FT-NIR Analysis of Fatty Acid Ethyl Esters in Olive Oil

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Guarantee of quality and commercial frauds are major concerns in the field of extra virgin olive oil. Among the chemical markers indicated by the European legislation (Reg. EU 2016/2095), the content of fatty acid ethyl esters (FAEE) can be useful to discriminate authentic products of high quality. However, the official method (Reg. EU 2011/61) is highly demanding in terms of time and reagents. Thus, the application of Fourier-transform near infrared (FT-NIR) spectroscopy to assess the concentration of FAEE can represent a rapid and valid alternative.

The work aims at evaluating the performance of FT-NIR spectroscopy in predicting the FAEE content of olive oil. Olive oil samples (170) with a FAEE content ranging from 2.44 to 109.9 mg/kg were analyzed in 8 mm-pathlength glass cuvettes by using a FT-NIR spectrometer (MPA, Bruker), in the spectral range 10000-4520 cm-1, with 8 cm-1 resolution, and 16 scans. Two aliquots of each sample were analyzed in duplicate. For the FAEE content prediction, Partial Least Squares (PLS) models were calculated, using raw and pre-treated average spectra. The models were calibrated and cross-validated using a dataset with 113 samples; the external validation was performed with the remaining 57 samples selected by Kennard Stone algorithm. Data elaborations were performed by using PLS toolbox and Matlab R2021b environment.

The best PLS model was obtained using 6 latent variables with spectra pre-treated with smoothing and standard normal variate. The determination coefficient and root mean square error in prediction resulted 0.86 and 8.69 mg/kg, respectively. The results are better than those reported by Cayuela (2017), who found a standard error of prediction ranging from 25.6 to 67.2 mg/kg. However, since the official method for the evaluation of FAEE content can give lower errors, depending on the level of FAEE, future data elaborations will consider the possibility of using selected spectral variables to reduce noise and improve the prediction ability of the FT-NIR method.

**Keywords:** olive oil, quality, prediction, ethyl esters.

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