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MÉTODOS DE ANÁLISE DE ALIMENTOS

Identification of almond's variety based on FTIR spectra of ground samples

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Attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) was employed to develop multivariate discriminant models for almond cultivar identification. For that, raw transmittance spectra were recorded for ground almonds in the range from 4000 to 500 cm^{-1} (**Figure 1a**). As can be inferred from the figure, The ATR-FTIR analysis unveiled distinct transmittance band spectral profiles, particularly emphasizing bands within the wavenumber ranges of 3700-2750 cm^{-1} and 1800-600 cm^{-1}. Remarkably, no visible peaks were observed in the wavenumber ranges of 4000-3700 cm^{-1}, 2750-1800 cm^{-1} and 600-500 cm^{-1}, which are considered neutral spectral regions. The spectra analysis of the ground almond samples exhibited characteristic bands, namely at 3290, 2975, 2925, 2855, 1640, 1380, 1265, 1235, 1095, 1050, 995 and 905 cm^{-1}. An accurate multivariate linear discriminant model (LDA) was established using transmittance data recorded at 30 wavenumbers, selected by applying the simulated annealing algorithm, which is a meta-heuristic variable selection algorithm. The model successfully discriminated the seven almond cultivars with correct classifications of 100%, 99.2% and 98.9% for training (**Figure 1b**), leave-one-out cross-validation and repeated K-fold cross-validation (10 repeats and 4 folds, which ensured keeping at least 25% of the initial dataset for cross-validation purposes). The predictive performances achieved in the present study are in line with those previously reported in the literature but for a smaller number of cultivars. Indeed, García et al.[1] described the successful discrimination (LDA coupled with a stepwise variable selection algorithm: 100% of correct classifications for training) of three almond cultivars (one American: *cv*. Butte; and two Spanish: *cvs*. Marcona and Guara). Also, Cortés et al.[2], applied the FTIR technique to differentiate four Spanish almond cultivars (*cvs*. Guara, Rumbeta, Marcona, and Planeta) based on absorbance spectra, being to accurately predict (external dataset) the almond cultivar with a success rate of 94.45% using a Partial Least Square Regression-Discriminant Analysis model. The same research team demonstrated the successful application of the FTIR technique in discriminating whole almonds based on their bitterness levels (sweet almonds versus bitter almonds).[3] In conclusion, the proposed a FTIR-LDA-SA classification approach based on raw transmittance spectra recorded for ground almonds was shown to be a rapid, cost-effective, and minimally invasive tool for almond cultivar traceability that can be of utmost relevance for producers and industrial stakeholders throughout the almond chain.

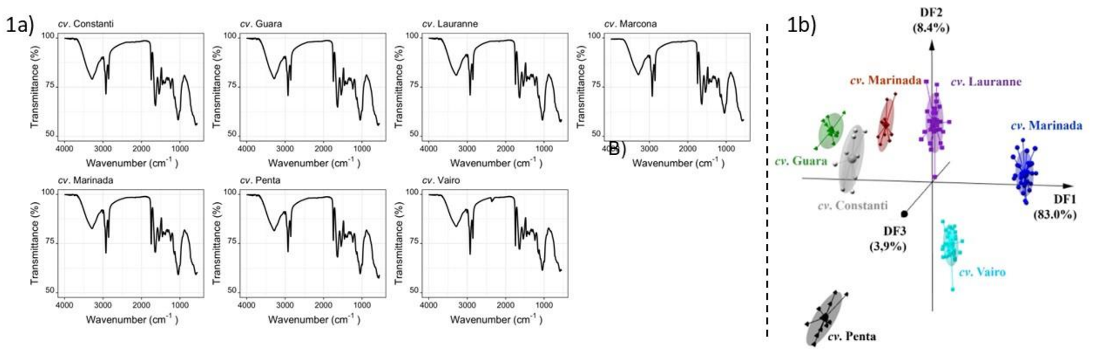

Figure 1: A) FTIR spectra (wavenumbers ranging from 4000 to 500 cm^{-1}) for ground almonds (cultivars: Constanti, Guara, Lauranne, Marcona, Marinada, Penta and Vairo); **B)** Almonds supervised discrimination (3D-LDA-SA plot) according to the seven studied cultivars FTIR raw data (transmittance %).

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