

Rapid quantification of 3-monochloropropane-1,2-diol in deep-fat frying using palm olein: using ATR-FTIR and chemometrics

ABSTRACT

Fourier transform infrared spectroscopy (FT-IR) was studied as an alternative technique for the estimation of the 3-monochloropropane-1,2-diol (3-MCPD) ester level in palm olein. The samples were the frying oils of potato chips with the addition of a synthetic or natural antioxidant. The same samples were evaluated by both the conventional method (GC-MS) and FTIR. Principal component analysis (PCA) was used to group the frying oils according to the level of the 3-MCPD esters. The results obtained by FTIR were consistent with the findings using an indirect determination method by GC-MS. Chemometric analysis was applied to correlate the content of 3-MCPD esters with the FTIR spectrum data. A partial least squares (PLS) model was able to predict the concentrations of 3-MCPD esters at the 95% confidence level with R² values higher than 0.90.