VIS-NIR spectroscopy to predict selected chemical parameters in unopened bottles of Sauvignon Blanc wines

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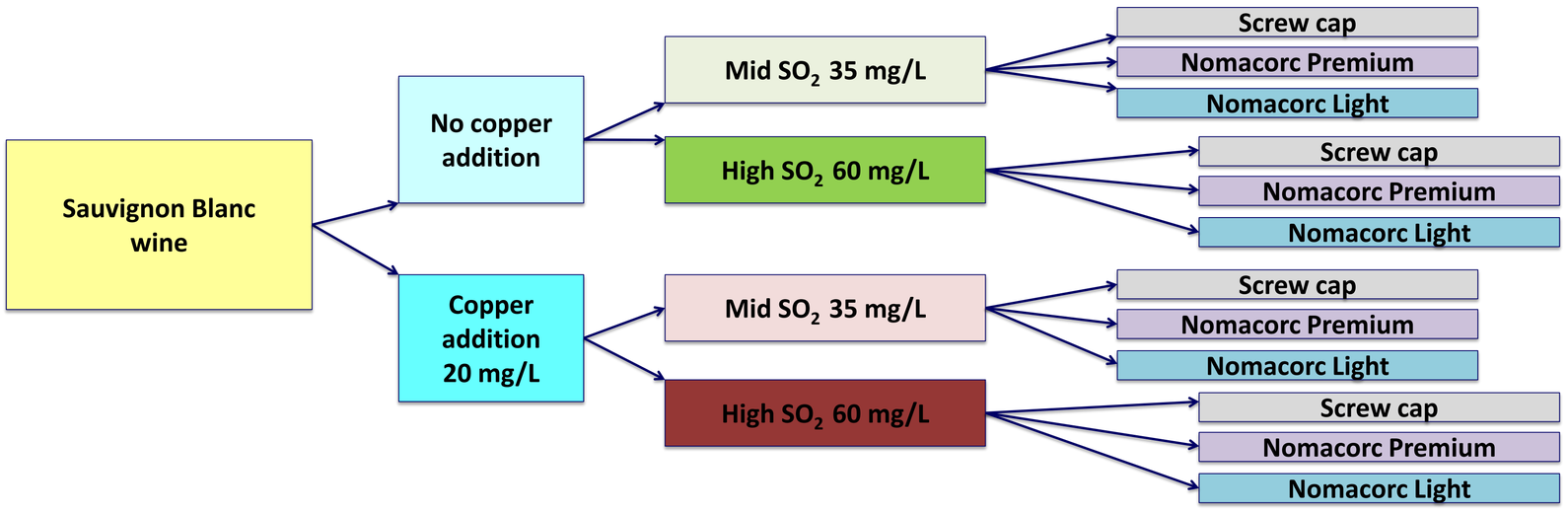
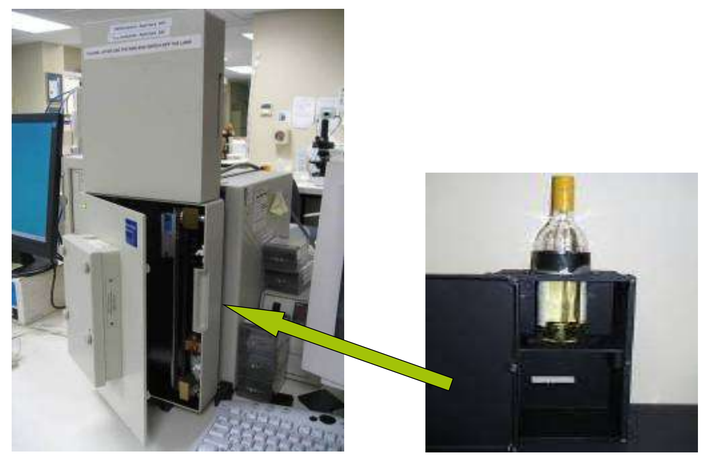
AIM OF STUDY

- To test a non-destructive spectral method to predict chemical parameters of Sauvignon Blanc wines in unopened bottles during storage.



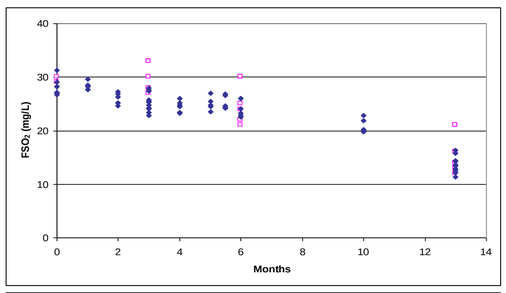


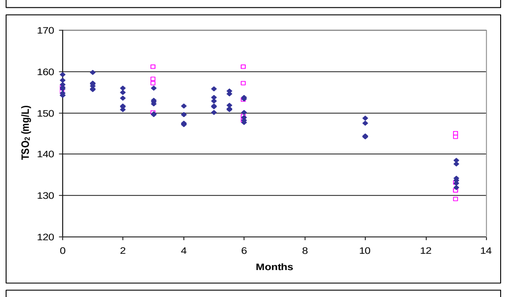
ANALYSES

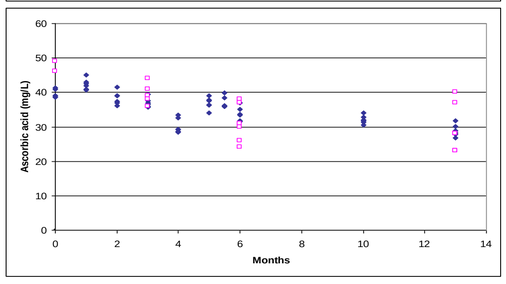
- Free (FSO_2) and total sulfur dioxide (TSO_2) and ascorbic acid were analysed using standard analytical techniques.
- Wines were scanned (400-1100 nm, transflectance mode) using a modified monochromator FOSS NIR Systems 6500 in bottle [1].
- Triple bottles replicates of each treatment were scanned and then opened for the analyses at bottling and 3, 6, and 13 months after bottling. Two-third of each data set (mid SO_2 and high SO_2 , kept separately) was used for calibration and one-third for validation of the model. In addition, a separate lot of 12 replicate bottles of each treatment (n=144 bottles at ten time points) were also scanned at the time of opened bottles analyses, and about every month in the periods between the opened bottle sampling points. These bottles were never opened.
- *Vision* software was used to collect spectral data.
- Partial Least Square (PLS1) with full cross-validation regression models between spectra and chemical reference data were obtained using *The Unscrambler* software.

Parameters predicted by VIS-NIR versus reference

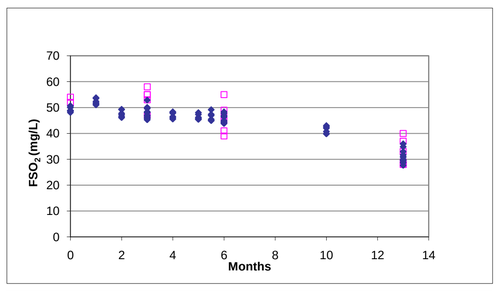
Mid SO_2

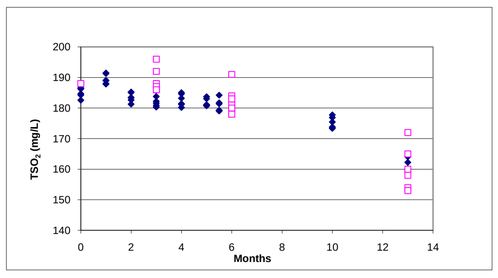


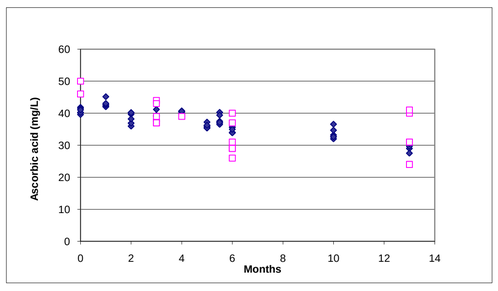




High SO_2







LEGEND
Reference □ Predicted ◆

PLS statistics

	CALIBRATION									VALIDATION					
	n	T	R^2	*SECV*	Mean	*SD*	Min	Max	RPD	n	T	R^2	*SEP*	Slope	Bias
TSO_2															
mSO_2	46	3	**0.81**	*4.6*	**145**	*10.3*	124	165	**2.3**	19	3	**0.75**	*5.6*	0.74	-3.22
hSO_2	46	2	**0.77**	*6.4*	**173**	*13.4*	152	197	**2.1**	20	3	**0.64**	*6.4*	0.58	-0.91
mSO_2 hSO_2	96	2	**0.40**	*14.5*	**159**	*18.6*	124	197	**1.3**	39	2	**0.46**	*14.1*	0.42	-2.56
FSO_2															
mSO_2	44	3	**0.84**	*2.6*	**21**	*6.4*	9	30	**2.5**	18	3	**0.77**	*3.2*	0.81	-2.83
hSO_2	46	3	**0.83**	*4.1*	**40**	*9.8*	23	60	**2.4**	20	3	**0.78**	*4.7*	0.72	-2.13
mSO_2 hSO_2	90	3	**0.43**	*9.7*	**31**	*12.9*	9	60	**1.3**	38	3	**0.44**	*9.8*	0.42	-1.77
Ascorbic acid															
mSO_2	40	3	**0.65**	*4.5*	**33**	*8.2*	20	50	**1.8**	18	3	**0.61**	*5.2*	0.53	0.57
hSO_2	46	2	**0.67**	*4.4*	**35**	*8.2*	20	50	**1.9**	18	2	**0.53**	*5.3*	0.56	2.41
mSO_2 hSO_2	90	3	**0.57**	*5.0*	**34**	*8.2*	20	50	**1.6**	39	3	**0.39**	*6.0*	0.46	0.53

- PLS1 regression was performed between the 2nd derivative (Savitzky-Golay) of the VIS-NIR wine spectra in a bottle and chemical reference data.
- Notes: n=number of reference samples, T= number of PLS terms, R^2= coefficient of determination, SECV= standard error of cross-validation, SEP= standard error of prediction, Residual Predictive Deviation RPD= SD/SECV (where SD= standard deviation of the sample set).
- Wine spectra of unopened bottles (mSO_2, hSO_2, n=720 each set) were collected during storage; predicted values of chemical parameters were averaged (12 bottle replicates per closure) and both sets were kept separately at each time point.
- Chemical parameters used in PLS1 were standardised by 1/SD.

CONCLUSIONS

- PLS1 regression models showed that predicting of free and total sulphur dioxide and ascorbic acid in unopened bottles of wine was possible.
- RPD values were smaller than three thus the method is considered as acceptable for screening purpose.
- Due to the wine matrix better calibration parameters were obtained when PLS1 analyses were performed separately on the mid SO_2 (mSO_2) and high SO_2 (hSO_2) data sets.

VIS-NIR IN THE BOTTLE KEY MESSAGES

- It has potential to predict free and total sulfur dioxide and ascorbic acid concentration of wines in unopened bottles during storage.
- It can save time and reduce analytical workload thus reduce the overall cost.

References:

1. *Cozzolino, D.; Kwiatkowski, M.J.; Waters, E.J.; Gishen, M. (2007) A feasibility study on the use of visible and short wavelengths in the near- infrared region for the non-destructive measurement of wine composition. Analytical and Bioanalytical Chemistry, 387 (6): 2289-2295*

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