Ultraviolet-visible Spectroscopy and Chemometrics for Simultaneous Evaluation of Minor Components in differently Processed Olive Oils

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Spectroscopic techniques coupled with chemometrics are an alternative to classical chemical methods used in oil analysis. The ease and simplicity of measurements are the most attractive features of spectroscopy from a practical point of view. The use of spectroscopy allows the development of analytical procedures that are fast and clean, avoiding extensive sample preparation and the use of reagents.

The UV spectral range covers the wavelength range from 200 to 350 nm, and the VIS range - from 350 to 700 nm. Absorption spectra of olive oils in the UV-VIS spectral region show intense bands, attributed to molecules with high electron density groups such as carbonyl and nitro groups, double and triple bonds, conjugated double bonds, etc.

This poster presents the application of UV-VIS spectroscopy combined with chemometrics for the quality analysis of olive oil. UV-VIS absorption spectra were recorded for a set of differently processed olive oils. Principal component analysis (PCA) used for exploratory studies of spectra revealed different absorption properties of oils. Partial least squares regression (PLS) was used to develop calibration models for predicting total phenol content, total tocopherols, carotenoids, chlorophylls and antioxidant activity. Calibration models were optimized using different methods for processing input data and variable selection was performed using jack-knife method. The highest predictive ability was obtained for models related to total phenol content (R^2 = 0.955, RPD = 4.7), total tocopherols (R^2 = 0.894, RPD = 3.1) and pheophytin (R^2 = 0.898, RPD = 3.2). Models for predicting carotenoids (R2 = 0.722, RPD = 1.9) and antioxidant activity (R^2 = 0.644, RPD = 1.7) were rather suitable for semi-quantitative analysis. The results show the potential of UV-VIS spectroscopy for quality analysis of olive oil. The developed regression models enabled the simultaneous quantification of several quality parameters in olive oils and the presented results may be important for future practical applications.