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CHEMOMETRICS METHODS TO DETERMINE PALM OILS IODINE VALUE (IV) USING FT-NIR AND FTIR SPECTRA

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ABSTRACT

The authentication of the palm oils quality is indirectly crucial to consumer health. There are issues in palm oils quality within consumer macrocosm such as recycled and adulteration of cooking oils. Recently in Malaysia, there are claims of used cooking oils reprocessed and sold as new with lower price to consumers. This creates a threat to consumer health because they might use the reprocessed cooking oils unknowingly. In this study, the palm oils quality was determined through the iodine value (IV) which measured the total unsaturation of the oils. The characteristic of double bond in the oils was examined before and after oxidation process through the combination of spectroscopic method of Fourier Transform Near Infrared (FT-NIR) and Fourier Transform Infrared (FTIR) analysis and chemometrics methods. The IV was chemically determined through MPOB P3.2: 2004 method which later incorporated in the chemometrics models. The chemometrics multivariate approach of Partial Least Squares (PLS) regression model was applied to predict the IV of palm oils. The models were developed with the application of the data preprocessing, variable selection, data splitting and multiblock analysis. The performance of each method was assessed throughout the model development in the IV determination process. From the result, different data preprocessing provided different quality of prediction model. Either the application of the row scaling, column scaling individually or a combination of both might have improved the quality of the model. It is concluded that data preprocessing is dependent on the nature of the dataset and there can be no single method for general use. In this study, for the FT-NIR spectra data of non-fried palm oils, mean centre is the best data preprocessing with R^2_{cv} of 0.9472 and *RMSECV* of 0.3496. Meanwhile for the FT-NIR spectra data of fried palm oils, standardisation is the best data preprocessing with R^2_{cv} of 0.9105 and *RMSECV* of 0.4435. For the FTIR spectra data of non-fried palm oils, mean centre is the best data preprocessing with R^2_{cv} of 0.9614 and *RMSECV* of 0.2966. Meanwhile for the FTIR spectra data of fried palm oils, mean centre and application of row scaling produced the best PLS model with R^2_{cv} of 0.9551 and *RMSECV* of 0.3181. In comparison of variable selection methods, correlation coefficient (COR) variable selection method is the best method compared to PLSRC and PLSW in all PLS model. Variable selection is proven improved PLS model compared to the full spectrum model. On other hand, the best data splitting method for non-fried model is Kennard-Stone (KS) method while Duplex is the best method for fried palm oils PLS model. In the FT-NIR spectra data of non-fried palm oils, KS method give the best PLS model with R^2_{test} of 0.9355 and *RMSEP* of 0.6813. Meanwhile, Duplex method resulted the best PLS model in the FT-NIR spectra data of fried palm oils with R^2_{test} of 0.9701 and *RMSEP* of 0.2153. In the FTIR spectra data of non-fried palm oils, KS method give the best PLS model with R^2_{test} of 0.9693 and *RMSEP* of 0.2871. Meanwhile, Duplex method resulted the best PLS model in the FTIR spectra data of fried palm oils with R^2_{test} of 0.9734 and *RMSEP* of 0.3192. In multiblock analysis, similarity analysis through Mantel test, Procrustes Error Analysis, R_v and R_v modified showed both spectra are very similar. Multiblock analysis to predict the IV showed PLS model with single block was found to be advantageous compared to the multiblock PLS (MBPLS). FTIR block showed the best performance, followed by employing the FT-NIR block and employing both blocks in MBPLS.

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