Title Prediction of colour and pH in grapes using a diode array spectrophotometer (400-110 nm)

Author D. Cozzolino, M.B. Esler, R.G. Dambergs, W.U. Cynkar, D.R. Boenm, I.L. Francis and M. Gishen

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Abstract

One hundred and twenty thawed samples of homogenized and whole frozen grape berries were analysed using a diode array spectrophotometer (400-1100 nm) (CORONA 45VISNIR, Carl Zeiss, Germany). The spectra and the analytical data were used to develop partial least squares calibrations to predict colour and pH in both presentation modes to the instrument. The visible (vis: 400-700 nm), near infrared (NIR: 700-1100 nm) and vis + NIR (400-1100 nm) regions were used to perform the calibrations. Cross validation models for colour and pH on homogenized samples gave a coefficient of determination in validation (R^2_{val}) and the root mean square error f cross-validation (*RMSECV*) of 0.92 and 0.07 mg g⁻¹ for colour, and 0.90 and 0.04 for pH, respectively, using the vis region. Presentation of intact whole grape berries gave R^2_{val} and RMSECV values of 0.50 and 0.14 mg g⁻¹ for colour, 0.60 and 0.08 for pH using the NIR region. It was concluded that homogenized samples gave the best calibration statistics. More research needs to be done to improve calibration on whole samples if the technology is to be used for rapid analysis for either on-farm or on-harvester applications.