



# Evaluation of extra virgin olive oil stability by artificial neural network



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## ABSTRACT

The stability of extra virgin olive oil in polyethylene terephthalate bottles and tinfoil cans stored for 6 months under dark and light conditions was evaluated. The following analyses were carried out: free fatty acids, peroxide value, specific extinction at 232 and 270 nm, chlorophyll,  $L^*C^*h$  color, total phenolic compounds, tocopherols and squalene. The physicochemical changes were evaluated by artificial neural network (ANN) modeling with respect to light exposure conditions and packaging material. The optimized ANN structure consists of 11 input neurons, 18 hidden neurons and 5 output neurons using hyperbolic tangent and softmax activation functions in hidden and output layers, respectively. The five output neurons correspond to five possible classifications according to packaging material (PET amber, PET transparent and tinfoil can) and light exposure (dark and light storage). The predicted physicochemical changes agreed very well with the experimental data showing high classification accuracy for test (>90%) and training set (>85). Sensitivity analysis showed that free fatty acid content, peroxide value,  $L^*C^*h$  color parameters, tocopherol and chlorophyll contents were the physicochemical attributes with the most discriminative power.

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## 1. Introduction

Auto-oxidation and photo-oxidation are the main oxidation mechanisms during processing and storage of edible oils (Choe, Lee, & Min, 2005). Lipid oxidation is unleashed by factors, such as oxygen availability, the presence of light and temperature. If certain limits of lipid oxidation products (hydroperoxides, conjugated dienes and trienes) are exceeded and/or rancid off-flavors occur, the olive oil may lose the permission to carry the label “extra virgin” or even “virgin” (Hrnčirik & Fritzsche, 2005). Furthermore, the protective role of olive oil in fighting certain diseases has been attributed to its fatty acid composition and the presence of minor constituents, mainly phenolic compounds, tocopherols and squalene. The oxidation process can reduce the content of its antioxidants components, decreasing the stability and the nutritional characteristics of the oil. However, it can be said that auto-oxidation of virgin olive oil during storage is an extremely slow process if technology delivers products with low initial peroxide/ $K_{232}$  values and high levels of polar phenols/ $\alpha$ -tocopherol content. Exclusion of air in bottled virgin olive oil is a prerequisite (Tsimidou, 2006).

The effect of some storage conditions and/or packaging material on extra virgin olive oil quality was studied by several authors (Cecchi, Passamonti, & Cecchi, 2010; Lozano-Sánchez et al., 2013; Méndez & Falqué, 2007; Pristouri, Badeka, & Kontominas, 2010; Psomiadou & Tsimidou, 2002; Sacchi et al., 2008). Psomiadou and Tsimidou (2002) studied the photo-oxidation of virgin olive oil and concluded that to preserve the precious characteristics of the oil, it is necessary to change practices of bottling and use dark glass bottles or paper bags as much as possible. The container can directly influence the olive oil quality, by protecting the product from oxygen and light. The materials used for packing olive oil include glass, metal and, more recently, plastics. Tinfoil cans have long been used to package oils and continue to show promise due to a variety of advantages. They offer total protection against light, oxygen and water vapor, and resist various types of mechanical damage. The inside of the can is coated with resins which protect the metal surface against corrosion (Piergiovanni & Limbo, 2009). Of the plastics, polyethylene terephthalate (PET) has conquered a large slice of the retail market for olive oil storage due to its numerous advantages, including transparency, chemical inertness and excellent mechanical properties. Consumers usually prefer transparent packaging because the oil is visible, but this is not scientifically advisable since photo-oxidation takes place easily in transparent glass.

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Artificial neural network (ANN) is a mathematical algorithm with the capability of relating the input and output parameter, learning from examples through iteration without requiring a prior knowledge on the relationships between the process variables (Cevoli et al., 2011). The use of the ANN for data processing can be characterized by analogy with biological neurons (Kruzlicova et al., 2009). The main advantages of ANN are its nonlinearity, allowing better fit to the data; noise insensitivity, providing accurate prediction in the presence of uncertain data and measurement errors; high parallelism, which implies fast processing and hardware failure tolerance; learning and adaptability, allowing the system to update (modify) its internal structure in response to changing environment and generalization, enabling application of the model to unlearned data (Debska & Guzowska-Świder, 2011).

Nowadays, there is an increasing interest application of neural networks as problem solving algorithms to perform mapping, regression, modeling, clustering, classification and multivariate data analysis (Marini, Bucci, Magrì, & Magrì, 2008; Marini, Magrì, & Bucci, 2007). The flexibility of neural network predestines them to deal with highly non-linear problems and any kind of data. The artificial neural networks have also been applied in quality control of many food products (Berrueta, Alonso-Salces, & Héberger, 2007; Debska & Guzowska-Świder, 2011; Huang, Kangas, & Rasco, 2007), including rice (Marini, Balestrieri, Bucci, Magrì, & Marini, 2003), coffee (Bona, Da Silva, Borsato, & Bassoli, 2011), olive oil (Cajka, Riddellova, Klimankova, et al., 2010; Torrecilla, Cancilla, Matute, & Díaz-Rodríguez, 2013), tea (Cimpoi, Cristea, Hosu, Sandru, & Seserman, 2011; McKenzie, Jurado, & de Pablos, 2010; Palacios-Morillo, Alcázar, de Pablos, & Jurado, 2013), fruit juices (Gestal et al., 2004, 2005), wine (Baykal & Yildirim, 2013), beer (Cajka, Riddellova, Tomaniova, & Hajslova, 2010; Cetó, Gutiérrez-Capitán, Calvo, & Del Valle, 2013) and other alcoholic beverages (Alonso-Salces et al., 2004; Ceballos-Magaña et al., 2013; Jack & Steele, 2002).

This work aimed to evaluate the influence of packaging material (tinplate cans, transparent and amber-colored PET bottles) and light exposure conditions (under light and in the dark) on the stability of physicochemical characteristics of extra virgin olive oil using artificial neural network as discriminative and classification technique.

## 2. Materials and methods

### 2.1. Sample preparation

The experiment was carried out with a sample of extra virgin olive oil of Portuguese origin, from the same batch and manufacturer. The olive oil was manually divided into the following containers: transparent and amber-colored PET 275 ml bottles with a wall thickness of  $0.4 \pm 0.07$  mm; and in cylindrical tinplate cans with a total volume of 350 ml. The olive oil was filled into 36 units of each type of PET bottles and 18 units of tinplate cans, leaving a 10% headspace. The PET bottles were closed by induction using a laminated seal with aluminum foil and a polypropylene (PP) screw-top cap.

### 2.2. Storage

The olive oil subsamples filled into PET bottles were divided into two groups and stored under different conditions: in cardboard boxes protected from the light ( $52 \pm 8\%$  RH/ $25 \pm 2$  °C); and with incidence of light for 12 h/day ( $47 \pm 10\%$  RH/ $26 \pm 2$  °C). The subsamples evaluated in the photo-oxidation trial were stored in a  $200 \times 100 \times 100$  cm light chamber adapted with two 32 W power fluorescent lamps (Osram FO 840 Lumilux Cool/White) with

light intensity of 3000 lux, at a distance of 70 cm. The subsamples were rearranged weekly to guarantee uniformity of light exposure. The olive oil filled into cans was only stored in the dark. The subsamples were stored for 6 months. The storage was performed under accelerated conditions, using higher values of light intensity than that used in commercial storage.

### 2.3. Physicochemical analyses

#### 2.3.1. Free fatty acids (FFA)

These were determined using method Ca 5a-40 (AOCS, 2004), and the results for free fatty acid content expressed as percent oleic acid.

#### 2.3.2. Peroxide value

This was determined using method Cd 8b-90 (AOCS, 2004), and the results expressed as milliequivalents of active oxygen per kilogram of olive oil (meq O<sub>2</sub>/kg).

#### 2.3.3. Specific extinction coefficient

This was determined using method Ch 5-91 (AOCS, 2004) in a Beckman model DU-70 UV/Visible spectrophotometer, reading the absorption at wavelengths of 232 and 270 nm using 1 cm thick quartz cuvettes and a reference of isooctane.

#### 2.3.4. Chlorophyll content

This was determined using method Ch 4-91 (AOCS, 2004) in a Perkin Elmer model Lambda 20 UV/Visible spectrophotometer, and estimated using the equation:  $C$  (mg Pheo a/kg of oil) =  $345.3 (A_{670} - 0.5A_{630} - 0.5A_{710})/L$ , where  $A_{\lambda}$  is the absorbance of the oil at the respective wavelength and  $L$  the thickness of the cuvette in mm.

#### 2.3.5. $\alpha$ -Tocopherol

This was determined using method Ce 8-89 (AOCS, 2004) by high performance liquid chromatography (HPLC) in a Perkin Elmer Series 200 chromatograph with isocratic elution in a mobile phase of n-hexane/2-propanol (99:1 v/v) and a Hibar RT  $250 \times 4$  mm Li Chrosorb Si 60.5 mm analytical column, mean flow rate of 1.0 ml/min, and LC 240 Perkin Elmer fluorescence detector programmed for excitation at 290 nm and emission at 330 nm.

#### 2.3.6. Total phenolic compounds

An adaptation of the method proposed by Gutfinger (1981) was used. The phenolic compounds were measured in the polar fraction obtained from 10 g olive oil dissolved in hexane and extracted by washing three times with a methanol:water (60:40 v/v) solution. The procedure consisted of reacting a 0.5 ml aliquot of the extract with 0.5 ml Folin-Ciocalteu reagent plus 1.0 ml of a saturated Na<sub>2</sub>CO<sub>3</sub> solution, leaving the mixture at rest for 1 h in the dark. Subsequently the adsorption was read in the visible region (760 nm) of a UV/Visible spectrophotometer. The result was expressed in equivalents of gallic acid using a standard curve from 10 to 100  $\mu$ g gallic acid/ml.

#### 2.3.7. Instrumental color analysis

This was carried out using the Hunterlab model Colorquest II, hue of 10°, illuminant D65 and the CIE L\*a\*b\* color system for the total transmittance of each sample in an optically clean glass cuvette with a 10 mm optical path.

#### 2.3.8. Squalene

This was determined by high performance liquid chromatography (HPLC) in a Perkin Elmer Series 200 chromatograph according to the method proposed by Nenadis and Tsimidou (2002), with isocratic elution in a mobile phase of acetone/acetonitrile (40:60 v/v)

in a Nucleosil C18 (250 mm × 4.0 mm × 5 μm) (Hichrom, Berkshire, UK) analytical column with a mean flow rate of 1.0 ml/min and UV/Visible detector at a wavelength of 208 nm.

### 2.3.9. Luminous transmittance

Determined using Agilent 8453 spectrophotometer UV/Visible transmittance spectrum with the scanning range of 190–1100 nm according to the methodology ASTM D1003-07 (2007).

### 2.3.10. Oxygen transmission rate

Determined by coulometric method using Oxygen Permeability OX-TRAN model 2/61 MJ (Modern Company Inc. – MOCON) according to the methodology ASTM F1307-02 (2007).

## 2.4. Artificial neural network modeling

The role of the ANN is to transform the input information into the output one. During the training process the weights are corrected to produce output values as close as possible to the target values (Kruzlicova et al., 2009). The main advantages include a high modeling performance, being especially suited to nonlinear sensor responses, and being very much related to human pattern recognition (Cetó et al., 2013). The propagation of the signal through the network is determined by the weights associated to the connections between the neurons, which represent the synaptic strengths in biological neurons. The goal of the training step is to correct the weights  $w_{ij}$  so that they will give a correct output vector  $y$  (as close as possible to the known target vector ( $d$ )) for the input vector  $x$  from the training set. After the training process has been completed successfully, it is hoped that the network will give a correct prediction for any new object  $x_n$ , not included in the training set (Kruzlicova et al., 2009). The hidden ( $x_i$ ) and output ( $y_i$ ) neuron activities are defined as follow:

$$x_i = f(v_i) \quad (1)$$

$$y_i = f(v_i) \quad (2)$$

where  $f(v_i)$  is the activation function applied in the hidden or output layers. In this study, the activation functions evaluated in the hidden and output layers were: linear function, logistic sigmoid function, hyperbolic tangent function, softmax function, exponential function and Gaussian function, which are described in Eqs. (3)–(8), respectively.

$$f(v_i) = v_i \quad (3)$$

$$f(v_i) = \frac{1}{1 + e^{-v_i}} \quad (4)$$

$$f(v_i) = \frac{e^{v_i} - e^{-v_i}}{e^{v_i} + e^{-v_i}} \quad (5)$$

$$f(v_i) = \frac{e^{v_i}}{\sum_{j=1}^n e^{v_j}} \quad (6)$$

$$f(v_i) = e^{-v_i} \quad (7)$$

$$f(v_i) = ae^{-\frac{(v_i-b)^2}{2c^2}+d} \quad (8)$$

where  $a$ ,  $b$ ,  $c$  and  $d$  are some constants,  $e$  is the Euler's number ( $e \approx 2.71828$ ), and  $v_i$  is the net signal which correspond to the sum of the weighted inputs from the previous layer given by:

$$v_i = \sum_{j=1}^p w_{ij}x_j + b_i \quad (9)$$

where  $j = 1, p$  concerns neurons  $x_j$  in the previous layer which precede the given neuron  $i$ ,  $w_{ij}$  is the weight and  $b_i$  is the bias (offset).

The bias is an extra input added to neurons which allows a representation of phenomena having thresholds. Each neuron consists of a transfer function expressing internal activation level. Output from a neuron is determined by transforming its input using a suitable transfer function, which can be linear or nonlinear depending on the network topology (Bahramparvar, Salehi, & Razavi, 2013).

The ANN modeling was performed by software STATISTICA 8.0 (StatSoft Inc., Tulsa, OK, USA), using a multilayer perceptron (MLP) (Maren, Harston, & Pap, 1990) and radial basis function (RBF) (Debska & Guzowska-Świder, 2011) network, to predict the packaging material and storage conditions of extra virgin oil samples through physicochemical analyses (Cruz et al., 2011, 2009). During training, weighting functions for the inputs to each ANN were determined, such that the predicted outputs best matched the actual outputs from the dataset. Multiple ANN topologies were assayed employing different numbers of hidden layers (1–3) and hidden neurons (4–34 neurons). The number of neurons in the hidden layer was obtained by trial and error. The number of input neurons was fixed as the number of input variables into the neural network, which in this case was comprised by eleven physicochemical attributes: free fatty acids content, peroxide value, extinction coefficients  $K_{232}$  and  $K_{270}$ , chlorophyll content,  $L^*C^*h$  color parameters, tocopherol, squalene and total phenolic contents. The output layer was made of five neurons corresponding to five possible classifications according to packaging material (PET amber, PET transparent and tinplate can) and light exposure (dark and light storage).

The dataset used in ANN modeling was composed of 6 replicates of each 5 storage conditions studied, which were analyzed from 0 to 6 months, totalling 210 data. These data were randomly allocated into training set (75%) and test set (25%) for all network topologies tested. The use of replicates instead of mean values during ANN modeling helps to evaluate not only the mean variation, but also their deviation range in the model. The training set was used to calculate the transfer function parameters of the network and the test set is used to estimate correct classification, which indicates if the neural network is performing well. An ideal network would classify all sets correctly. The aim of the neural network training is to minimize the error function by changing the weights and offsets. In the error functions estimative, each predicted output value ( $O_i$ ) is compared against the experimental target value ( $T_i$ ) to test of network performance. They can either be the mean square error (MSE) (Eq. (10)), such as when BP-MLP is being used, or cross entropy (CE) (Eq. (11)) for the RBF model. The training step was finished when the MSE and CE converged and was less than 0.0001. If the error function did not converge, training was completed after 500,000 epochs, where an epoch represents one complete sweep through all the data in the training set:

$$MSE = \frac{\sum_{i=1}^N (O_i - T_i)^2}{N} \quad (10)$$

$$CE = \frac{\sum_{i=1}^N T_i \ln O_i + (1 - T_i) \ln (1 - O_i)}{N} \quad (11)$$

where  $O_i$  is the  $i$ th predicted output value,  $T_i$  is the  $i$ th observed target value and  $N$  is the number of data.

## 2.5. Statistical analysis

A random block design was used with a minimum of 3 repetitions, fixing the storage time and type. The results were submitted to an analysis of variance with an  $F$  test at 5% of probability, the means being compared by Tukey's test at 5% of probability. Sensitivity analysis was conducted to provide a measure of the relative impact of each input of the neural network model on the outputs.

**Table 1**  
Peroxide values, extinction coefficients and total phenolic compound concentrations in extra virgin olive oil during storage time.

Time (months)	PV (meq O <sub>2</sub> /kg)						K <sub>232</sub>						K <sub>270</sub>					
	Light			Dark			Light			Dark			Light			Dark		
	PET	PET	Can	PET	PET	Can	PET	PET	Can	PET	PET	Can	PET	PET	Can	PET	PET	Can
	amber	transparent	transparent	amber	transparent	transparent	amber	transparent	transparent	amber	transparent	transparent	amber	transparent	transparent	amber	transparent	transparent
0	7.27 A d	7.27 A c	7.27 A d	7.27 A d	7.27 A c	7.27 A d	1.85 A b	1.85 A b	1.85 A b	1.85 A b	1.85 A b	1.85 A c	0.17 A d	0.17 A c	0.17 A b	0.17 A b	0.17 A bc	0.17 A
1	17.40 A a	17.64 A a	15.30 B	15.30 B	10.24 C b	10.06 C c	2.54 A a	2.42 A a	2.42 A a	2.47 A a	2.47 A a	2.48 A ab	0.22 A bc	0.24 A ab	0.22 A a	0.22 A a	0.21 AB a	0.18 B
2	13.39 A	12.77 A b	12.85 A c	12.85 A c	14.12 A a	12.51 A	2.11 BC	1.93 C ab	2.29 BC	2.29 BC	2.29 BC	2.82 A a	0.22 A bc	0.22 A b	0.19 A ab	0.19 A ab	0.20 A ab	0.19 A
3	12.93 A c	12.26 A b	12.68 A c	12.68 A c	12.34 A a	11.55 A	2.09 A ab	2.30 A ab	2.46 A a	2.46 A a	2.46 A a	2.21 A bc	0.20 B cd	0.25 A ab	0.16 C b	0.16 C b	0.18 BC abc	0.17 C
4	14.90 AB	11.90 C b	15.81 A a	15.81 A a	13.45 BC a	14.26 AB	2.27 A ab	2.23 A ab	2.40 A a	2.40 A a	2.40 A a	2.19 A bc	0.24 A b	0.26 A ab	0.16 B b	0.16 B b	0.14 B c	0.16 B
5	13.18 A	11.27 B b	13.61 A	13.61 A	13.20 A a	10.84 B	2.18 A ab	2.05 A ab	2.47 A a	2.47 A a	2.47 A a	2.11 A bc	0.25 A b	0.26 A ab	0.16 B b	0.16 B b	0.19 B ab	0.17 B
6	13.54 A	12.67 A b	13.44 A	13.44 A	12.84 A a	12.38 A	2.56 A a	2.03 B ab	2.52 A a	2.52 A a	2.52 A a	2.33 AB	0.29 A a	0.26 A a	0.19 B ab	0.19 B ab	0.18 B ab	0.18 B
	bc	bc	bc	bc	bc	ab						abc						a

\* Means followed by the same capital letter in the same line and by the same small letter in the same column do not differ at the 5% level of probability according to Tukey's test.

### 3. Results and discussion

#### 3.1. Characteristics of PET bottles

PET containers used to bottle the olive oil showed irregular thickness, and the means for transparent and amber bottles were  $0.40 \pm 0.09$  mm and  $0.34 \pm 0.06$  mm, respectively. The transmittance of the amber packaging showed a peak of 20% in the visible light region (>600 nm) and the transparent ones showed high levels of transmittance (>75%) in the UV (300 nm) and throughout out the visible light region. The bottles showed low oxygen permeability of  $0.03 \pm 0.001$  cm<sup>3</sup>/(pkg day).

#### 3.2. Stability of the extra virgin olive oil

The sample of extra virgin olive oil was conformed to the classification criteria of the [European Regulation \(2013\)](#) for extra virgin olive oil.

The free fatty acid content was not greater than 0.18 g/100 g (expressed as oleic acid) in any of the treatments, a value considered characteristic of extra virgin olive oil. The statistical difference between the results did not represent great alterations in relation to the quality and stability of the extra virgin olive oil. The free fatty acid content showed a slight increase to 0.32 g/100 g during the first two months of storage. However no differences were observed in relation to the type of storage or container.

In this experiment the peroxide value varied little in relation to the type of container and storage. With respect to time, it showed a more pronounced increase during the first 30 days, followed by little alteration up to the end of storage. However, on observing the values found for each treatment as shown in [Table 1](#), it can be seen that the can presented the smallest value. The evolution of peroxide values was found to be more rapid in plastic subsamples under light in the first month of storage and then it stabilized. This behavior can be explained by the fact that hydroperoxides are formed quickly, but are very unstable when oxygen and light are available. The results obtained are in agreement with a study published by [Sacchi et al. \(2008\)](#), in which extra virgin olive oil was filled into glass bottles and into PET bottles with an oxygen absorber in proportions from 0.1% to 5%, and stored exposed to light for 6 months. The authors stated there was no variation in peroxide values in relation to the type of container, since all the results increased during the first 35 days and then decreased up to the sixth month.

The degree of oxidation of olive oil can also be evaluated by analyzing the specific extinction of the oil samples. According to the values for K<sub>232</sub> presented in [Table 1](#), the treatments behaved in a similar way throughout the experiment, the main difference occurring in relation to storage time, with a discreet increase during the first 30 days, subsequently altering very little. The analysis of K<sub>270</sub> measures the products of secondary lipid oxidation, such as conjugated trienes. [Table 1](#) shows that the type of storage had the greatest influence on the values for K<sub>270</sub>. It is evident that the treatments exposed to light radiation presented higher values than those stored in the dark or in cans. With respect to time, the treatments showed slightly increased values during the first month, but then remained stable for the rest of the storage period. The high value shown for the K<sub>270</sub> of the olive oil at the start of the experiment could be related to oxidation of the oil during the time it remained stored after production, before the start of the analyses. The olive oil filled into cans remained the most stable of all the treatments, presenting no significant differences with time.

Regarding the results obtained for the total phenolic compound content, there was no effect of the type of container or of the different storage environments. There was a small reduction in the total

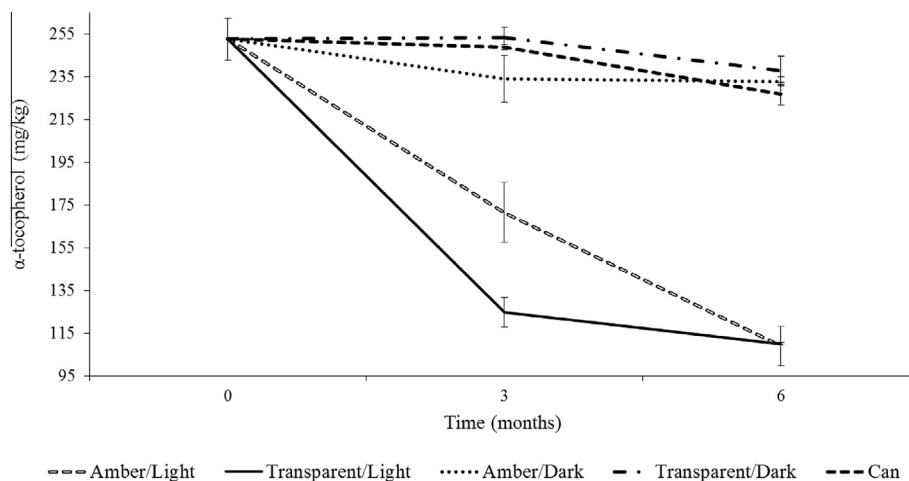


Fig. 1. Behavior of the extra virgin olive oil samples with respect to their  $\alpha$ -tocopherol contents during 6 months of storage for the five different treatments.

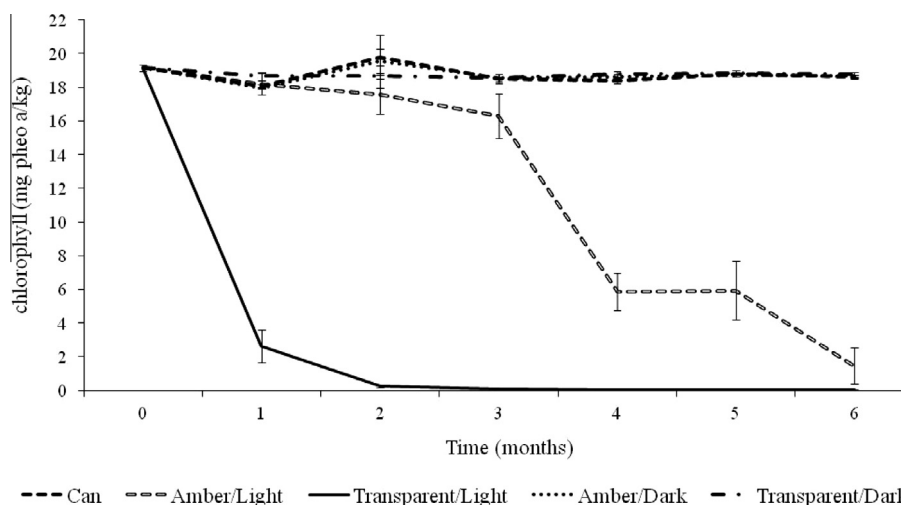


Fig. 2. Behavior of the extra virgin olive oil samples with respect to their chlorophyll contents during 6 months of storage for the five different treatments.

Table 2

Neural networks architectures with highest training and test set classification coefficients generated and selected from among 500 networks generated by the automatic network designer (AND) module from Statistica 8.0 (StatSoft Inc., Tulsa, OK, USA).

ANN index	Neural network topologies (X–Y–Z)	Classification accuracy (%)		Training algorithm	Error function	Activation function	
		Training set	Test set			Hidden neurons	Output neurons
1	MLP (11–22–5)	85.12	90.48	BFGS (31)	CE	Tanh	Softmax
2	<b>MLP (11–22–5)</b>	<b>88.10</b>	<b>90.48</b>	<b>BFGS (40)</b>	<b>CE</b>	<b>Tanh</b>	<b>Softmax</b>
3	MLP (11–13–5)	86.90	90.48	BFGS (43)	CE	Tanh	Softmax
4	MLP (11–25–5)	85.71	90.48	BFGS (63)	MSE	Tanh	Exp
5	<b>MLP (11–18–5)</b>	<b>87.50</b>	<b>92.86</b>	<b>BFGS (36)</b>	<b>CE</b>	<b>Tanh</b>	<b>Softmax</b>
6	MLP (11–13–5)	85.71	90.48	BFGS (70)	MSE	Logistic	Exp
7	RBF (11–12–5)	73.21	80.95	RBFT	CE	Gauss	Softmax
8	RBF (11–28–5)	70.83	83.33	RBFT	CE	Gauss	Softmax
9	RBF (11–18–5)	77.38	80.95	RBFT	MSE	Gauss	Identity
10	RBF (11–21–5)	72.02	83.33	RBFT	CE	Gauss	Softmax

Neural network topology (X–Y–Z) signifies X neurons in input layer, Y neurons in hidden layer and Z neurons in output layer); MLP, multilayer perceptron; RBF, radial basis function; BFGS (number of training epochs) signifies Broyden–Fletcher–Goldfarb–Shanno algorithm; CE, cross entropy; MSE, mean square error; Tanh (hyperbolic tangent function); Softmax (softmax function); exp (exponential function); logistic (logistic sigmoid function); Gauss (gaussian function); identity (linear function). The best networks are marked in bold.

phenolic compound content in the sixth month, from 55.22 mg of caffeic acid/kg, to 53.13 (PET amber under light), 54.90 (PET transparent under light), 54.54 (PET amber under dark), 52.01 (PET transparent under dark) and 52.31 (can). It can be considered that quantitatively the total phenolic content remained stable.

According to the analysis of variance of the values obtained for the squalene content, the results were only significant when evaluated in relation to storage time ( $p < 0.01$ ). Thus, the changes in squalene content were not affected by the type of container or different storage environments. There was a notable and significant



**Table 3**  
Classification performance of MLP 11–18–5 network with respect to light exposure condition and packaging material used in the storage of extra virgin oil obtained from artificial neural network modeling.

Data set	Light exposure condition	Packaging material	Classification accuracy (%)
Training set	Dark	Amber PET	85.0
		Transparent PET	93.0
	Light	Amber PET	87.0
		Transparent PET	85.0
		Tinplate can	85.0
Test set	Dark	Amber PET	100.0
		Transparent PET	100.0
	Light	Amber PET	77.0
		Transparent PET	85.0
		Tinplate can	100.0
Total dataset	Dark	Amber PET	88.0
		Transparent PET	95.0
	Light	Amber PET	85.0
		Transparent PET	85.0
		Tinplate can	88.0

decrease in the squalene content during the first three months of storage, from 3221.27 mg/kg initially to 2597.23 mg/kg.

Analyzing Fig. 1, it can be seen that the decrease in  $\alpha$ -tocopherol content was related to the variables of time and storage environment. The bottles stored under light suffered a significant decrease in  $\alpha$ -tocopherol content, being more extensive under transparent bottles. The effect of light radiation was less accentuated on the oil in amber bottles, but nevertheless more expressive when compared to the treatments stored in the dark. The decrease in  $\alpha$ -tocopherol content was subtle in the subsamples stored in the dark and in cans.

The chlorophyll content was estimated as pheophytin *a*, the main pigment in the olive oil. It can be seen in the Fig. 2 that the variables influencing the chlorophyll content were the type of storage and time. The chlorophyll content remained constant in the subsamples stored in the dark. The effect of photo-oxidation on the chlorophyll content stored in the light is evident, especially when filled into transparent PET bottles. It can be seen that the subsamples stored in both transparent and amber PET bottles lost chlorophyll during storage, but the reduction was more accentuated in the transparent containers. This result was expected since the pigmentation of the amber bottle serves as a barrier to light. Nevertheless it can be seen that this pigmentation was not efficient for the six months of storage under a light intensity of 3000 lux.

Regarding color analysis using the  $L^*C^*h$  system, it was noted the luminosity ( $L^*$ ) increased pronouncedly in the subsamples filled into transparent PET bottles and stored in the light, these subsamples already differentiated themselves from the other treatments during the first month of storage. The subsamples in the amber PET bottles and stored in the light also showed an increase in luminosity, but only became differentiated from the others as from the third month. The saturation ( $C^*$ ) increased for all treatments in the first month of storage, but it remained stable from the second to the sixth months for the treatments stored in the dark. The value for  $C^*$  was affected by light exposure. The subsamples in transparent PET showed greater increase than the other treatments, differentiating themselves as from the first month. With respect to hue ( $h$ ), the subsamples were found in the yellow region (close to the 90° angle) and suffered little alteration during the experiment. Thus it can be said that using the  $L^*C^*h$  model, the treatments stored in the dark and in the cans did not show any significant alterations during the experiment. On the other hand, the subsamples stored in the light were influenced by the time, storage environment and type of container.

### 3.3. Artificial neural network

The ANN design is relatively simple, presenting connections in parallel and sequence between neurons, which results in a short

time and a high-potential to compute robustness and adaptive performances (Palancar, Aragón, & Torrecilla, 1998). The ANN algorithm is able to model chemical processes based on linear or nonlinear dynamics (Mellit, Benghanem, & Kalogirou, 2007).

In order to generate neural networks that classify extra olive oil subsamples efficiently with respect to packaging material and storage conditions, the automatic network designer search (ANDS) module from Statistica 8.0 has been used to generate MLP and RBF neural networks in subsequent cycles. In a generated set of best networks in a given cycle it saved 5 that had the best training and test set classification performance. During the training process of a MLP network, the ANDS module searched for a proper hidden neuron activation functions among Eqs. (3)–(7). In the case of radial base functions (RBF), the hidden layer activation functions were isotropic Gaussian functions (Eq. (8)). The type of implemented error function imposes the type of output neuron activation function in Statistica 8.0. With cross entropy (CE) as an error function classification, the output activation function for RBF and MLP networks a softmax function has been employed. Using the MSE as an error function by ANDS for RBF networks has always determined the use of output neuron linear activation function. In the case of using MSE as an error function for MLP networks, ANDS software searched for a proper output neuron activation function. The created neural networks, as highly nonlinear tools, were trained using iterative techniques such as RBF, BFGS (Broyden–Fletcher–Goldfarb–Shanno), scaled conjugate gradient and gradient descent training algorithms (Debska & Guzowska-Swidler, 2011).

Table 2 shows the ten best classification results of ANN modeling selected by ANDS module according to its topology, classification accuracy, training algorithm, error function, hidden and output neurons activation functions used. It is notable that MLP networks showed better performances for training (85–88%) and test set (90–92%) than RBF, which classification accuracy varies from (70–77%) and (80–83%) for training and test set, respectively. This result was already expected since many MLP networks have been reported to be very good at solving pattern recognition and classification problems (Palancar et al., 1998; Torrecilla, Aragón, & Palancar, 2005; Torrecilla, Mena, Yáñez-Sedeño, & García, 2007, 2008; Torrecilla, Otero, & Sanz, 2004; Torrecilla, Otero, & Sanz, 2005; Torrecilla et al., 2013). Table 2 also shows the two best networks (marked in bold) whose classification accuracy were 88.1 and 87.5% for training set and 90.5% and 92.9% for test set, respectively. For both networks, the ANDS module chose BFGS as an optimal teaching algorithm using hyperbolic tangent as hidden neuron activation function. The output neurons were activated with a softmax function for both architectures, which, according to Statistica

**Table 4**  
Weight and bias values for input, hidden and output layers of the MLP 11–18–5 network.

	Input neurons											Output neurons					
	FFA content	Peroxide value	$K_{232}$	$K_{270}$	Chlorophyll content	$L^*$	$C_{ab}^*$	$h_{ab}$	Tocopherol content	Squalene content	Total phenolic content	Input bias	Dark PET amber	Dark PET transparent	Light PET amber	Light PET transparent	Tinplate can
Hidden neurons	1	-2.95	6.47	-2.24	-2.29	0.43	-1.13	-1.22	4.52	6.86	-12.54	-2.01	0.32	3.61	-1.28	0.49	2.52
	2	-0.13	2.96	-7.23	-0.94	-2.04	-1.81	-2.00	5.04	2.54	-2.48	2.27	-1.46	5.06	-5.48	-3.04	-0.42
	3	-2.35	3.60	5.03	-0.26	-1.58	-1.79	4.78	-7.88	1.80	3.56	1.76	2.96	-0.73	6.94	1.92	-2.26
	4	2.17	0.95	3.08	-3.54	-5.49	3.42	1.30	-0.30	5.11	-1.68	-1.05	-2.29	0.96	5.61	-5.27	2.95
	5	-10.76	-5.72	-3.80	2.34	-5.20	0.65	1.91	-0.73	-5.42	-0.08	-2.58	4.20	-0.97	-0.98	-1.87	5.32
	6	7.82	-0.31	1.93	0.16	0.59	1.55	1.26	-0.04	0.10	-2.47	-0.80	2.78	7.25	-1.01	-3.30	5.84
	7	4.83	0.16	-0.66	4.30	-5.05	1.46	-1.37	3.19	0.29	4.78	-0.98	-1.96	-1.89	-10.39	-5.25	-0.82
	8	-6.48	-1.42	-0.09	-5.92	1.60	2.90	4.95	0.54	-7.85	-10.67	-3.25	-2.19	-5.40	-2.47	0.01	3.55
	9	-5.94	1.83	-1.94	-3.24	-2.28	3.85	3.91	-1.86	-0.32	6.41	0.71	0.23	-3.74	7.07	0.22	-6.07
	10	-0.76	-2.71	-0.63	-4.16	1.17	-0.97	4.99	1.71	-6.13	3.63	0.46	-1.97	-0.88	-0.91	1.91	-1.21
	11	2.86	4.18	-0.34	0.81	-6.03	-0.70	-0.04	-3.45	-1.92	-4.72	-2.24	3.41	7.01	5.50	-3.05	-1.38
	12	2.29	-2.51	-1.82	5.90	-2.58	-0.93	2.51	5.63	0.71	-11.13	2.97	2.52	-5.01	7.43	3.67	-2.39
	13	1.82	-0.91	-0.75	1.93	-6.44	0.14	3.89	4.03	-2.84	-1.88	-3.17	2.57	-12.40	2.72	4.92	-2.68
	14	3.27	0.01	-1.41	1.64	10.37	-2.32	3.34	3.75	6.84	-1.06	-4.12	0.48	-1.88	-9.33	-6.21	9.47
	15	-0.56	4.16	-0.97	1.97	1.44	0.36	-0.34	-2.49	-15.75	-2.15	7.87	-1.79	-0.02	0.66	1.76	-1.62
	16	9.80	-1.50	-3.16	0.30	-2.14	-0.10	-0.60	0.46	12.64	-2.34	-2.23	-3.10	3.91	4.48	-5.49	1.72
	17	-7.30	0.15	0.47	-0.39	-0.60	-2.07	2.86	2.48	8.20	-2.00	2.04	-2.69	1.87	4.92	8.69	-5.09
	18	-4.28	-0.89	-3.24	-2.10	-1.80	-2.09	-2.30	4.31	-6.89	-1.52	1.43	-2.26	-4.60	-3.91	-0.15	2.86
Hidden bias													-2.21	-7.99	1.59	-0.35	8.97

8.0 presuppositions, is used together with cross entropy as an error function to evaluate the net performance. The classification training procedure required 40 epochs in case of the network topology with 22 hidden layer neurons (MLP 11–22–5) and 36 epochs with 18 hidden layer neurons (MLP 11–18–5).

The best ANN model was considered to be the MLP 11–18–5 because this topology achieved higher classification accuracy for test set using less hidden layer neurons than MLP 11–22–5. This topology with a single hidden layer has been considered sufficient to solve similar or more complex classification problems (Torrecilla et al., 2004; Torrecilla, Otero, et al., 2005). Besides, more hidden layers may cause over-fitting (Ruan, Almaer, & Zhang, 1995). The performance analysis of the optimum network selected by ANDS module is showed in Table 3. The classes composed by amber and transparent PET bottles exposed to light showed great heterogeneity of physicochemical characteristics presenting low classification accuracy for training set (85–87%), test set (77–85%), and 85% of total data set, respectively. On the other hand, the tinplate can, amber and transparent PET bottles stored in the dark showed high accuracy for training set (85%, 85% and 93%) and test set (100%), respectively. This result can be explained by the higher stability of the physicochemical characteristics of the extra virgin olive oil stored in the dark.

ANNs have been used for many purposes in food technology, such as: to control/simulate nonlinear chemical process (Palancar et al., 1998), to estimate food treatment properties at high-pressure (Torrecilla, Otero, et al., 2005), to predict variable values at relatively high temperature (Torrecilla, Aragón, et al., 2005), to solve adulteration, pattern recognition and classification issues (Berrueta et al., 2007; Cajka, Hajslova, Pudil, & Riddellova, 2009; Cajka, Riddellova, Klimankova, et al., 2010; Cordella, Militão, Clément, & Cabrol-Bass, 2003; González-Arjona, López-Pérez, González-Gallero, & González, 2006; Padin et al., 2001; Palit et al., 2010), and to predict sensory attributes (Bardot, Bocherreau, Martin, & Palagos, 1994; Cruz et al., 2011; Jack & Steele, 2002; Krishnamurthy, Srivastava, Paton, Bell, & Levy, 2007). The ANN modeling results of the present work are in accordance with the literature data toward its moderate accuracy (85–95%) and robustness of the parameters evaluated. On the other hand, the use of ANNs in phenolic compounds quantification has also been reported in the literature (Torrecilla et al., 2008). Table 4 exhibits weight and bias values input-hidden-output node connections obtained for MLP 11–18–5 network. There are a total of 288 weights, which correspond to the sum of 198 and 90 connections between input-hidden and hidden-output nodes, respectively. Besides, one can see that 23 bias were used to help model adjustment corresponding to 18 connections between input bias and hidden neurons and 5 connections between hidden bias and output neurons.

In order to examine which variables have the biggest influence on classification process, a sensitivity analysis (Table 5) was performed in the MLP 11–18–5 network to identify the critical parameters (in bold) and their degree of importance on the model outputs. The results show that the network output changes according to the inputs, providing information about the more sensitive parameters, which should be measured more accurately. The results of such an analysis would also provide useful details about the “robustness” of the model parameters, leading to a better decision-making process. The sensitivity analysis showed that free fatty acid (FFA) content, peroxide value,  $L^*C^*h$  color parameters, tocopherol and chlorophyll contents were the physicochemical attributes with the most discriminative power presenting variable of importance in projection (VIP) scores of 4.73, 5.45, 11.25, 6.21, 13.62, 10.71 and 15.41, respectively. The low values of VIP for squalene and total phenolic content can be correlated to ANOVA, which no significant variations were observed with respect to 5 storage conditions studied. On the other hand, the physicochemical

**Table 5**

Overall sensitivity analysis computed for each of the physicochemical attributes.

Variable	VIP <sup>1</sup> (%)		
	Train set	Test set	Total dataset
<b>Free fatty acid content</b>	<b>4.94</b>	<b>3.81</b>	<b>4.73</b>
<b>Peroxide value</b>	<b>5.28</b>	<b>6.16</b>	<b>5.45</b>
<i>K</i> <sub>232</sub>	1.11	2.02	1.28
<i>K</i> <sub>270</sub>	1.60	1.91	1.66
<b>Chlorophyll content</b>	<b>15.50</b>	<b>14.99</b>	<b>15.41</b>
<i>L</i> <sup>*</sup>	<b>11.14</b>	<b>11.69</b>	<b>11.25</b>
<i>C</i> <sub>ab</sub> <sup>*</sup>	<b>6.03</b>	<b>6.98</b>	<b>6.21</b>
<i>h</i> <sub>ab</sub>	<b>14.12</b>	<b>11.45</b>	<b>13.62</b>
<b>Tocopherol content</b>	<b>10.17</b>	<b>13.05</b>	<b>10.71</b>
Squalene content	1.10	1.22	1.12
Total phenolic content	2.58	1.53	2.38

<sup>1</sup> VIP – variable of importance in projection. The most discriminative variables are highlighted in bold.

analysis with most discriminative power, such as tocopherol (Fig. 1) and chlorophyll content (Fig. 2), showed the most significant results. These results indicate physical chemical attributes as color and chlorophyll content, which are measured by simple techniques such as spectrophotometry, can easily be used as quality control and adulteration parameters of extra virgin olive oil.

#### 4. Conclusion

Although the olive oil analyzed in this study presented values for acidity above 0.5% and indicators of oxidation such as the peroxide value and coefficient of extinction, conforming to the standards accepted for extra virgin olive oils, it could be seen that a considerable fraction of the minority components degraded during the first months of exposure to light. Thus, the PET bottles tested under the conditions of this study are not recommended for use with extra virgin olive oil when exposed to light, neither the transparent nor the amber models, since the subsamples did not maintain oxidative stability or the nutritional compounds characteristic of extra virgin olive oil. The artificial neural network showed high classification performance for tinplate cans, amber and transparent PET bottles stored in the light and dark using BFGS algorithm with 11 input neurons, 18 hidden neurons and 5 output neurons. The high classification accuracy for the training set and test set may be related to the fact that subsamples are from the same batch. More robust results can be obtained by evaluating the physicochemical attributes of extra virgin olive oil obtained from different batches. The sensitivity analysis showed that free fatty acid content, peroxide value, *L*<sup>\*</sup>*C*<sup>\*</sup>*h*<sup>\*</sup> color parameters, tocopherol and chlorophyll contents were the physicochemical attributes with the most discriminative power. It also showed the “robustness” of the model indicating which physicochemical analyses could be used to solve clustering, pattern recognition, classification and adulteration issues related to extra virgin olive oil production.

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