Thesis abstract

Coffee is one of the most popular beverages all over the world. Coffee's quality refers to sensory properties and healthy properties. One of the factors affecting sensory properties is the roasting process. During roasting, a series of chemical and physical reactions lead to the formation of components which are responsible for coffee sensory qualities. The criterion used to evaluate roasting process is the roasting degrees. The functional compounds presenting in coffee contribute to health benefits for human. One of the functional quality characteristics attracting increasing interest is its antioxidant properties. Within this class of antioxidant phenolic compounds, chlorogenic acid (CGA) has been proved to play an important role in human health, as well as contribute to the acidity and overall quality of the final cup of coffee.

Recently, near infrared (NIR) spectroscopy technology has been used as a fast and non-destructive method to detect food quality. NIR spectroscopy records the response of the molecular bonds of chemical constituents, such as C-H, N-H, and O-H bonds, which are primary structural components of organic molecules. Most absorption bands in NIR region correspond to overtones and combinations of fundamental vibrations. For food analysis which contains complex mixture of chemical constituents, the absorption peaks in NIR region are broad and overlapping, making visual examination of the NIR spectra difficult discriminate between authentic and adulterated products. Therefore, chemometric methods are needed, such as preprocessing methods (multiple scattering correction (MSC), orthogonal signal correction (OSC), standard normal variate (SNV), 1st derivation, 2nd derivation and so on) and regression methods (partial least square (PLS) regression, interval partial least square (iPLS) regression and multiple linear regression (MLR)).

Coffee roasting degrees and CGA concentration prediction were investigated based on NIR spectroscopy, combined with chemometric methods in this study. Roasting degrees were studied in terms of weight loss in ground roast coffee and the reference value of

weight loss was measured by the electronic balance (SHIMADZU AUW220D). CGA concentration was discussed in both ground coffee and aqueous solution respectively. The reference value of CGA concentration was measured by high performance liquid chromatography (HPLC) method. A batch of Arabica green coffee originating from Antigua Island was purchased from a supermarket. In order to obtain a wide range of weight loss and CGA concentration to develop a universal prediction model, the green coffee samples were roasted at different temperature and time for all experiments. The NIR spectra of coffee samples were obtained from UV-VIS/NIR spectrophotometer (JASCO, V-670). Calibration models of roasting degrees and CGA concentration were developed between NIR spectral data and the reference value. Different preprocessing methods were applied to eliminate noise and extract useful information from raw NIR spectral data. Linear regression methods, such as PLS regression, iPLS regression and MLR, were used to develop calibration models based on raw and preprocessed NIR spectra. The full cross validation method was performed to evaluate the calibration models' performance. The accuracy and predictive ability of the obtained models were assessed by root mean square error of cross validation (RMSECV), determination coefficient of cross validation (Rcv^2), and ratio prediction to deviation (RPD) and so on.

In the first experiment, the calibration model of roasting degrees was developed by MLR method based on the selected wavebands. Five characteristic wavebands (1111 nm, 1225 nm, 1450 nm, 1725 nm, and 1940 nm) were selected from the optimal principle components of the best PLS regression model. Various combinations of these five wavebands were tested to obtain the best MLR calibration model. Finally, the best MLR model was achieved with RMSECV of 0.61 and Rcv^2 of 0.98, based on only three wavebands (1225 nm, 1725 nm, 1940 nm), which were assigned to the compounds releasing during roasting.

In the second experiment, PLS regression method was used to develop the calibration model of CGA concentration in ground coffee. MSC preprocessing method was used to eliminate the effect of scattering before calibration model development. For comparison,

different preprocessing methods were applied on NIR spectral data, including 1st derivation, 2nd derivation, SNV and so on. The best PLS prediction model was obtained with RMSECV=1.10% and Rcv^2 of 0.76.

Finally, CGA concentration in coffee aqueous solution was determined by iPLS regression method. OSC preprocessing method was applied on the raw spectral data to eliminate water interference. iPLS regression method was used to select informative spectral region. For comparison, a PLS regression model based on a full wavelength range was also developed. The final model was developed by iPLS regression method, with RMSECV of 0.62 and Rcv^2 of 0.68, covering a wavelength range of 800 nm – 950 nm, 1000 nm – 1150 nm, 1350 nm -1400 nm, 1550 nm -1650 nm. The results in this dissertation show that NIR spectroscopy, combined with chemometric methods, has a potential to evaluate coffee roasting degrees and CGA concentration.