Classification of edible oils based on ATR-FTIR spectral information during a long heating treatment

Abstract

Identification of oil type and its QC are important concerns in food control laboratories. Classifying edible oils that have not been used (i.e., unheated) with the aid of vibrational spectroscopy has previously been reported. However, the classification of used (i.e., heat-treated) oils needs special attention. The effect of long heating times on the classification of four kinds of edible oils (canola, corn, frying, and sunflower) based on attenuated total reflectance (ATR)-FTIR spectra was surveyed. The sampling was done on the oils during a 36 h heating process (at 170°C). The ATR-FTIR spectra of the samples were collected in the range of 4000-550 cm⁻¹. Interval extended canonical variates analysis (ECVA), as a variable selection and classification tool, was used to determine the best intervals during the heating procedure for classification. Principal component analysis discriminate analysis, partial least-squares discriminate analysis, and ECVA were performed on the selected intervals and on the total heating time. The effect of autoscaling and mean-centering, as data preprocessing methods, was also investigated. The ECVA method resulted in the best performances for classification, with a 94% cross-validated nonerror rate (one misclassification) for the heating process times of 24-27 and 33-36 h.