FTIR coupled with chemometrics as a non-invasive tool for PDO olive oils' discrimination

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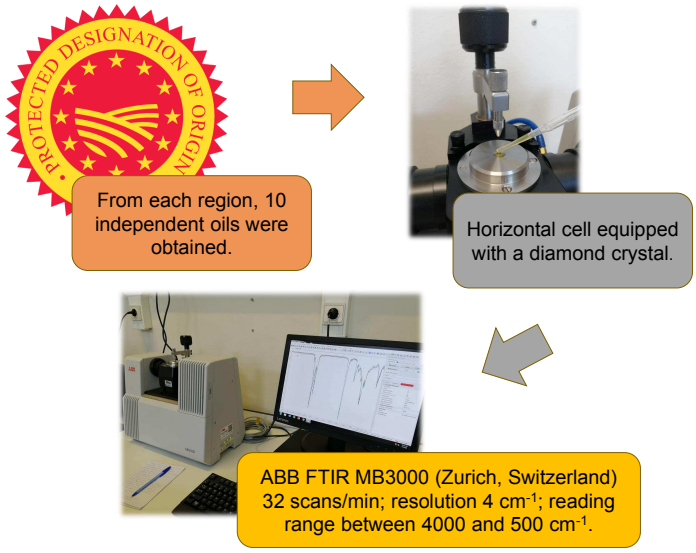
Introduction and objectives

Quality schemes protect the diversity of traditional European foods, such as the Protected Designation of Origin (PDO) and the Protected Geographical Indication (PGI). Only the olive oils from extra virgin and virgin commercial categories can be labelled with a PDO or PGI. In Portugal, currently, there are six PDOs. Olive oils labelled as PDO present a superior chemical-sensory quality. Therefore, from a commercial point of view it is of paramount importance to be able to identify them according to the correct label, avoiding fraud and ensuring the consumer regarding the exact origin of the purchased oil. Non-invasive and fast techniques, like Fourier transform infrared spectroscopy (FTIR), have been applied to assess olive oil origin and to detect fraud and adulterations. Thus, this work aimed to use FTIR spectra coupled with linear discriminant analysis-simulated annealing algorithm (LDA-SA) to classify commercial olive oils belonging to three Portuguese PDOs, namely, 'Alentejo Interior', 'Beira Interior', and 'Trás-os-Montes'.

Material and methods



Results and discussion

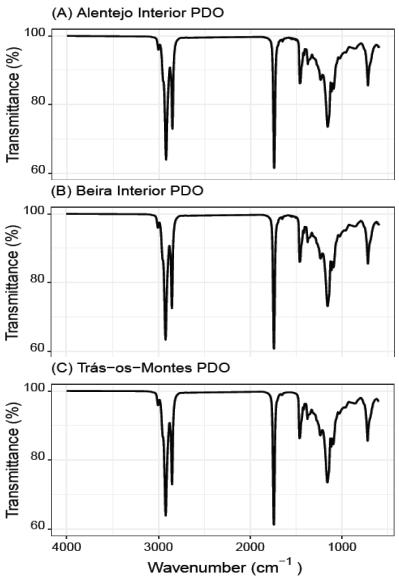


Figure 1. FTIR spectra: transmittance (%) values recorded for olive oils from three Portuguese PDOs olive oils in the wavenumber region of 4000 to 500 cm^{-1}). (A) 'Alentejo Interior', (B) 'Beira Interior', and (C) 'Trás-os-Montes'.

The vibration bands of the FTIR spectra recorded for the studied Portuguese olive oils of the three PDOs were in-line with those reported for other Portuguese olive oils from different cultivars and geographical origins, namely from the geographical regions studied in the present work (Figure 1). Two main absorption regions could be identified in all olive oils, namely between 3100 and 2750 cm^{-1} and 1850-600 cm^{-1}, showing typical bands that could be related to the known vibration modes of the molecular bonds. The transmittance raw data (Figure 1) were further treated by applying LDA-SA allowing to establish a classification model based on the raw spectral information. The model allowed to correct classify all the olive oils according to the certified PDO (100% of sensitivity and specificity), for training (Figure 2) and LOO-CV internal validation. A correct classification average rate of 97.5% was obtained for the 40 random subsets of data used (4 folds × 10 repeats, in which one subset, comprising 25% of the data, i.e., 2-3 olive oils per PDO region, were kept for assessing the predictive performance of the model established using the remaining 75% of the data), confirming the potential use of the proposed FTIR-chemometric approach.

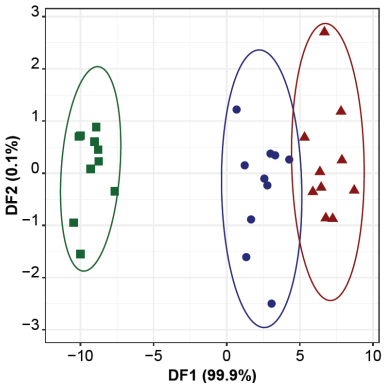


Figure 2. PDO olive oils supervised discrimination (2D LDA-SA plots) achieved with the FTIR-LDA-SA model based on the transmittance (%) data recorded at six wavenumbers selected by the SA algorithm; ■ 'Alentejo Interior' PDO's olive oils; ● 'Beira Interior' PDO's olive oils; and, ▲ 'Trás-os-Montes' PDO's olive oils.

Conclusion

The overall results clearly pointed out the feasibility of applying the developed FTIR- LDA-SA model as a predictive tool to identify the correct PDO of the studied Portuguese olive oils, confirming that FTIR is a powerful non-invasive tool for olive oil authentication in terms of geographical origin.

Acknowledgments

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