**High-quality edibles oils: use of spectroscopic techniques in combination with chemometrics as a powerful strategy in the adulteration detection analysis**

Much D\*(1), Azcarate S(2), Alcaraz M(3)

(1) Agencia de Investigación Científica (AIC-CONICET), Santa Rosa, La Pampa, Argentina.

(2) Instituto de Ciencias de la Tierra y Ambientales de la Pampa (INCITAP-CONICET-UNLPam), Santa Rosa, La Pampa, Argentina.

(3) Laboratorio de Desarrollo Analítico y Quimiometría (LADAQ) FBCB-UNL, Santa Fe, Santa Fe, Argentina.

\* diego.much@conicet.gov.ar

In the last decade, the consumption of edible seed oils, such as sesame, flax or chia, has been increasing due to their particular nutritional characteristics. Their high demand, high cost, and low regulations make them a target for fraudulent actions, in particular, adulteration with refined oils such as sunflower, corn or soybean. Currently, research in the food safety field is oriented toward the development of strategies that provide fast, non-destructive, low-cost and environmentally friendly solutions. In this aspect, techniques based on spectroscopic measurements seem to be the most attractive alternatives. Likewise, chemometrics has shown synergy with these analytical techniques having a positive impact on the experimental development, mainly, in the reduction of analysis times and the solvent consumption, but, importantly, in the enhancement of the chemical information of the systems under study in comparison to conventional techniques. The aim of this work was to determine the adulteration degree of five high-quality edible oils: sesame, flax, chia, canola and extra virgin olive oils. Refined oils used as adulterants (sunflower oil, corn oil and soybean oil) were evaluated at low concentration levels (2-15%). For the analysis, three multidimensional spectroscopic techniques (UV-Vis, NIR and excitation-emission matrix (EEM) Fluorescence) were used and the data were then subjected to chemometric analysis. For the quantitation of adulterant oil, partial least squares (PLS) analysis was used to build the predictive models for the data set obtained by each individual technique. Furthermore, to exploit the individual particularities of each instrumental dataset, two data fusion strategies (low- and medium-level) were evaluated. A total of twenty-five models (five for each seed oil) were analyzed. The predictive capacity of each model was evaluated through the analysis of the statistical parameters regression coefficients of the calibration (R2), percentage error of prediction (REP%) and mean square errors of calibration (RMSEC), cross-validation (RMSECV) and prediction (RMSEP). In general terms, EEM provides more information about the system in a single measurement due to the multidimensional structure of the data. This property allows obtaining more sensitive models profiting from the multidimensional information comprised in the EEM, entailing REP% values (<20%) lower than those obtained by the analysis of individual spectroscopic techniques (<40% and <60% for UV-Vis and NIR, respectively). This observation is in accordance with the results obtained from the analysis of the fused data, where the combination of the instrumental information leads to an improvement in the model efficiency (REP% <15% and 16% for low- and mid-level, respectively). The results showed that the combination of the spectral information leads to a substantial improvement in the predictive ability of the chemometric models compared to those obtained from individual instrumental signals. Last, the feasibility of spectroscopic techniques combined with chemometrics for authenticity analyzes in quality oils was again demonstrated.

Keywords: food safety, multi-instrumental data, data fusion, discriminant analysis, linear regression model.