

Chemometric Tools to Highlight Possible Migration of Compounds from Packaging to Sunflower Oils

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ABSTRACT: Polyethylene terephthalate (PET) could be considered for the packaging of vegetable oils taking into account the impact of its oxygen permeability on the oxidation of the oil and the migration of volatile organic compounds (VOC) from the polymer matrix. After accelerated aging tests at 40 °C for 10, 20, and 30 days, the headspace of three sunflower oils packed in PET with high density polyethylene caps was carried out using solid phase microextraction. VOCs such as benzene hydrocarbons, ethylbenzene, xylene isomers and diethyl phthalate were identified in vegetable oils by gas chromatography coupled to mass spectrometry. Chemometric tools such as principal components analysis (PCA), independent components analysis (ICA), and a multiblocks analysis, common components and specific weight analysis (CCSWA) applied to analytical data were revealed to be very efficient to discriminate between samples according to oil oxidation products (hexanal, heptanal, 2-pentenal) and to the migration of packaging contaminants (xylene).

KEYWORDS: polyethylene terephthalate, HS-SPME, volatile organic compounds, independent components analysis, common components and specific weight analysis, vegetable oil

■ INTRODUCTION

Food packaging preserves food quality and gives it greater safety assurance against microorganisms and biological and chemical changes from the moment of conditioning to the time of consumption, such that packaging can extend the shelf life of foods.^{1,2} In order to meet the huge demand of the food industry, there has been a remarkable growth in the development of food packaging in the past decades. Nowadays, a large range of plastics are being used as packaging materials, displacing traditional materials such as glass and tinplate.

This growth has been based mainly on the properties of plastic materials, such as low weight, flexibility, competitive cost, and transparency. This versatility was reached by formulations in order to obtain a wide range of properties well adapted for each kind of foodstuff. Packaging materials are made of polymers and include additives such as antioxidants, plasticizers, stabilizers, lubricants, and antistatic and antiblocking agents which are added to maintain or to improve the performance of the polymer material either during processing and fabrication or throughout the shelf life of the packed food.²

Nevertheless, plastics intended to be in contact with food are not inert, and interactions with the packaged food may cause mass transfers from the polymeric structure or from the food in contact. Plastic packaging–food interactions that take place during the shelf life originate in three phenomena: the sorption of food constituents by the packaging, the migration of packaging additives into food, and the permeation which describes the phenomenon of solubilization–diffusion of volatile molecules, organic compounds, water vapor, and gas as oxygen originating from the packaged food and from outside the container.^{3–5}

The existence of food and packaging interactions has led, at the international level (European Union, United States Food and Drug Administration, and Mercosur), to the definition of strict regulations regarding the use of plastic materials that are suited to be in contact with foods. For example, European Union (EU) regulations state that food contact materials (FCM) must not transfer their constituents to foodstuffs in quantities that could endanger human health or bring about an unacceptable change in the composition or deterioration of its organoleptic characteristics.^{6–8}

Vegetable oils, such as olive oils, are usually packed in glass, tinplate, aluminum, or stainless steel containers. Polyethylene terephthalate (PET) bottles are nowadays competitive packaging material for vegetable oils mainly for their low degree of formulation, their transparency, and their ability to be recycled.⁹ Although PET does not contain many additives in comparison with other polymers, some studies identified phthalates (di-2-hexyl ethyl phthalate (DEHP), di-*n*-butyl phthalate (DBP), and diisooctyl phthalate (DiOP)) in PET bottles.^{8,10} Moreover, volatile organic compounds (VOC) are widely distributed in the environment and can also be present in foods either naturally or as contaminants. In particular, benzene, toluene, ethylbenzene, xylene, and the three styrene isomers (ortho, meta, and para) named BTEXs are a subclass of highly volatile organic compounds with boiling points between 80 and 150 °C that

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could contaminate olive oils.¹¹ Komolprasert et al. reported that benzene might migrate into food from contaminated PET bottles.¹² It was also demonstrated that benzene and alkylbenzene could be generated from several types of food contact plastics in high temperature applications.⁵

Methodologies for the characterization of these volatile contaminants were developed using headspace techniques. Several researchers have used headspace gas chromatography mass spectrometry (HS-GC/MS) for the analysis of benzene hydrocarbons in virgin olive oil.^{11,13,14} BTEXs were extracted from other matrices such as soils and water using an headspace-solid phase microextraction (HS-SPME) procedure with a carboxen/polymethylsiloxane fiber (CAR/PDMS).^{15,16} The goal of these analytical approaches was usually to identify the volatile organic compounds and to quantify each substance by means of calibration curves. However when different parameters play a role or are cross-linked in the evolution of the samples, that is, during storage of packed sunflower oil, it is quite difficult to distinguish their effects on the samples. So our approach of using the whole chromatogram as an analytical fingerprint of oil samples, combined with chemometric tools, is quite original. The importance of this methodology lies in conserving all of the information contained in the chromatograms and highlighting the relevant information which allows the discrimination of the samples, here the oxidation of the product during aging and the migration phenomena.

The objective of our work is to develop an HS-SPME procedure to assess the volatile organic compounds present in sunflower oils, aged in accelerated conditions and in contact with PET as a packaging material. Multivariate approaches as principal components analysis (PCA), independent components analysis (ICA), and common components and specific weights analysis (CCSWA) were then applied in order to extract relevant information on the change in sunflower oils from the large GC-MS data set.

MATERIALS AND METHODS

Sunflower Oils Sampling. Three types of sunflower oils were used: an oil "A" (production date: April 2009), an oil "O" (production date: March 2010), an oil "L" (production date: January 2011). They were bought on the Lebanese market and bottled in 1-L PET bottles with HDPE caps. During this study, approximately 200 mL of each oil was packed in three different glass bottles. An accelerated aging was applied to all the samples, in an oven at 40 °C; the analyses were done every 10 days; the aging conditions were chosen according to CE directive 94/48 in order to simulate natural aging, over a period of 30 days, for all oil samples (bottled in PET with HPDE caps and in glass).¹⁷ A total of 21 samples were analyzed in this work.

Headspace Sampling with SPME and GC-MS Analysis. Extraction of volatile compounds was done with a SPME fiber with CAR/PDMS 75 μm at 90 °C. After a preincubation period of 5 min, the volatiles were extracted from the headspace with the SPME fiber during 30 min. The trapped volatiles were then desorbed from the fiber for 5 min at 200 °C in the GC injector port, in split/splitless mode. The instrument used was a HS-SPME coupled to a gas chromatograph (GC, Agilent 6890) with a mass detector (MS, Agilent 5975). Compounds were separated on a fused silica capillary column DB5MS (J & W Scientific 123-5536 IU) 30 m \times 320 μm \times 0.5 μm . The initial oven temperature was 35 °C for 10 min and then a ramp of 5 °C/min until 60 °C which was held 1 min and then ramped up to 200 °C, 9 °C/min and maintained for 2 min. Electron impact mass spectra were recorded under the following conditions: mass range 29–500 m/z ; threshold: 150; sample number 2; scan rate: 4 scan s^{-1} ionization voltage 70 eV. Mass spectral matches were done by comparison with NIST and Wiley mass spectra libraries.

Chemometric Tools. GC-MS chromatograms were assembled in matrices, where each row was a chromatogram of an oil sample, and each column was the intensity at a given retention time. Three chemometric tools were employed: principal components analysis (PCA), independent component analysis (ICA), and a multiblock analysis method, common components and specific weight analysis (CCSWA). The first two techniques were applied to the total ion current chromatograms (TIC), the last one to selected m/z (75, 77, 91, 104, 105, 106, 177) ion chromatograms typical of BTEX and phthalate compounds. Matlab 2007b and the SAISIR toolbox 2008 were used for all the chemometric treatments of data.^{18,19}

Before any chemometric analysis of the data, each matrix was normalized by rows and centered by columns, in order to eliminate any uncontrolled intensity variation in the chromatograms and to highlight the differences among the samples.²⁰

Principal Components Analysis - Principle. PCA is an unsupervised exploratory method. It replaces the original variables (intensity), highly redundant, with synthetic variables, principal components, which contain almost all of the variability and are orthogonal to each other. They correspond to directions of greatest dispersion of samples that are projected onto this new dimension.²¹ In our case, PCA could help in highlighting similarity in studied sunflower oils according to the position of the samples on the scores of the principal components.

Independent Components Analysis - Principle. ICA is a tool for solving problems of blind source separation. The objective of ICA is to find physically significant vectors. ICA attempts to recover original sources, "pure" signals, from a set of measured signals where they are mixed in unknown proportions, by estimating a linear transformation, using a criterion that measures statistical independence among the sources. This may be achieved by the use of higher-order information that can be extracted from the densities of the data. ICA calculates a demixing matrix, W , that approximates the inverse mixing matrix. The pure component signals are recovered from the measured mixed signals by $S = WX$, where X is the data matrix.^{22,23}

Joint approximate diagonalization of eigenmatrices (JADE) is a blind source separation method to extract independent non-Gaussian sources from signal mixtures with Gaussian noise, based on the construction of a fourth-order cumulant array from the data. This algorithm can be used to calculate W .^{24,25} The number of independent components (ICs) can be calculated using the ICA by blocks procedure.²⁶

ICA aims to extract pure signals from a set of mixtures of signals. In this work, sunflower oils samples are characterized by a mixture of pure compounds from HS-SPME analysis, and some of these compounds could result from oil oxidation. ICA will help in distinguishing between these samples according to pure compound signals.

Common Components and Specific Weight Analysis Method - Principle. Common dimension analysis is an implementation of common components and specific weights analysis (CCSWA).²⁴ Several matrices with different numbers of variables describing the same samples are simultaneously studied. CCSWA describes m data tables observed for the same n samples: a set of m data matrices (X) each with n rows, but not necessarily the same number of columns. CCSWA determines a common space for all m data tables, each matrix having a specific contribution ("salience") to the definition of each dimension of this common space.^{22,27}

In this paper the matrices considered for the CCSWA method are the selected ion chromatograms for the different m/z values of the sunflower oil samples. This data analysis method will help in understanding which ions contribute in the distinction between oils due to migration or even oxidation mechanisms.

RESULTS AND DISCUSSION

Migration tests in food contact materials are well established by food authorities (EU Directives 82/711/EC; 85/572/CEE; UNE-EN 1186 of 2002; 2007/19/CE); however, the particular approach applied in this study was a preliminary work to highlight the evolution of these oils in PET bottles comparatively to glass bottles using chemometric tools.

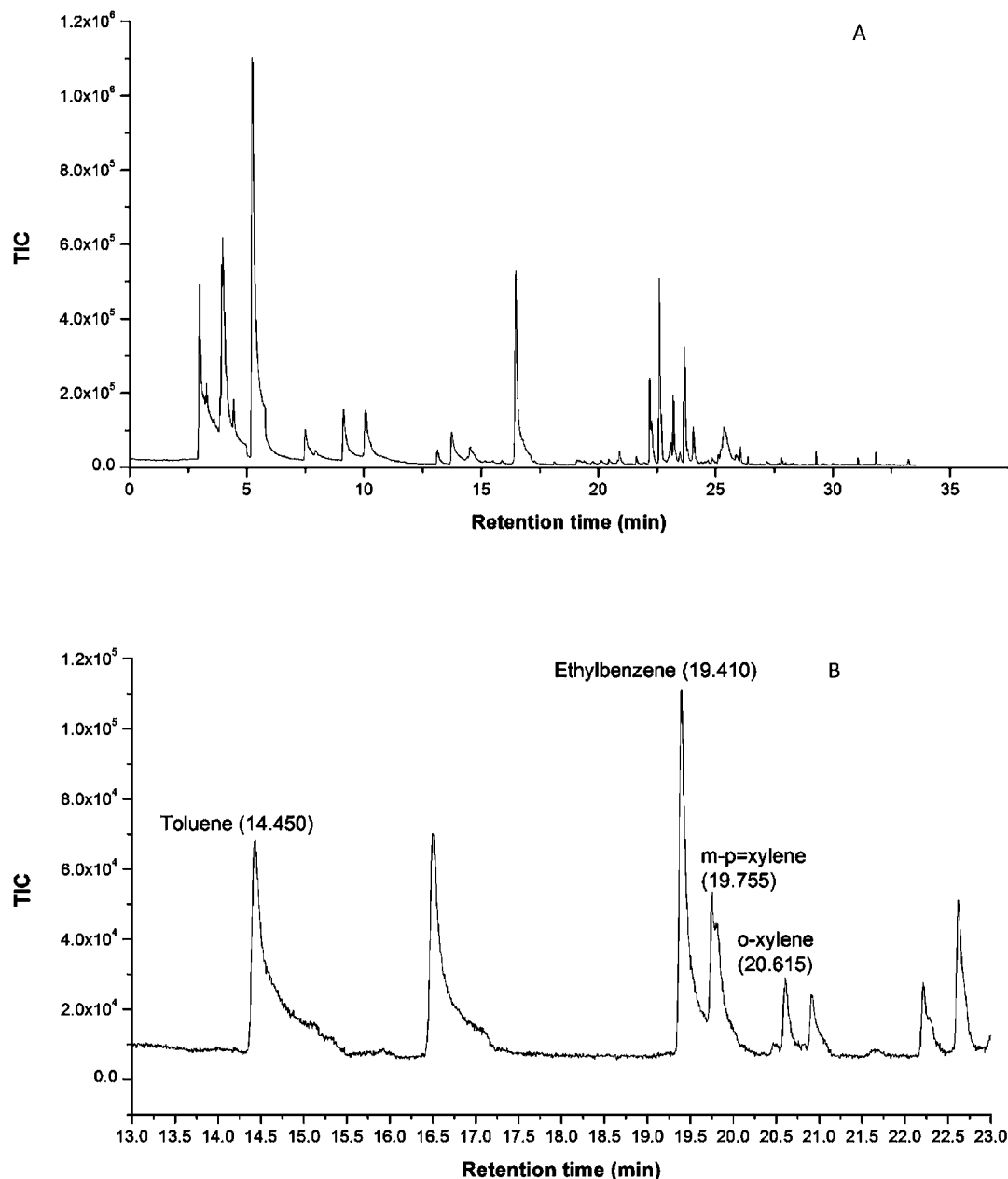


Figure 1. (A) Total ion current (TIC) chromatogram of an oil sample analyzed by HS-SPME-GC-MS, (B) detail of the volatile organic compounds (VOC) area.

Figure 1 is a typical total ion current (TIC) chromatogram of the VOCs analyzed by HS-SPME-GC-MS. The chosen GC area for all the samples is related to the volatile organic compounds (VOC) and phthalates. Table 1 shows an attempt at the identification of the GC peaks present in Figure 1 and their Kovats indices (INRAMASS database). This table highlights that almost all of peaks present in the TIC, such as 2-butenal and hexanal, are related to the oxidation of the studied oils, the others are related to oil natural composition, and there is no apparent information about potential migration of molecules from packaging material. In order to extract this hidden information, we have intentionally chosen several m/z ions of VOCs which are described as potential migrants from packaging materials, as shown in Table 2.^{10,11}

Principal Components Analysis Results. Figure 2A,B represents the main results of the PCA. Four principal

Table 1. Attempt of Identification of GC-MS Peaks and Their Kovats Indices

T_r (min)	tentatively identified component	retention index
7.54	2-butenal	618/627
9.17	1-penten-3-ol	651
10.11	pentanal	674
13.19	2-ethylpropenal	
13.78	2-pentenal	724
15.91	1-octene	782/785
16.50	hexanal	769/771
20.91	<i>n</i> -heptanal	882/879
22.21	1-(1-cyclohexen-1-yl) ethanone	931
22.62	2-heptenal (E)	942
23.21	1-octen-3-ol	959
23.69	2,4-heptadienal (E,E)	966

Table 2. Major Fragments Attribution of Compounds Identified in the Headspace of Sunflower Oils^a

<i>m/z</i>	ion
51	benzene, ethyl-benzene
65	toluene
75	benzene fragment
77	benzene fragment
78	benzene, styrene
91	toluene, ethyl-benzene, <i>o</i>-, <i>m</i>-, <i>p</i>-xylene
92	toluene
103	styrene
104	styrene
105	<i>o</i>-, <i>m</i>-, <i>p</i>-xylene
106	<i>o</i>-, <i>m</i>-, <i>p</i>-xylene, ethyl-benzene
149	diethyl-phthalate (DEP)
150	diethyl-phthalate (DEP)
177	diethyl-phthalate (DEP)

^aIn bold *m/z* ions attribution of the chosen ions.

components (PC) were chosen, representing more than 95% of the variability present in the TICs. The matrix (21*1560) studied had 21 rows (samples) and 1560 columns (intensities at the 1560 retentions times). Three different labels are applied for the same samples: numbers "0", "10", "20", and "30" indicate time, in days,

spent by the samples in the oven at 40 °C; letters "P" and "V" indicate whether they are bottled in PET or in glass respectively, and letters "A", "L" and "O" are the different oils.

Differences between samples are highlighted in their projection on PC1 and PC3 scores (Figure 2A,B) when the presentation is made according to the packaging, even if the three sunflower oils considered in this work have three different packing dates ("A", April 2009; "O", March 2010; "L", January 2011). Hexanal that elutes at 16.26 min is at the origin of the separation between samples bottled in PET or in glass and highlighted in PC1 and PC3. Hexanal is an oxidation product of linoleic acid present in sunflower oil; it seems that when using PET, the oxidation of this polyunsaturated fatty acid is accelerated giving rise to hexanal.²⁸ Our accelerated aging study was done at 40 °C, a relatively moderate temperature. The study by Velasco et al. on virgin olive oil highlighted that at low or moderated temperatures the formation of carbonyl compounds is promoted since the solubility of oxygen is higher in the oil.²⁹ In fact, at this temperature, the solubility of oxygen is important, and it could be that when using PET instead of glass, oxygen transfer through PET bottle occurs and could increase the degradation of molecules sensitive to oxygen. Berlinet et al. showed that the degradation of vitamin C increased when orange juice was packed in PET instead of glass.^{30,31}

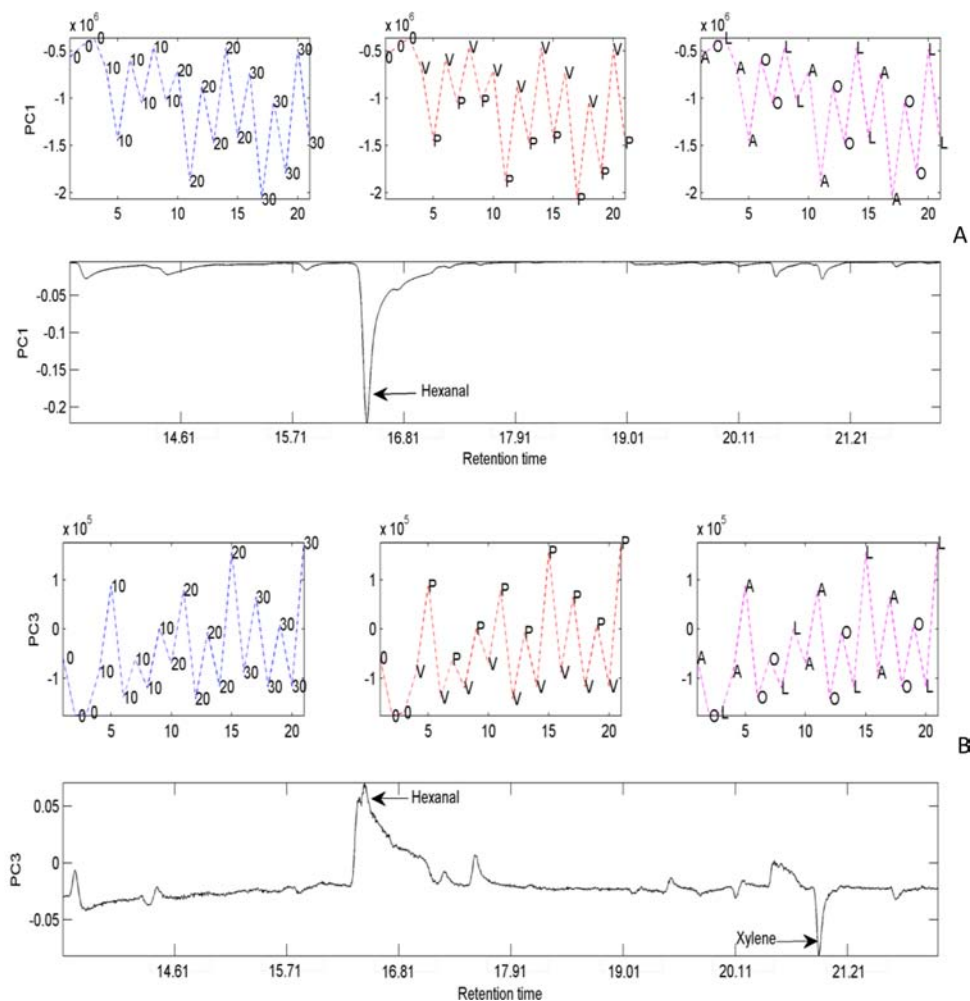


Figure 2. Scores and loadings of PC1 (A) and PC3 (B) resulting from PCA applied on total ion current chromatograms of three types (A, O, L) of sunflower oil samples stored for 0, 10, 20, and 30 days at 40 °C in PET (P) and glass (V).

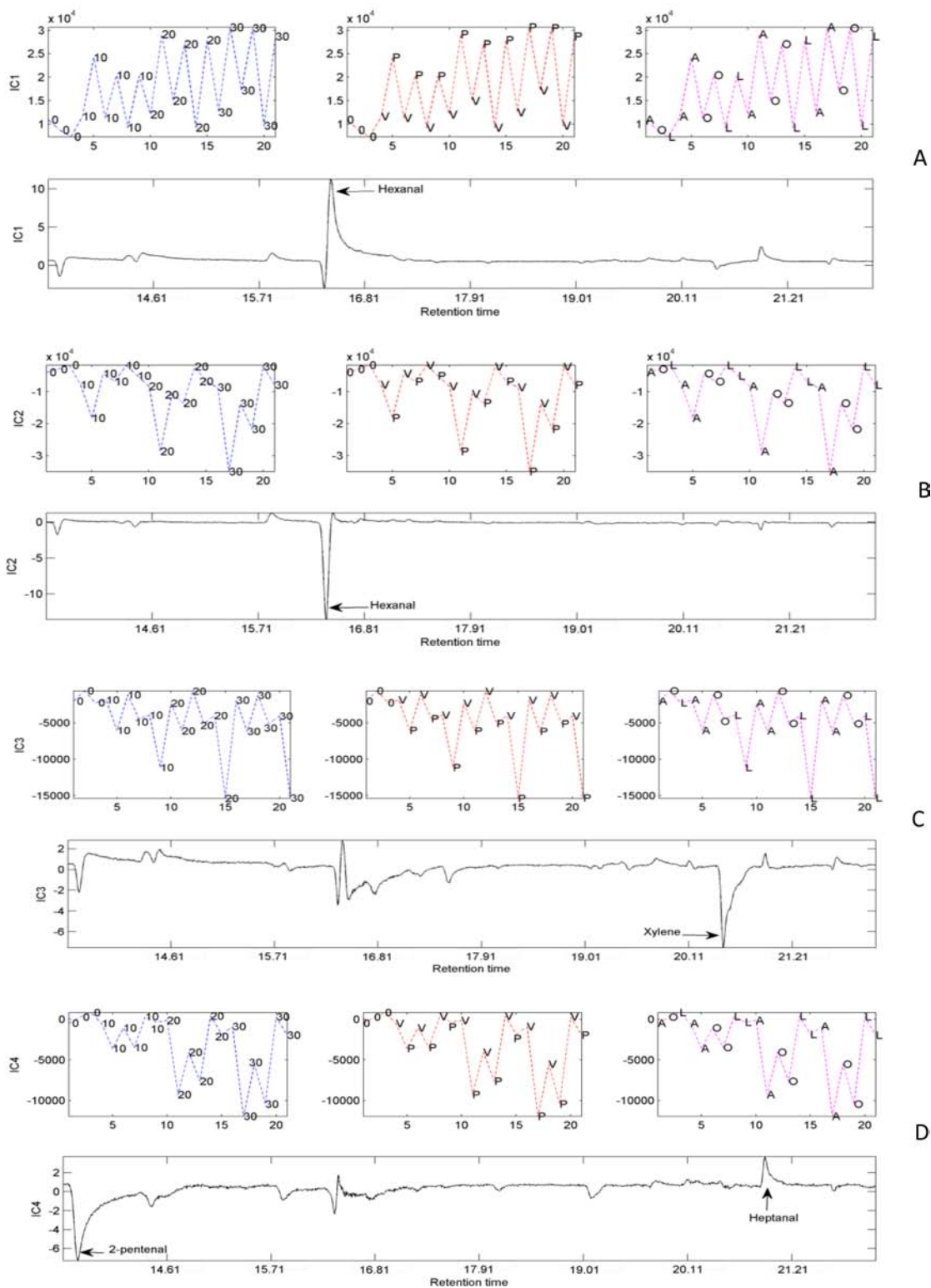


Figure 3. Results of an ICA applied on total ion current chromatograms of three types (A, O, L) of sunflower oil samples stored for 0, 10, 20, and 30 days at 40 °C in PET (P) and glass (V): (A) IC1, (B) IC2, (C) IC3, (D) IC4.

Although PC3 (Figure 2B) shows a second peak at 20.4 min due to xylene, its presence in these oils is probably due to its migration from PET, knowing that xylene is used as a raw material in the production of terephthalic acid, a monomer of the PET. Fabris et al. reported the presence of xylene in Brazilian samples of postconsumer PET flakes.³² PC3 also separates oils bottled in PET from those bottled in glass. PCA only revealed a

limited amount of information, particularly on the molecules which can migrate from PET bottles. Nevertheless the presence of xylene in sunflower oil cannot be unambiguously assigned to packaging as Gilbert-Lopez et al. reported that the BTEXS in olive oils could be due to a biological process in the fruit or the production technology and even a contamination by fuel vapors.¹¹

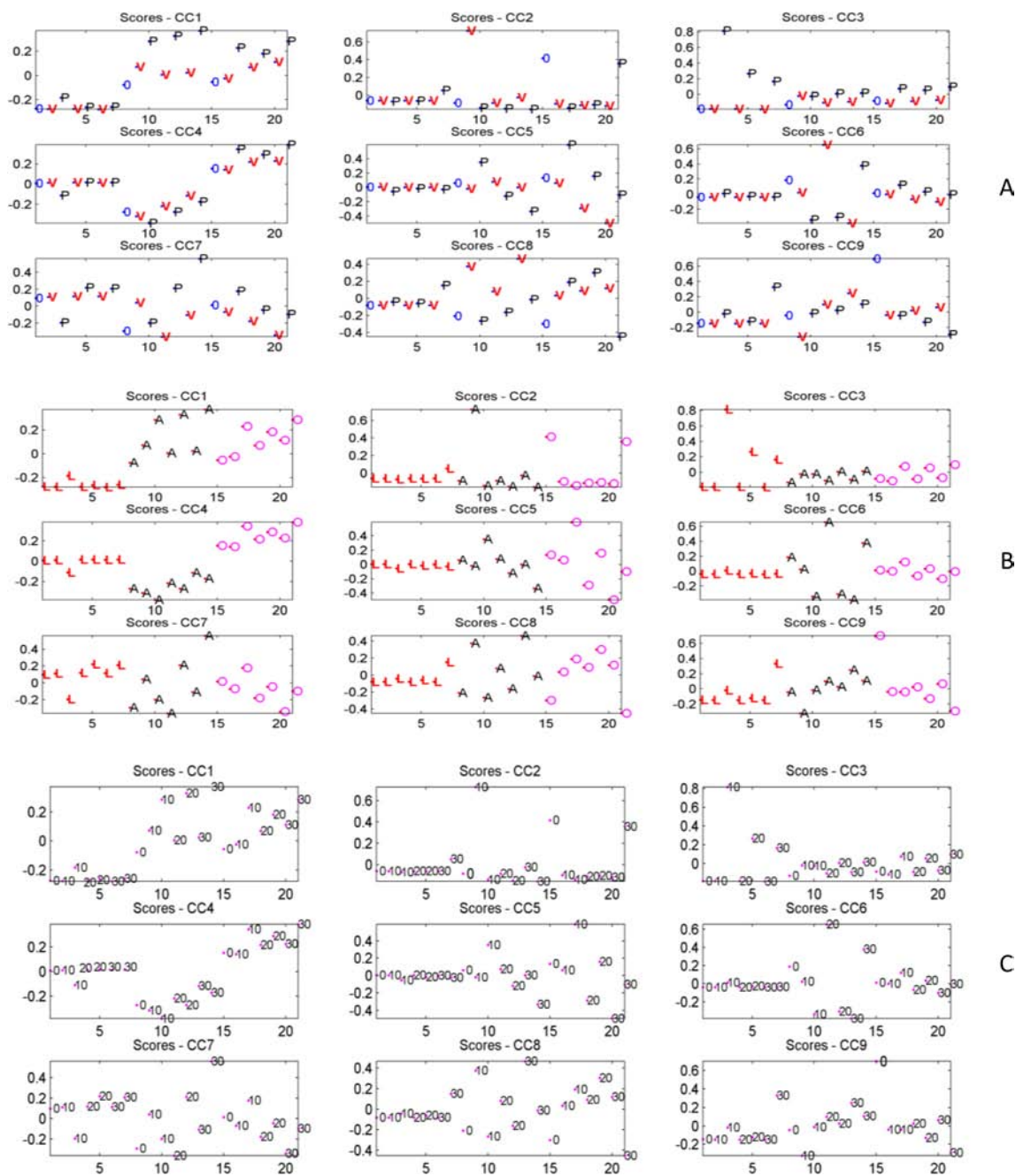


Figure 4. Scores of the nine CCs of CCSWA applied on *m/z* ion chromatograms: (A) Scores labeled according to packaging (P or V), (B) scores labeled according to oil types (A, O, L), (C) scores labeled according to aging time (0, 10, 20, or 30 days).

PCA results highlighted the presence of different degradation and decomposition products in oil issuing from PET manufacturing. The presence of oxygen in the PET melt process at high temperature can promote thermo-oxidative reactions. Belonging to the family of polyesters, the presence of water during the melt process can also induce PET hydrolysis. PET thermal degradation generates subproducts such as oligomers and diethylene glycol. Volatile organic compounds such as aldehydes (formaldehyde, acetaldehyde, benzaldehyde), C_1 – C_4 aliphatic hydrocarbons, aromatic hydrocarbons (benzene, toluene, ethylbenzene, and styrene), esters (vinyl benzoate, methyl acetate), methanol, and acetophenone have been identified in PET samples subjected to temperatures between 200 and 300 °C.³³ These volatile compounds can migrate into

food in contact, in particular, acetaldehyde that leads to sensory defects in drinking water due to its low sensory threshold.³⁴ Some of these molecules such as acetophenone, linear aldehydes, and benzaldehyde were identified in strawberry syrup bottled in PET after 225 days of storage.³⁴

Because of the limited results obtained using PCA, two other chemometric tools, ICA and CCSWA, were applied to the data.

Independent Components Analysis Results. The number of independent components (ICs) was determined by ICA-by-blocks; the data set was divided into two representative blocks and the signals extracted by applying ICA on each block were compared.²⁶ Four ICs were shown to be present in both blocks of samples. The JADE algorithm was used for the ICA. The first IC (Figure 3A) shows that the hexanal peak eluting at

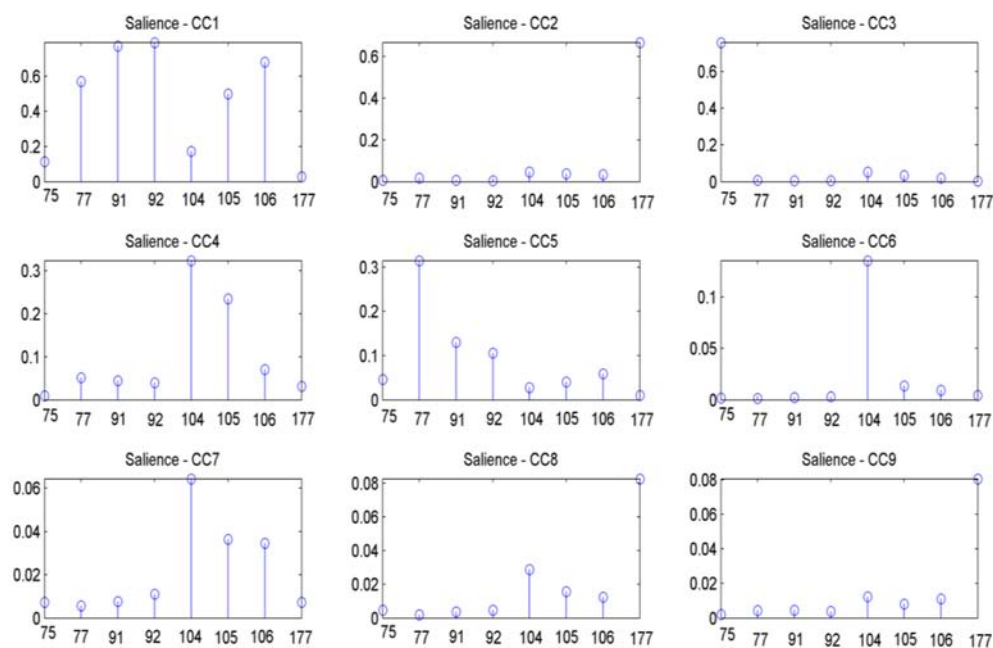


Figure 5. Saliences of the nine CCs of CCSWA results applied on eight m/z ions chromatograms. (75; 77; 91; 92; 104; 105; 106; 177).

16.26 min is at the origin of the separation between oils bottled in PET and in glass, independently of the duration of aging and of the oil sample. This result is comparable to PC1 results; however, the separation between samples is clearer. In the same way, samples packed in PET can be distinguished from other samples by IC2 (Figure 3B). This distinction is due to hexanal that is present in higher concentrations in samples bottled in PET and in the older oil "A". According to IC2, at each analysis time, oils bottled in PET are positioned below oils bottled in glass. For the oldest oil A packed in PET, one can notice its discrimination from the others accordingly to the increase of the hexanal amount during the aging. IC3 (Figure 3C) shows a clear separation of oil samples due to the xylene peak at 20.4 min. It clearly appears that the oil "L" (production date: 2011) is more affected by the migration of xylene from plastic packaging. Knowing that the diffusion coefficient of xylene in PET is in the range of 10^{-17} to 10^{-18} m^2/s , it is theoretically very difficult to highlight its presence in this youngest oil.³⁵ However Figure 3C indicates a particular behavior of this oil related to xylene which migrates after 10 days of accelerated aging. The effect of xylene on the oil "L" is significantly different from that on the oils "A" and "O" (Figure 3C). IC3 highlights the migration that occurred after 10 days aging in the younger oil. Comparing the information in IC2 and IC3, it is clear that IC2 is related to the oxidation that happened in the oils during the aging and IC3 to the migration. After the first 10 days, according to IC3, the position of both old oils has changed due to a change in xylene for these two oils. An equilibrium is established due to the partition coefficient of this molecule between the oil and its packaging that could be considered as having two parts: the PET bottle and the HDPE caps, each of which could release contaminant molecules. Both origins could be considered for the presence of xylene into the oils. The manufacture of PET, semicrystalline polymer, involves several steps among them synthesis which has the potential to leave some residues in the resin.³³ In particular, *p*-xylene is primarily used as a feedstock for terephthalic acid and thus is a key component in PET resins. Another contamination source for xylene could be the caps that are used for PET bottles.

Indeed these caps, made of polyolefin, could easily absorb contaminants such as BTEX and phthalates since they have a rubber structure at room temperature. Xylene could have passed from a contaminated cap through the head space into the bottled oil.

IC4 (Figure 3D) reveals a comparable behavior of samples "A" and "O" (2009 and 2010) according to the duration of accelerated aging and packaging. 2-Pentenal discriminates between oils "A" (bottled in PET) and "O" (bottled in PET and glass) from oil "L". 2-Pentenal is an oxidation product of vegetable oils and responsible for off-flavors in olive oil and indicator of rancidity.³⁶ Heptanal also plays a minor role in the discrimination of the three oils. The content of this aldehyde is higher in the youngest oil L. Hämäläinen et al. reported in 2002 that a probable origin of the heptanal could be the β -scission of the alkoxy radical formed from 12-hydroperoxy-*trans*-8, *trans*-10-octadecadienoate, in turn reported to be one of the hydroperoxides formed in oxidized *cis*-9, *trans*-11 conjugated linoleic acid.³⁷

In summary, ICA highlighted a double packaging effect, on the degradation (composition) of the oils, that is, the migration of volatile organic compounds and the oxidation of oils exacerbated by the entrance of oxygen through the packaging, resulting in the development of oxidation products such as hexanal and heptanal.

Common Components and Specific Weight Analysis – CCSWA – Results. Nine common components (CC) were extracted. Three presentations for these CCs are shown in Figure 4A–C: the first one according to packaging material ("P" or "V"), the second for oils type ("L", "A", "O"), and the third for aging time (10, 20, and 30 days). Scores on the first Common Component (CC1) highlights a distinction between samples bottled in PET and in glass (Figure 4A) for oils "A" and "O", the oldest oils; however this behavior is not shown for oil "L" (Figure 4B). Looking at the salience of CC1 (Figure 5) it can be seen that ions with m/z equal to 77, 91, 92, 105, and 106 corresponding to three VOCs, benzene fragment, ethyl-benzene, and xylene are practically the only ions contributing to CC1. These volatile compounds are present in larger amounts in older oils due to

their migration from the packaging throughout storage at room temperature before aging test.

The third common component (CC3), presented in Figure 4A, distinguishes oils bottled in PET from those packed in glass, the main difference being for oil "L", the youngest oil (Figure 4B). When examining CC3 in Figure 4C, the scores of L decrease with aging. The salience of CC3 (Figure 5) shows that the ion with m/z equal to 75 is the only fragment contributing to this salience. After investigating the extracted ion chromatogram of the oils L packed in PET bottles, according to $m/z = 75$, 2-*tert*-butyl benzoquinone was identified as the compound probably contributing to the discrimination. The presence of this molecule in oils L packed in PET could be due to two factors. According to the first one, 2-*tert*-butyl-benzoquinone is the primary and major oxidation product of 2-*tert*-butylhydroquinone used as antioxidant in vegetable oils.^{38,39} The second reason relates the presence of this molecule to a migration from PET packaging since it could be a degradation product of antioxidants along with 2,6-di-*tert*-butyl benzoquinone which have structures similar to antioxidants such as Irganox and Irgafos used in plastic formulations.⁴⁰

Knowing that benzene is a volatile organic compound, with the lowest boiling point 80 °C of all the studied VOC (toluene, 111 °C; ethylbenzene, 136.5 °C; xylene, 137–144 °C), it is very likely that during the accelerated aging benzene evaporates from the oil probably due to permeation through the caps used. The benzene fragment could be an oxidation product of the sunflower oil. Indeed, Guillen et al. reported the presence of a benzene fragment in the headspace of two sunflower oils bottled at room temperature for 112 months having different air/oil volume ratio.⁴¹ Both IC3 and CC1 results highlight migration phenomena. IC3 emphasizes the xylene role, while CC1 emphasizes complementary information related to other migrating molecules, benzene and ethylbenzene. It is also possible that the presence of benzene results from its migration from HDPE caps as Skjevraak et al. identified it as one of the VOCs migrating from HDPE pipes into drinking water.⁴²

CC4 discriminates between the three studied oils independently from the aging. This distinction is due to the presence of styrene and xylene, probably due to an external contamination of the oils not related to packaging nor aging.

The presence of phthalates in packaging materials and their migration into packaged foods were confirmed by numerous authors from various packaging materials.^{43–47} Moreover, exposure to phthalates has been of increasing concern due to the findings from toxicology studies on animals and identified as endocrine disruptors for humans.^{47,48} So information on levels of phthalates in food is important for human exposure assessment, and one way to reach this goal is to develop new methodological approaches. Even though phthalates were present in our oil samples, they did not contribute to the discrimination between these samples; their presence is probably due to an ubiquitous contamination.

In the case of CC5 and CC8, it can be seen that they do not discriminate the different sunflower oil samples. Information contained in these CCs is not specific for an aging time, an oil type, or a packaging material.

CONCLUSION

In our study we combined GC data and the chemometric tools PCA, ICA, and CCSWA. These three techniques were very efficient in extracting relevant information from GC chromatograms of volatile organic compounds present in sunflower oils.

PCA and ICA applied on the TIC profiles highlighted the impact of the packaging storage on the composition of the sunflower oil. Discrimination between the migration and oil oxidation phenomena can be revealed by the presence of xylene and hexanal. Moreover, the ICA results brought additional information on the importance of 2-pentenal and heptanal as oxidation products in the oil samples discrimination. CCSWA suggested that the presence of VOCs such as xylene and benzene fragments could be due to an external contamination and/or potential migration from the packaging material, bottle, or cap.

In this paper, a hyphenated methodology of HS-SPME-GC-MS followed by multivariate analysis was developed and proved effective in the context of the interaction of food with packaging. The originality of this hyphenated methodology was that it was able to highlight separately different phenomena such as migration of specific VOCs from the glassy polymer PET and polyolefin caps into sunflower oils, external contamination of the samples, and the oxidation of oil during storage.

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Notes

The authors declare no competing financial interest.

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