* fatty acid composition into consideration when consuming French fries.

### 3.2. Chemometric approach to classify the samples

#### 3.2.1. PCA

Table 3 reports the eigenvalues and percentages of variance of the PCs generated from PCA. According to Kaiser's rule, eigenvalues higher than 1.0 are accepted as descriptors of variance in the data set. The first 3 PCs had eigenvalues higher than 1.0. The eigenvalue is proportional to the explanation of the variance in the data set, which means that the higher the eigenvalue is, the more it accounts for variability in the data set. PC1, with the highest eigenvalue (5.46), explained 54.605% of the variance in the data set. PC2 and PC3, which had eigenvalues of 1.66 and 1.38, accounted for 16.609% and 13.747% variability in the data set, respectively. These PCs jointly accounted for 84.961% of the variance of the data set. They were sufficient for qualitative purposes because this percentage (84.961%) was higher than 70% (Larrigaudiere et al., 2004). The most significant loading values of the 3 PCs are highlighted in bold in Table 4. As seen in this table:

- Among the fatty acids, C18:2 *cis*, C14:0, C16:0, C12:0, C18:1 *cis*, and C18:0 explained the variation in PC1.
- C16:1 and C20:1 accounted for the variance in PC2.
- *Trans* fatty acids (C18:1 and C18:2) were responsible for the variation in PC3.

The score plots of PC1 versus PC2, PC1 versus PC3, and PC2 versus PC3 are presented in Figure 1. These plots provide information about the correlation between the variables. This correlation is shown in Table 5. A significant negative correlation ($r = -0.908$, $P < 0.05$) was observed between the oleic acid (C18:1 *cis*) and linoleic acid (C18:2 *cis*). Shin et al. (2010) reported that there was a significant negative correlation ($r = -0.997$, $P < 0.001$) between oleic and linoleic acids in runner-type peanut cultivars. There was a positive correlation between C14:0 and C16:0 variables. No correlation was determined between the C18:2 *trans* and C12:0 fatty acids. The sample score plots for PC1 versus PC2, PC1 versus PC3, and PC2 versus PC3 are presented in Figure 2. There

**Table 3.** Results of PCA analysis using data on the fatty acid composition of the lipids.

| PC | Eigenvalue | Variance (%) | Cumulative variance |
|---|---|---|---|
| 1 | 5.460 | 54.605 | 54.605 |
| 2 | 1.661 | 16.609 | 71.214 |
| 3 | 1.375 | 13.747 | 84.961 |
| 4 | 0.941 | 9.406 | 94.367 |
| 5 | 0.362 | 3.624 | 97.991 |
| 6 | 0.098 | 0.978 | 98.969 |
| 7 | 0.053 | 0.530 | 99.498 |
| 8 | 0.046 | 0.461 | 99.959 |
| 9 | 0.004 | 0.037 | 99.996 |
| 10 | 0.000 | 0.004 | 100.000 |

**Table 4.** Loadings of the significant principal components and contributions of components.

| Component | PC1 | Contributions (%) | PC2 | Contributions (%) | PC3 | Contributions (%) |
|---|---|---|---|---|---|---|
| C18:2 *cis* | **–0.975*** | 14.999 | –0.113 | 0.009 | –0.107 | 1.066 |
| C14:0 | **0.934** | 15.988 | 0.243 | 3.563 | –0.066 | 0.313 |
| C16:0 | **0.922** | 15.563 | 0.312 | 5.855 | –0.156 | 1.769 |
| C12:0 | **0.905** | 0.000 | –0.012 | 51.006 | 0.121 | 7.553 |
| C18:1 *cis* | **0.901** | 11.204 | –0.248 | 0.408 | 0.276 | 2.177 |
| C18:0 | **0.782** | 1.122 | 0.082 | 5.156 | –0.173 | 51.822 |
| C16:1 | 0.002 | 14.871 | **0.920** | 3.714 | 0.322 | 5.543 |
| C20:1 | –0.641 | 1.324 | **0.676** | 1.999 | 0.281 | 23.176 |
| C18:1 *trans* | 0.248 | 17.397 | –0.293 | 0.775 | **0.844** | 0.836 |
| C18:2 *trans* | 0.269 | 7.531 | 0.182 | 27.515 | **–0.564** | 5.745 |

*Most significant loadings are given in bold.

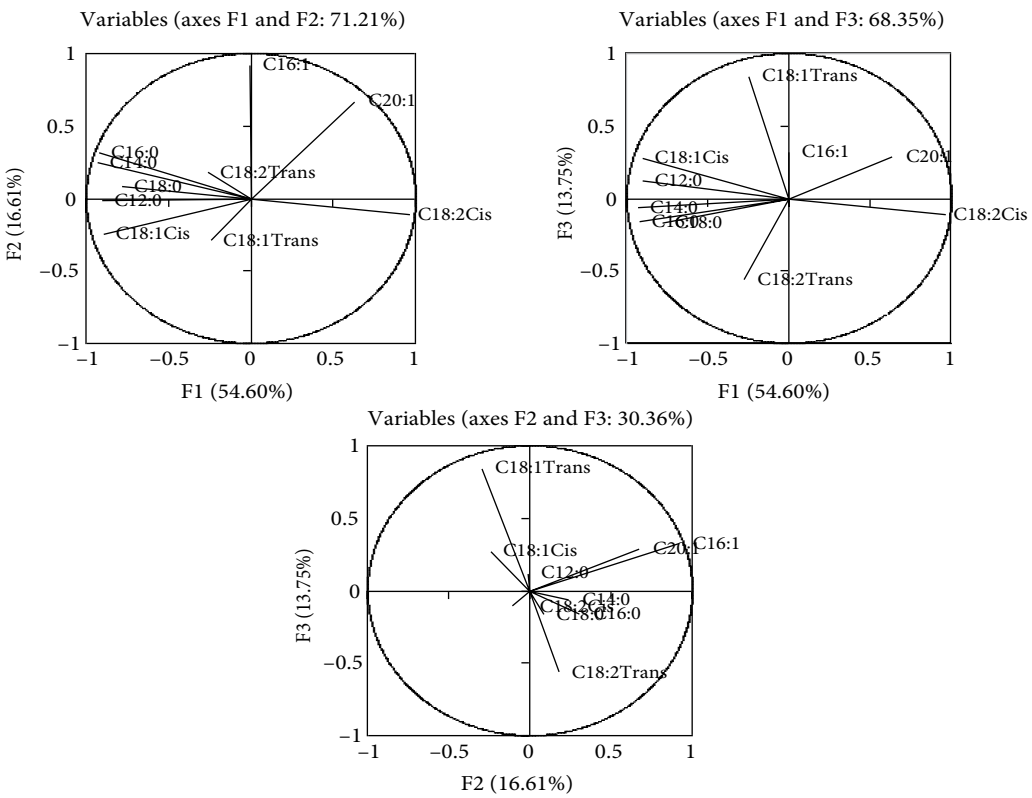


**Figure 1.** Plot of the first 3 principal component (PC) loading vectors.

**Table 5.** Correlations among the fatty acids.

| | C12:0 | C14:0 | C16:0 | C16:1 | C18:0 | C18:1 *trans* | C18:1 *cis* | C18:2 *trans* | C18:2 *cis* | C20:1 |
|---|---|---|---|---|---|---|---|---|---|---|
| C12:0 | 1 | | | | | | | | | |
| C14:0 | **0.879*** | 1 | | | | | | | | |
| C16:0 | **0.823** | **0.944** | 1 | | | | | | | |
| C16:1 | −0.019 | 0.172 | 0.228 | 1 | | | | | | |
| C18:0 | **0.664** | **0.720** | **0.733** | 0.064 | 1 | | | | | |
| C18:1 *trans* | 0.220 | 0.078 | −0.018 | 0.023 | −0.045 | 1 | | | | |
| C18:1 *cis* | **0.786** | **0.742** | **0.710** | −0.121 | **0.568** | **0.600** | 1 | | | |
| C18:2 *trans* | −0.006 | 0.289 | **0.363** | 0.012 | 0.080 | −0.190 | 0.194 | 1 | | |
| C18:2*cis* | **−0.864** | **−0.921** | **−0.932** | −0.137 | **−0.689** | **-0.331** | **−0.908** | **−0.302** | 1 | |
| C20:1 | **−0.522** | **−0.430** | **−0.420** | **0.664** | **−0.540** | −0.112 | **−0.672** | −0.181 | **0.509** | 1 |

*In bold, significant values (except the diagonal) at the level of significance alpha = 0.050 (2-tailed test).

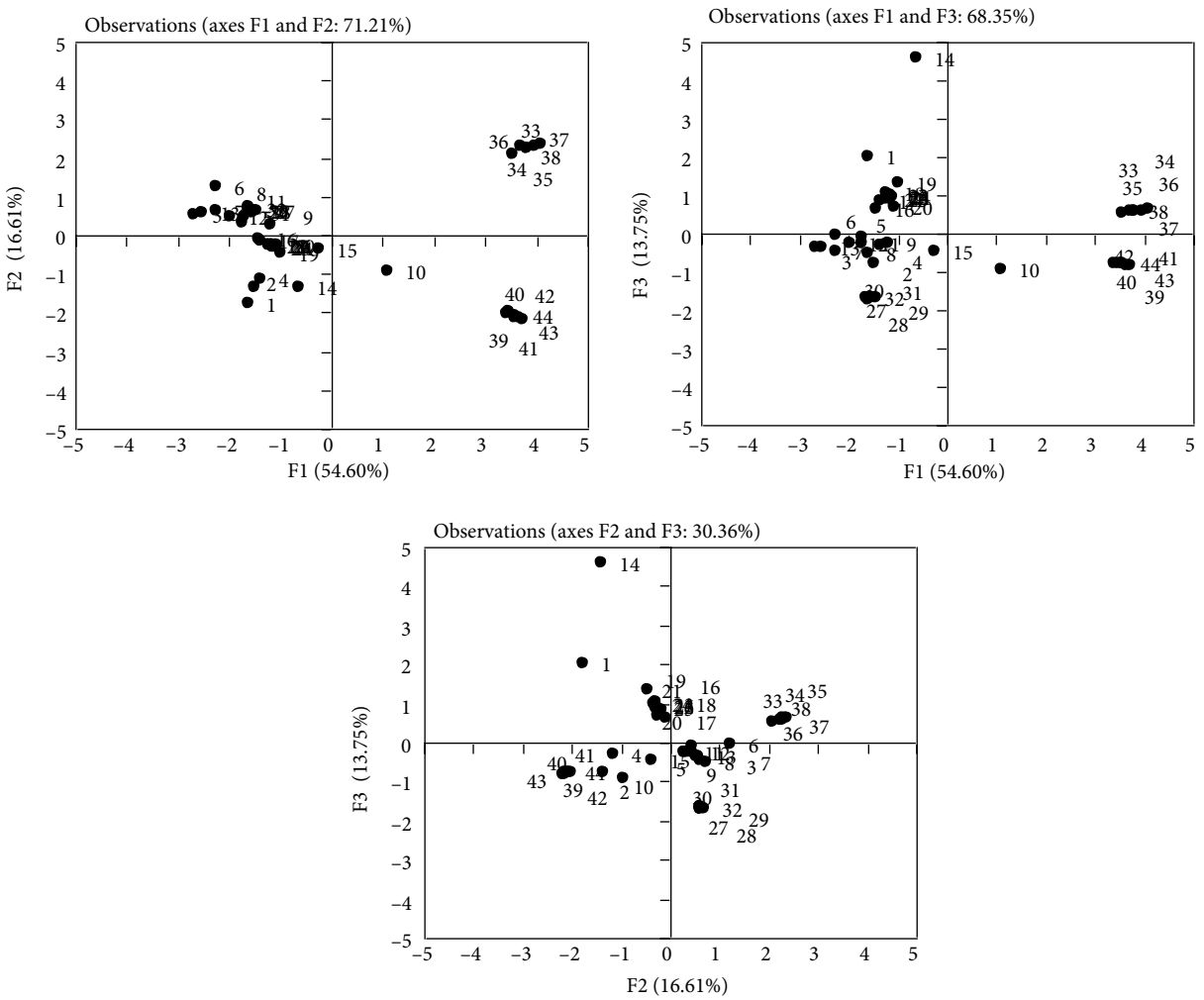


**Figure 2.** Plot of the first 3 principal component (PC) score vectors.

were 3 different clusterings on the PC1–PC2 plot, which accounted for 71.21% of the total variance in the data set. The oils extracted from potato samples fried in margarine for different time periods and the oils extracted from fried potatoes collected from different restaurants (except for sample 10) are located on the left half of the PC1–PC2 plot. Interestingly, sample 10 is located in the lower right quadrant of the plot, indicating that its fatty acid composition (at least one fatty acid) significantly differed from the other samples. For the determination of this differentiation Figures 1 and 2 were created. By using these plots, it is possible to suggest the reasons for the locations of the samples based on their fatty acid composition. The location of the oil and margarine samples obtained from restaurants can be explained by the higher C16:0, C14:0, and C18:1 *cis* contents of those oils when compared with the samples fried in mixed oil and sunflower oil. The diversion of sample 10 from those oils was due to its lower C14:0 and C16:0 content. The samples fried in mixed oil and sunflower oil were located in the upper and lower right quadrants of the plot, respectively. As seen in Figure 2, the length of frying time did not significantly change the fatty acid composition of the oil samples extracted from fried potatoes. A major factor influencing the location of mixed oil samples was C20:1 concentration, which was higher than that of the other oil samples analyzed in this study. The higher C18:2 *cis* content of the sunflower oil was also a primary factor affecting the location of those oil samples on the PC1–PC2 plot. In order to obtain more information about the relationship between fatty acid composition and the sample groups, the PC1–PC3 and PC2–PC3 plots were also investigated (Figure 2). The distance between the cluster of mixed oil samples and sunflower oil samples on the PC1–PC3 plots was less than that of the PC1–PC2 plots. This may have resulted from the PC1–PC3 (68.35%) grouping accounting for less of the total variability in the data set when compared to the PC1–PC2 plot (71.21%). Sample 14 was located on the top of the PC1–PC3 and PC2–PC3 plots due to its higher C18:1 *trans* fatty acid content. The location of sample 1 on the PC1–PC3 and PC2–PC3 plots was slightly different from the other samples owing to its higher C18:1 *cis* concentration. The samples fried in margarine were clearly clustered in the lower left quadrant of the PC1–PC3 plot due to C18:2 *trans* fatty acid content.

### 3.2.2. HCA

The dendrogram obtained from HCA is shown in Figure 3, where 4 main clusters are present. The dissimilarities between the samples are principles for grouping the samples based on the similarity of the fatty acid compositions of the oils extracted from the fried potato samples. Cluster 1, which has 4 main subgroups, is composed of the oil samples obtained from different restaurants. Cluster 2 includes samples fried in margarine for different lengths of time. The main factor that distinguishes cluster 1 from cluster 2 is the C18:2 *trans* fatty acid content of the samples

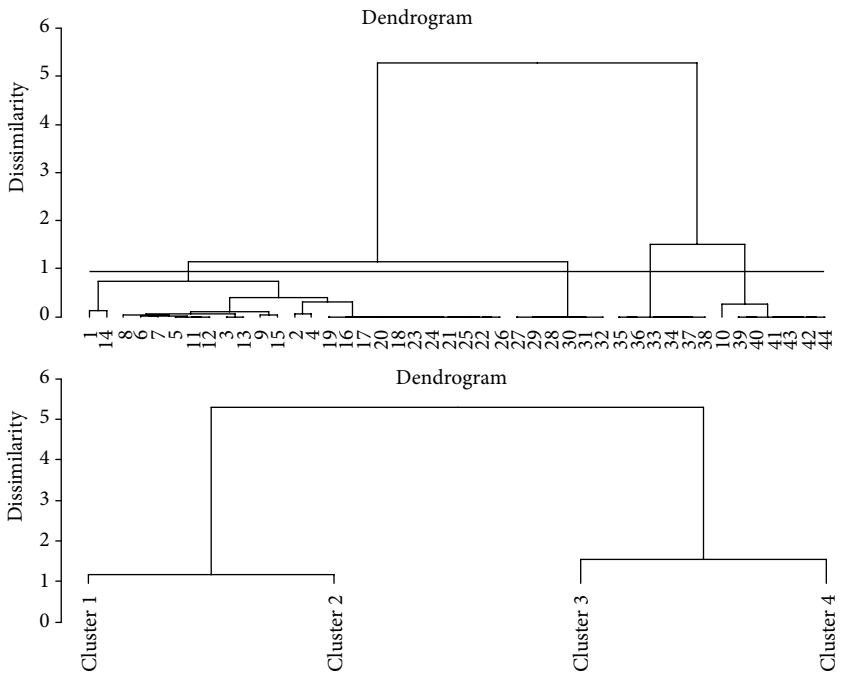


**Figure 3.** Dendrogram for the HCA results using Ward's clustering algorithm with Euclidian distance.

fried in margarine. This result is in accordance with the PCA results (PC1–PC3 plot). A similar result between PCA and HCA was also found in a previous study (Patras et al., 2011). Cluster 3 and cluster 4 consist of samples fried in mixed and sunflower oil, respectively. These findings are also in accordance with the PCA results. Due to its higher C18:2 *cis* and lower C18:1 fatty acid content, sample 10 is located in cluster 4.

In conclusion, this study focused on fatty acid compositions and control of the formation of *trans* fatty acids during the frying process of French-fried potatoes. It examined how the contributions of individual fatty acids are related to generated PCs. Furthermore, the fatty acid composition of French-fried potatoes collected from different restaurants was investigated, and *trans* fatty acid formation was monitored. In general, C18:2 *trans* fatty acid was detected in very small quantities in the samples fried in margarine. Among the samples collected from restaurants, no *trans* fatty acid was detected in the samples collected in the first week, while *trans* fatty acid (lower than 8%) was detected in the extracted oils from French-fried potatoes collected from the same restaurants in the second week. Three PCs that had eigenvalues of higher than 1.0 were constructed, and these were found to be explanatory of more than 84.96% of the total variability in the data set. Four main clusters were obtained from the cluster analysis and the results of HCA were parallel to the results of PCA.

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