

Determination of extra virgin olive oil in quaternary mixture using FTIR spectroscopy and multivariate calibration.

ABSTRACT

The purpose of this study was to optimize Fourier transform infrared (FTIR) spectroscopy in combination with multivariate calibrations (partial least square and principle component regression) for determination of extra virgin olive oil (EVOO) in quaternary mixture systems with grape seed oil (GSO), rice bran oil (RBO) and walnut oil (WO). FTIR spectra of EVOO in quaternary mixtures were subjected to several treatments including mean centering (MC), standard normal variate, and spectra derivatives. The combined frequency regions of 1200–900 and 2949–2885 cm^{-1} were used for determination of EVOO. Using partial least square calibration, FTIR normal spectra treated with MC model give the highest values of coefficient of determination (R^2) and the lowest values of root mean square error of calibration (RMSEC). The R^2 value obtained for the relationship between actual and FTIR predicted value of EVOO was >0.99 with RMSEC value of 1.55% (v/v). The developed PLS model was further used to calculate EVOO in prediction samples, and the root mean square error of prediction obtained was 3.65% (v/v).

Keyword: Extra virgin olive oil; FTIR spectroscopy; Partial least square (PLS); Principle component regression; Quaternary mixtures.