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Research Paper

Intelligent modelling to monitor the evolution of quality of extra virgin olive oil in simulated distribution conditions

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One of the main attributes of extra virgin olive oil (EVOO) is that it possesses multiple advantages for human health, which makes quality control of this functional food an attractive action. In the present research, samples of two different EVOOs (Almazara del Ebro and As Pontis) were held under three different temperature conditions (3 °C, 40 °C, and room temperature (~23 °C)). These different temperatures, as well as time, led to an alteration in the properties of the samples that were studied with visible spectroscopy and multilayer perceptrons (MLPs), which are non-linear mathematical tools. The absorption peaks representing the chlorophylls and carotenoids present in EVOO decrease with time and temperature. Generally, the results show that higher temperatures contribute more to the degradation of EVOO when compared to lower ones. The obtained information was used to design and optimise two MLPs. These tools were able to properly distinguish the time and temperature conditions that EVOO samples underwent. This technique is fast, user-friendly, inexpensive, and non-destructive, so it could be of great use for real-time quality control of olive oils during, for example, their storage and distribution, as ideal conditions could be potentially found.

1. Introduction

Olive oil, the juice obtained from olives, is the leading source of fat in the well-known and healthy Mediterranean diet (Visioli, Poli, & Galli, 2002). It has been shown that following a balanced Mediterranean diet has multiple beneficial effects such as a decreased incidence of major cardiovascular events (Estruch et al., 2013) or healthier cholesterol levels reflected in lower amounts of low-density lipoproteins (Kris-Etherton et al., 2002). These effects have been in part linked to the elevated amounts of antioxidants (especially mono-unsaturated fatty acids and phenolic compounds) present in olive oil (Covas et al., 2006) and, even more so, in its high-quality form: extra virgin olive oil (EVOO).

This high-quality product represents a relevant sector within the food market regarding its economical and gastronomical impact. Additionally, the seemingly beneficial effects

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of the consumption of EVOO towards human health has led to the development of numerous scientific studies to better understand this product, such as characterising its polyphenolic fraction (Carrasco-Pancorbo et al., 2006), designing methods to grade olive oils according to quality (Cancilla, Wang et al., 2014), or creating tools to locate adulterated EVOO samples (Aroca-Santos, Cancilla, Matute, & Torrecilla, 2015).

To qualify as extra virgin, an olive oil must be produced only through mechanical processes (in order to be "virgin") and possess a low free acidity (<0.8%), perceptible fruitiness, and an absence of any sensory defects (required to be "extra"). This is mentioned because EVOO is a fragile product, which is affected by light, temperature, and storage time (and other factors) (Pristouri, Badeka, & Kontominas, 2010), and if the conditions are not adequate, it may reach the consumer in a non-extra virgin status. Therefore, a proper distribution chain and shelf-life, with controlled conditions, must be established to ensure that the hard work behind the production of high-quality EVOO is not in vain.

During the present research, an attempt to simulate real conditions that are experienced in the distribution chain of EVOO has been carried out. A series of EVOO samples, which were obtained from bottles of different EVOO brands that are currently being exported overseas, were exposed to a set of temperature conditions during a three-month timespan, and their quality was assessed periodically through absorption spectroscopy. In the past, a clear relation between absorption measurements and EVOO quality has been proven, and, as a matter of fact, it has become one of the routine tests to evaluate olive oil samples as it provides data regarding quality, alterations induced by processing methods, and state of preservation (United States Standards for Grades of Olive Oil and Olive-Pomace Oil, 2010). In particular, photo- and thermal degradation of EVOO can be easily evaluated using mainly the variation of the concentrations of a few compounds such as chlorophyll pigments (chlorophyll-a and chlorophyll-b) and carotenoids (lutein and β-carotene) (Ayuso, Haro, & Escolar, 2004; Domenici et al., 2014), information which can be inferred from visible spectroscopic measurements.

Recently, our team has published research where this spectroscopic approach has been successfully used to quantify and identify adulterants in EVOO (Aroca-Santos et al., 2015) and to estimate the photo-degradation of pure and mixed samples (Torrecilla, Vidal, Aroca-Santos, Wang, & Cancilla, 2015), employing computational artificial intelligence to model the results. As a continuation of this work, after revealing that contaminants can be identified, and the effect of light assessed following this methodology, it seemed logical to monitor the consequences that different temperatures have on EVOO, with the goal of estimating the environmental conditions (time and temperature) that a specific product had experienced during its distribution or shelf-life.

To determine these conditions, a mathematical tool based on neural networks was designed to estimate the temperature at which certain EVOO samples had been kept, as well as the duration of this exposure, just using information extracted from the spectroscopic analyses. Achieving successful models in this regard would imply that an inexpensive and straightforward approach could be available to evaluate how an EVOO had been handled during its distribution, enabling the location of mistreated products or the least favourable phases of their shipment and/or storage.

2. Materials and methods

2.1. *Extra virgin olive oil samples*

Three samples (20 ml each) of two extra virgin olive oils (EVOO), Almazara del Ebro (Empeltre varietal) and As Pontis (Manzanilla Cacereña varietal), were kept in three different temperature conditions: 3 °C, 40 °C, and room temperature (~23 °C; controlled by a thermostat (minimum of 21 °C and maximum of 24 °C)). The room temperature samples were only measured twice (the first and last days of the experiment) simply to compare their degradation over time with the other four samples kept at 3 °C and 40 °C. The oils were both within their best before dates and the six samples were kept away from light to avoid the changes in quality caused by this variable (Torrecilla et al., 2015).

2.2. *Visible spectroscopy*

The absorption spectra of the four EVOO samples (two at 3 °C and two at 40 °C) were each measured 52 times within a time period of three months (from February 12th, 2017 to May 11th, 2017) using a Varian Cary 1E UV–Vis spectrophotometer operating between 350 and 750 nm (taking an absorption measurement for each nm band), which is the ideal range to detect the absorption peaks of the chlorophylls and carotenoids present in the EVOOs (Mínguez-Mosquera, Rejano, Gandul, Higinio, & Garrido, 1991). The hot and cold samples were taken out of the oven and fridge, respectively, 30 min before being measured to be sure that the measurements were always done at the same temperature. The samples were analysed in a 1 cm path length quartz cell. Each spectrum was measured three times and the average of the three spectra provided the data used to train a multilayer perceptron model.

2.3. *Multilayer perceptron*

In order to detect the degradation of the EVOOs with temperature and time, a non-linear mathematical tool known as a multilayer perceptron (MLP) was created. MLPs are artificial neural networks (ANNs) which are able to find suitable non-linear relationships between the different independent and dependent variables present in the analysed database (in this case, visible absorption peaks and the time and temperature conditions of the EVOO samples measured, respectively). ANNs are interpolating and estimating systems, so it is essential to highlight that they do not provide reliable or accurate extrapolations, as they rigorously rely on the range of the studied data (Nedic, Despotovic, Cvetanovic, Despotovic, & Babic, 2014).

The MLP-based model was chosen because it has proven to be a successful tool throughout many applications in different fields such as food technology (Torrecilla, Aroca-Santos, Cancilla, & Matute, 2016), chemistry (Aroca-Santos, Cancilla, Pariente, & Torrecilla, 2016), nanochemistry (Wang, Cancilla, Torrecilla, & Haick, 2014), and biochemistry (Cancilla,