

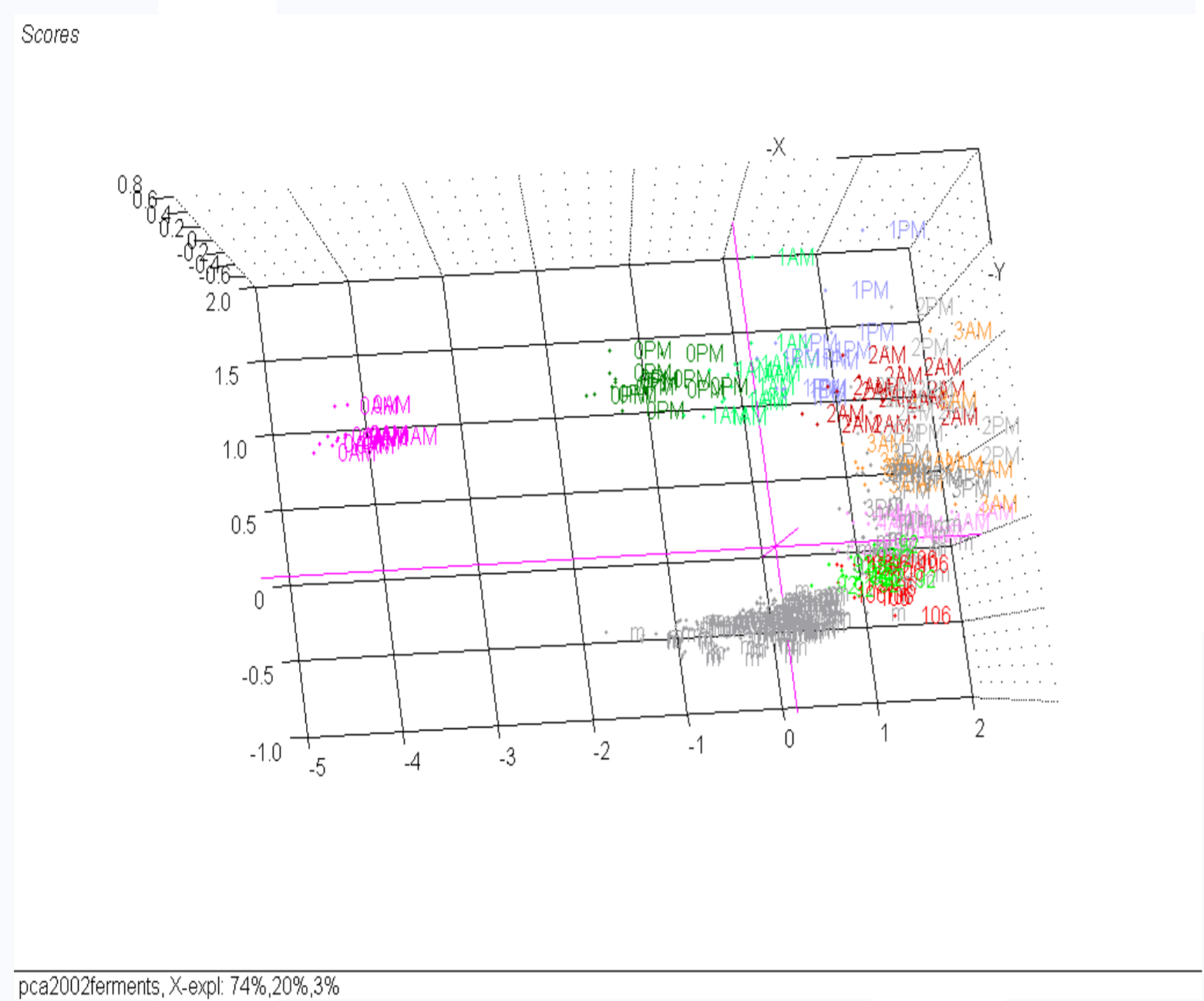


Quantitative analysis of phenolic compounds in red wine fermentation using near infrared spectroscopy

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Figure 1. Score plot for the first three principal components for replicate fermentations indicating the time course.



Introduction

During wine fermentation many grape constituents such as tannins and anthocyanins are extracted and modified by (bio) chemical reactions. The analysis of compounds affected by fermentation can in some cases require several steps of sample preparation that can result in delays in obtaining the result. The objective of this work was to determine the feasibility of near infrared (NIR) spectroscopy to rapidly monitor phenolic compounds during the red wine fermentation process.

Materials and methods

Samples taken from several different experimental wine fermentation trials conducted by the AWRI in the years 2001, 2002 and 2003, were scanned (400–2500 nm) in transmission mode in a 1 mm path length cuvette, using a monochromator spectrophotometer (FOSS NIRSystems6500). Calibration equations were developed for the concentration of malvidin-3-glucoside (M3G), tannins (T) and pigmented polymers (PP) using an HPLC method as the reference. Spectral data collection and manipulation were achieved using VISION software. Partial least square (PLS) regression models between spectral and HPLC data were developed using The Unscrambler software.

Results and conclusion

Figure 1 shows the changes that occur during fermentation in the scores for the first three principal components. This same type of pattern was observed for all fermentations monitored during the study. Figure 2 shows the eigenvectors for the first three principal components. The highest eigenvectors were observed around 520 nm (most likely caused by anthocyanins), around 2000 nm (OH tones most likely due to water and alcohol) and around 2200 nm (CH overtones, possibly due to phenolics). High coefficients of determination in calibration (R^2) and low standard error in cross validation (SECV) were obtained for M3G, T and PP (Figure 3). If the residual predictive deviation (RPD), defined as the ratio between the standard deviation of the population (SD) and the standard error of cross validation (SECV), is greater than three, a calibration model is considered as acceptable for analytical purposes.

Ø The results indicate that NIR spectroscopy shows promise as a means of rapidly monitoring the concentration of phenolic compounds during red wine fermentation.

Figure 2. Eigenvectors for the first three principal components.

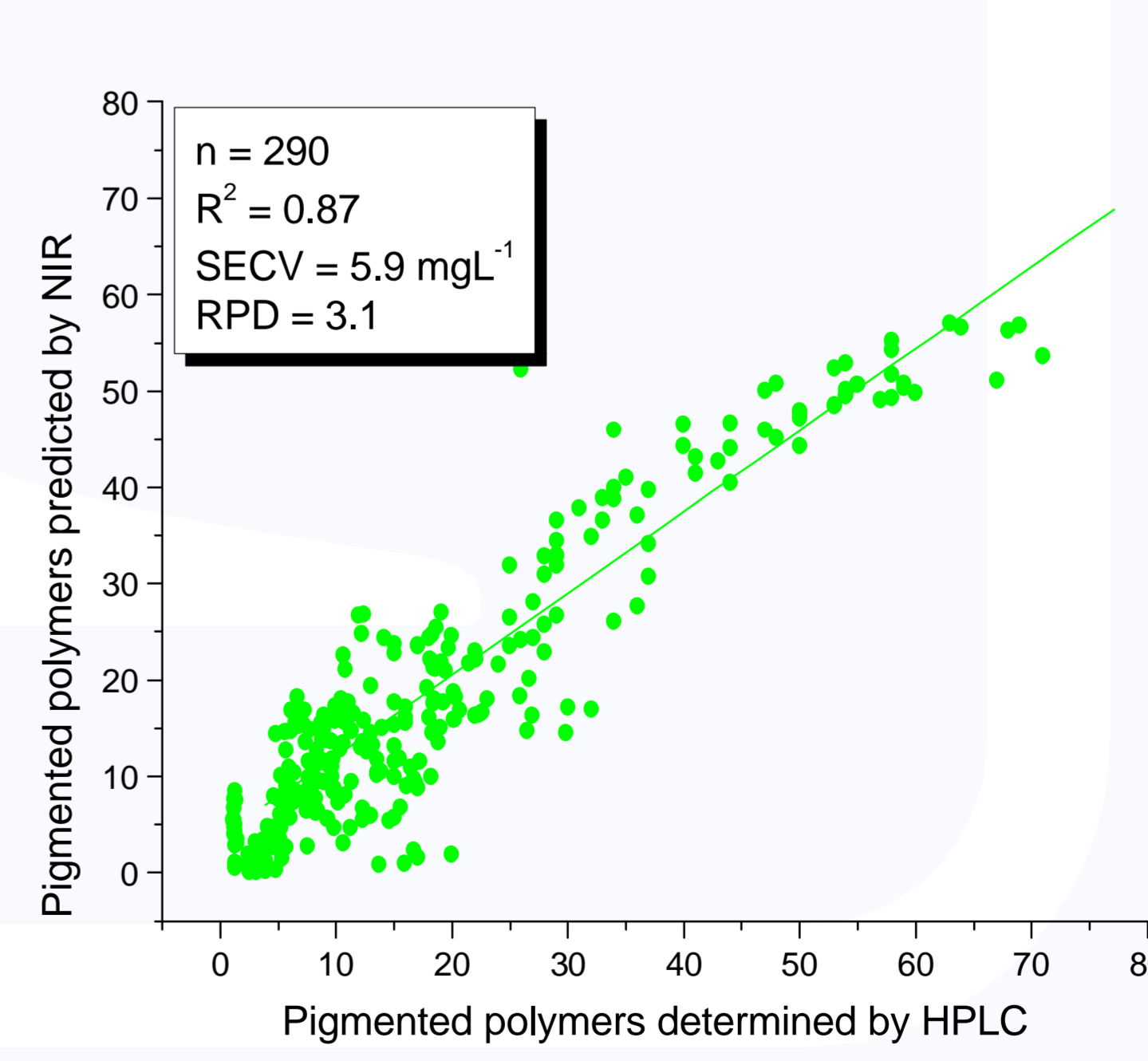
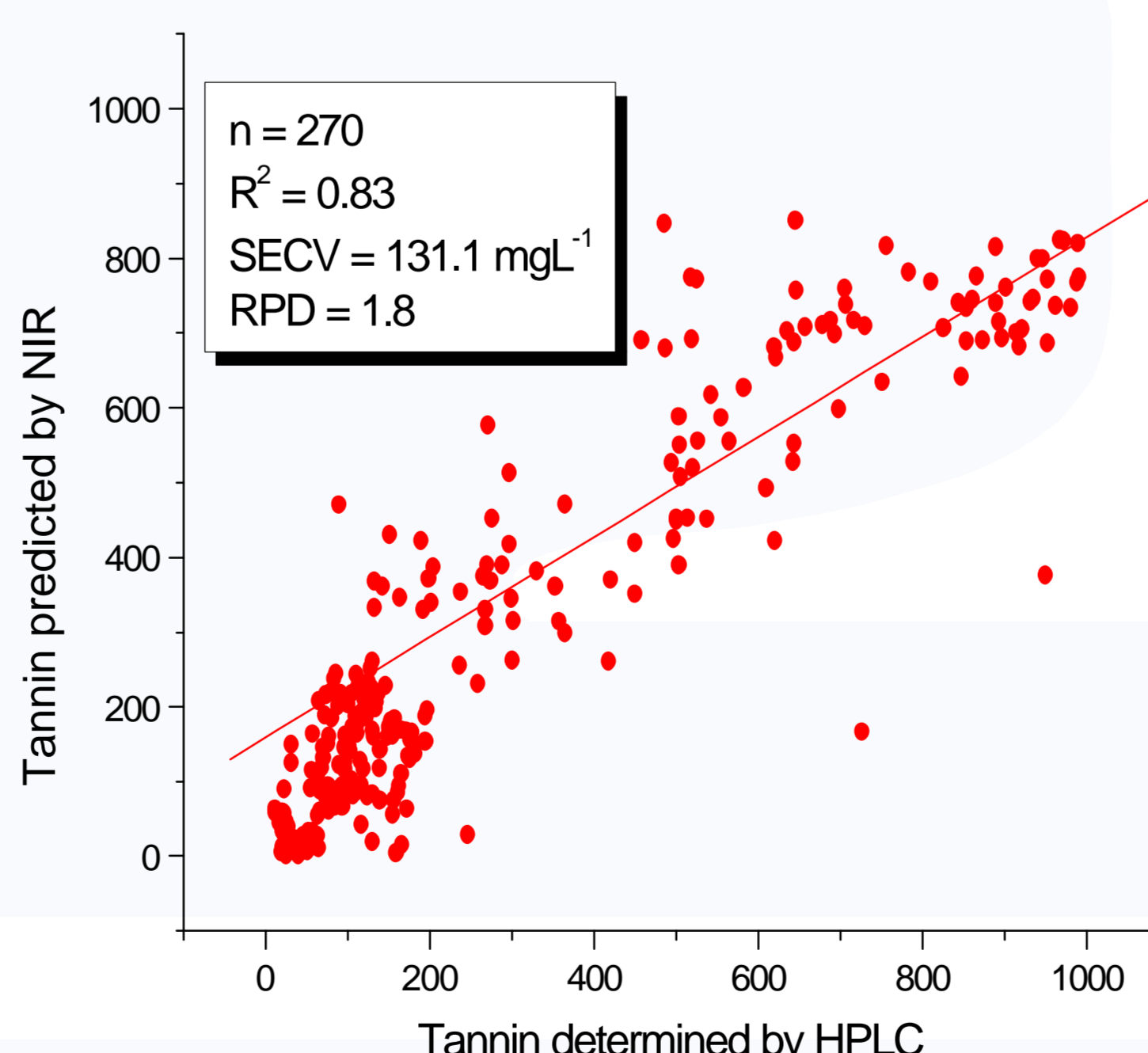
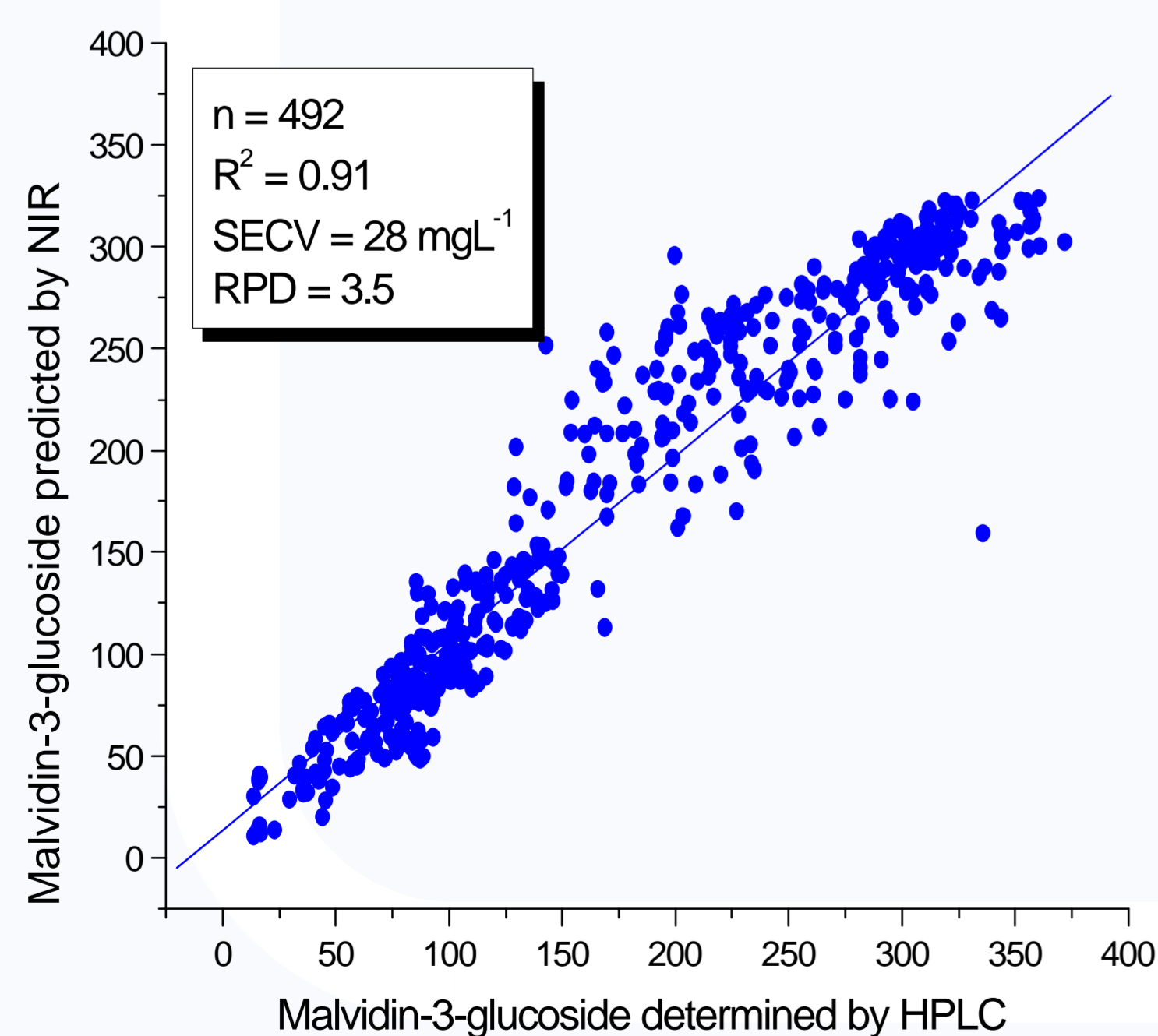
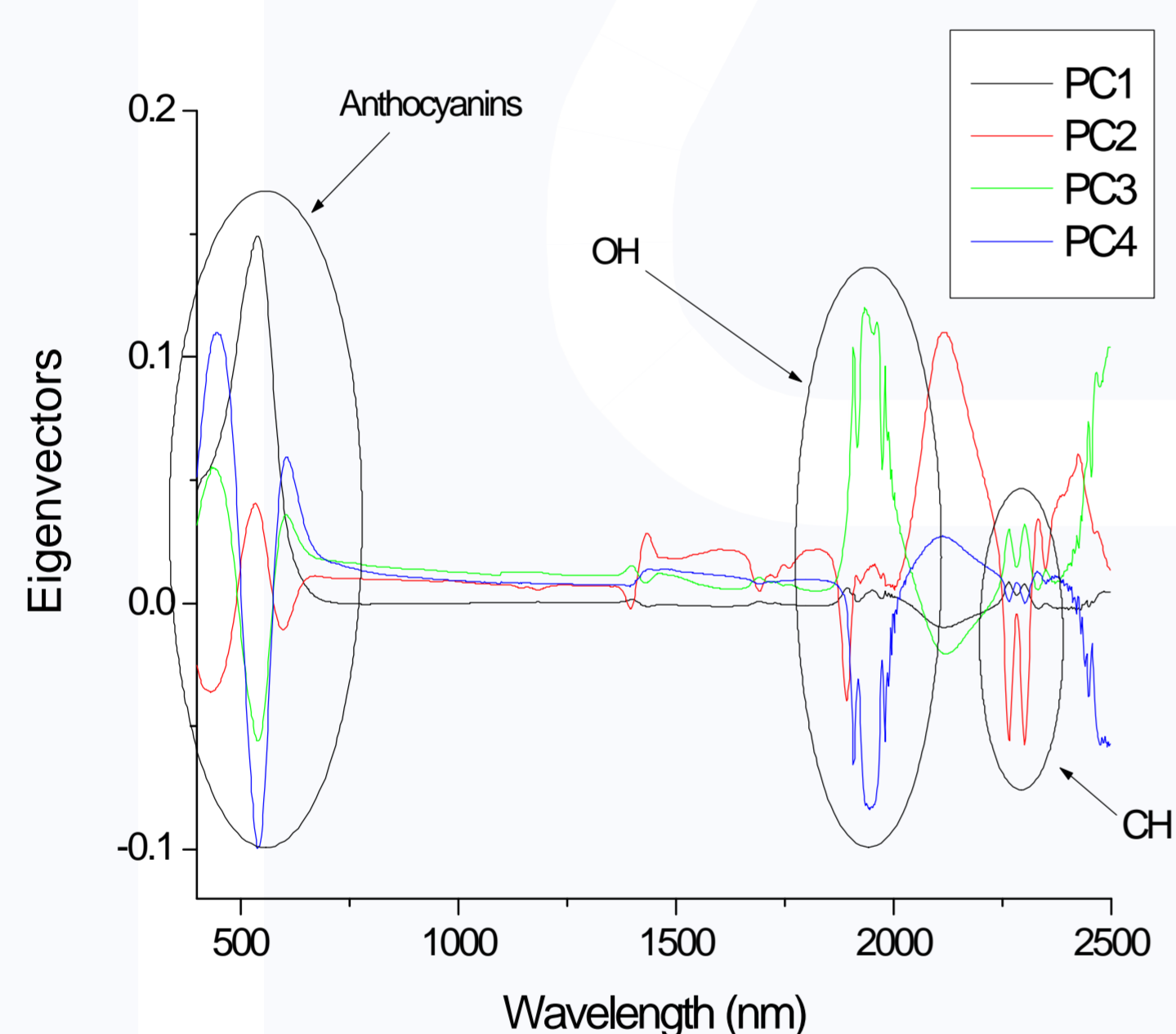


Figure 3. Correlation between NIR-predicted and reference method determinations for the concentrations of M3G, T and PP in red wine ferments. Note: RPD = SD/SECV