Rapid assessment of total MCPD esters in palm-based cooking oil using ATR-FTIR application and chemometric analysis

ABSTRACT

The technique of Fourier transform infrared spectroscopy is widely used to generate spectral data for use in the detection of food contaminants. Monochloropropanediol (MCPD) is a refining process-induced contaminant that is found in palm-based fats and oils. In this study, a chemometric approach was used to evaluate the relationship between the FTIR spectra and the total MCPD content of a palm-based cooking oil. A total of 156 samples were used to develop partial least squares regression (PLSR), artificial neural network (nnet), average artificial neural network (avNNET), random forest (RF) and cubist models. In addition, a consensus approach was used to generate fusion result consisted from all the model mentioned above. All the models were evaluated based on validation performed using training and testing datasets. In addition, the box plot of coefficient of determination (R^2), root mean square error (RMSE), slopes and intercepts by 100 times randomization was also compared. Evaluation of performance based on the testing R^2 and RMSE suggested that the cubist model predicted total MCPD content with the highest accuracy, followed by the RF, avNNET, nnet and PLSR models. The overfitting tendency was assessed based on differences in R^2 and RMSE in the training and testing calibrations. The observations showed that the cubist and avNNET models possessed a certain degree of overfitting. However, the accuracy of these models in predicting the total MCPD content was high. Results of the consensus model showed that it slightly improved the accuracy of prediction as well as significantly reduced its uncertainty. The important variables derived from the cubist and RF models suggested that the wavenumbers corresponding to the MCPDs originated from the –CH=CH_2 or CH=CH (990–900 cm^{-1}) and C-Cl stretch (800–700 cm^{-1}) regions of the FTIR spectrum data. In short, chemometrics in combination with FTIR analysis especially for the consensus model represent a potential and flexible technique for estimating the total MCPD content of refined vegetable oils.

Keyword: MCPD prediction; GC-MS; FTIR; Chemometric analysis; Consensus model