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Nondestructive Determination of Histidine in Oilseed Rape Leaves Using Near Infrared Spectroscopy

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Abstract. Histidine ($C_6H_9N_3O_2$) is one of the amino acids which are quite important indices for monitoring and indicating the growing status of oilseed rape. The traditional detection methods, such as HPLC or automatic amino acid analyzer were time consuming, laborious, and not convenient for fast and non-destructive determination. Nowadays, near infrared (NIR) spectroscopy is widely applied in quantitative and qualitative analysis for plant growing information detection. In this study, the oilseed rape leaf samples in calibration, validation and prediction sets were 80, 40 and 30, respectively. Linear and nonlinear chemometric methods were compared, including partial least squares (PLS) and least squares-support vector machine (LS-SVM). The performance of different spectral data pretreatments was compared, including Savitzky-Golay smoothing, standard normal variate, first and second derivatives. The correlation coefficient (R) and root mean square error (RMSE) were used as evaluation indices. Firstly, different pretreatments were implemented by PLS model. Secondly, certain wavelengths were selected by the regression coefficients plots. Simultaneously, for comparison, a newly developed informative information and relevant variable selection method, called successive projections algorithm (SPA), was employed to obtain the most effective wavelengths with least collinearity and redundancies. Thirdly, the selected wavelength by regression coefficients and SPA were used as the inputs of LS-SVM model, respectively. Finally, the performance of PLS and LS-SVM models were compared and the best model was achieved. The results indicated that a better prediction results were achieved by the LS-SVM model with correlation coefficient $R = 0.92$ for validation set. NIR spectroscopy combined with LS-SVM was successfully applied for the non-destructive determination of histidine in oilseed rape leaves. This method could be used for the on field monitoring of growing status and other physiological parameters of oilseed rape, and it also helpful for the development of portable instruments and sensors for plant growing information detection.

Keywords. Near infrared spectroscopy, oilseed rape, amino acid, least squares-support vector machine, successive projections algorithm.

Mead production improvements after using a factorial design

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Abstract. In North of Portugal, Trás-os-Montes region, honey production is a very important activity, contributing greatly to the economy of that area. Nevertheless, in certain situations there are difficulties in sell all honey produced, being this marketed at prices below cost of production. Thus, it is very important to find solutions in order to solve this problem. Mead production is one of the possibilities; however, most of the time, mead is not produced in a standardized, but empirically and handmade form.

Thus, in this work it was evaluated how factors, such as, temperature and salt concentration, as well as the yeast used, affects the fermentation process. Temperatures equal to 20, 25 and 30°C, and salt concentrations of 60, 90 and 120 g/hL, as well as two commercial strains of *Saccharomyces cerevisiae*, namely, Fermo[®] Reims Champagne and ICV[®] D47, used in oenological fermentations, were tested. A factorial design 3^2 was used, and the experimental data were analyzed by the Response Surface Method.

Generally, for both yeasts the temperature and salt concentration did not influenced greatly the production of ethanol in the ranges studied; however, the increase of the temperature above 24°C and a salt concentration between 70 and 115 g/hL may cause a higher production of glycerol and acetic acid. Nevertheless, it was verified that values of acetic acid over 0.8 g/L were difficult to obtain, not having the risk of exceeding the maximum admissible. It was in glucose and fructose that the greatest differences were observed between the yeasts; however, the models developed for both sugars, were not as suitable as for the other parameters.

The fits to the mathematical models developed for the ICV[®] D47 yeast were not so good as that obtained for the Fermo[®] Reims Champagne, since the first yeast showed a more irregular and less reproducible behavior.

In conclusion, in future mead production it is advisable to use the Fermo[®] Reims Champagne yeast. Moreover, a working temperature between 24 and 29°C and a salt concentration between 85 and 100 g/hL are recommended.

Keywords. Mead, Factorial Design, Response Surface Methodology, Ethanol, Sugars, Glycerol, Acetic acid.