CORRECTION OF THE EFFECT OF SEASONALITY THROUGH A DATA STANDARDIZATION STRATEGY IN THE AUTHENTICATION OF EXTRA VIRGIN OLIVE OIL

Glòria Rovira, M. Pilar Callao, Itziar Ruisánchez

Rovira i Virgili University, Chemometrics, Qualimetric and Nanosensors Group,
Department of Analytical and Organic Chemistry, Marcel·lí Domingo s/n, Tarragona,
43007, Spain
gloria.rovira@urv.cat

Extra Virgin Olive Oil (EVOO) is one of the principal ingredients of the Mediterranean diet. Because of its nutritional and sensory properties and the multiple health benefits, its use has increased significantly worldwide. As a consequence of this use, fraud also increased. The most studied types of fraud are framed, mainly, in two large blocks: adulteration with other cheaper oils and lack of authenticity due to fraudulent labeling [1,2].

To authenticate Arbequina EVOO from two Protected Catalan Designations of Origin (Les Garrigues and Siurana, Catalonia, Spain) we have developed and validated a two-class PLS-DA model from fluorescence spectra of the 2019 harvest samples.

In the case of the authentication of seasonal products (or their derivatives), the future samples may contain sources of variability not considered when the model was developed. Therefore, maintaining the performance parameters and making the model applicable to seasonal variability remains a challenge in the authentication field.

The correction of the differences between the measurements (spectra) performed under different conditions is done by chemometric methods known as standardization or transfer methods. Transfer methods calculate a transform function that corrects the measurements done in the new conditions according to the training set used to build the multivariate model (primary conditions). As a result, the model can be used to predict samples measured in the new conditions. This strategy aims to correct the
difference between measurements performed under different conditions to make a model transferable and useful at lower experimental costs.

In this work, a strategy to account for the season variability is proposed by adapting the Piecewise Direct Standardization (PDS) method. PSD transforms the response from second/new conditions to correspond to the response from the primary conditions from a subset of samples measured under both conditions [3]. Alternatives for the determination of the transfer function have been proposed when it is not possible to have a set of samples measured in both conditions [4]. We propose to obtain it from the average of the spectra in the first conditions concerning the mean of a set of spectra in the second conditions.

Samples from 2020, 2021, and 2022 harvests have been measured with the same instrument. The corresponding transfer functions have been established and the spectra have been corrected so that they can be predicted using the PLS-DA model established from 2019 harvest samples.

References