

The detection of glycidyl ester in edible palm-based cooking oil using FTIR-chemometrics and ¹H NMR analysis

ABSTRACT

Glycidyl ester (GE) is a process contaminant formed during the palm oil refining process. In this study, 156 spectra of palm-based cooking oil were recorded by Fourier transform infrared (FTIR) spectroscopy and resulting data were processed using chemometrics approach. The relationship between spectrum data and measured data of GE content was established using Cubist, Random Forest (RF), average neural network (avNNET), and artificial neural network (nnet) model. Then, a consensus regression model was established using a fusion of those four models. GE contents measured by gas chromatography-mass spectrometer (GC-MS) were between 1.338 and 18.362 mg/kg with mean value of 6.880 ± 3.767 mg/kg and median value of 6.480 mg/kg. In this study, FTIR spectrum served as data input and calibrated using measurements from GC-MS. NMR was then applied to verify the present and structural information of GE. Prediction results of GE using the consensus model showed -high coefficient of determination (R^2) value of 0.79. The contribution (in percentage) of each member model from highest to the lowest was in order Cubist > RF > avNNET > nnet. Further confirmation of the presence of GE in samples were performed using ¹H NMR spectroscopy. Comprehensive analyses based on FTIR chemometrics and ¹H NMR spectroscopy successfully determined GE in palm-based cooking oil.

Keyword: Palm oil; Glycidyl ester; FTIR chemometrics; GC-MS; ¹H NMR