Novel Digital Technologies to Assess Smoke Taint in Wine Using Non-Invasive Chemical Fingerprinting, a Low-Cost Electronic Nose, and Artificial Intelligence

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Introduction

Climatic anomalies, such as heatwaves and bushfires, are increasing in number, intensity, and severity worldwide due to climate change. Bushfires are especially problematic in wineproducing countries since smoke contamination can reach vineyards in critical periods of berry development, which is passed to the wine as smoke taint in the winemaking process. The only alternative for winemakers to assess berry or wine contamination is by sending samples to specialized laboratories, which can be time consuming and cost-prohibitive and only sentinel plants, bunches or wine batches can be monitored. These studies aimed to develop rapid, reliable and affordable methods using novel digital technologies to assess smoke taint in wine.

Methods

Two studies were conducted by applying different smoke treatments to grapevines (Cabernet Sauvignon; Study 1) and applying different amelioration treatments to non-smoked and smoke-tainted wines (Pinot Grigio; Study 2). Study 1 was conducted at the University of Adelaide's Waite campus in Urrbrae, South Australia (Figure 1a).

Treatments:

i. Control
ii. Control with misting
iii. Low-density smoke
iv. High-density smoke
v. High-density smoke with misting

Microvinification was used to develop wine samples to conduct analysis for this study. Triplicates of wine samples of each treatment were used to analyse chemical fingerprinting using a near-infrared (NIR) spectroscopy microPHAZIR™ RX Analyzer (Thermo Fisher Scientific, Waltham, MA, USA) within the 1596 – 2396 nm spectra. These samples were also analysed using a low-cost and portable electronic nose (e-nose) to assess volatile compounds present in the samples. As ground-truth data, samples were analysed for volatile phenols and glycoconjugates using the stable isotope dilution analysis (SIDA) method. Furthermore, a consumer sensory session was conducted to assess acceptability of different attributes. Gas chromatography mass-spectroscopy was used to assess aromatic volatile compounds in wine samples.

Study 2 was conducted using commercial wines supplied by a winery located at King Valley, Victoria, Australia.

Treatments:

i. Non-smoked control
ii. Non-smoked with activated carbon
iii. Non-smoked with activated carbon and enzyme
iv. Smoke-tainted control
v. Smoke-tainted with activated carbon
vi. Smoke-tainted with activated carbon and enzyme

Samples (Figure 1b) were analysed in triplicates using a low-cost and portable electronic nose (e-nose) to assess volatile compounds present in the samples.

(a) (b)

Figure 1. (a) Tent used to apply smoke treatments in vineyard for Study 1 and (b) two of the seven amelioration treatments (before filtration) used for study 2.

For both studies, machine learning models based on artificial neural networks were developed using Matlab® (Mathworks, Inc., Natick, MA, USA). Models 1 – 3 were developed using the Levenberg Marquardt training algorithm, Model 5 was constructed using the scaled conjugate gradient, while Models 4 and 6 used the Bayesian Regularisation algorithm.

Study 1:
Model 1: Inputs: NIR absorbance values; Targets: (regression): six volatile phenols and 17 glycoconjugates; *Model 2:* Inputs: e-nose outputs; Targets (regression): 10 volatile phenols and 20 glycoconjugates; *Model 3:* Inputs: e-nose outputs; Targets (regression): Sensory acceptability (12 attributes); *Model 4:* Inputs: e-nose outputs; Targets (regression): aromatic volatile compounds; *Model 5:* Inputs: e-nose outputs; Targets (classification): smoke treatment

Study 2:
Model 6: Inputs: e-nose outputs; Targets (classification): non-smoked treatments and smoke-tainted control treatment

Results

Figure 2 shows the overall regression machine learning models developed using NIR absorbance values (Model 1) and e-nose outputs (Models 2 – 4) as inputs. It can be observed that all models presented very high accuracies with correlation coefficients R > 0.98.

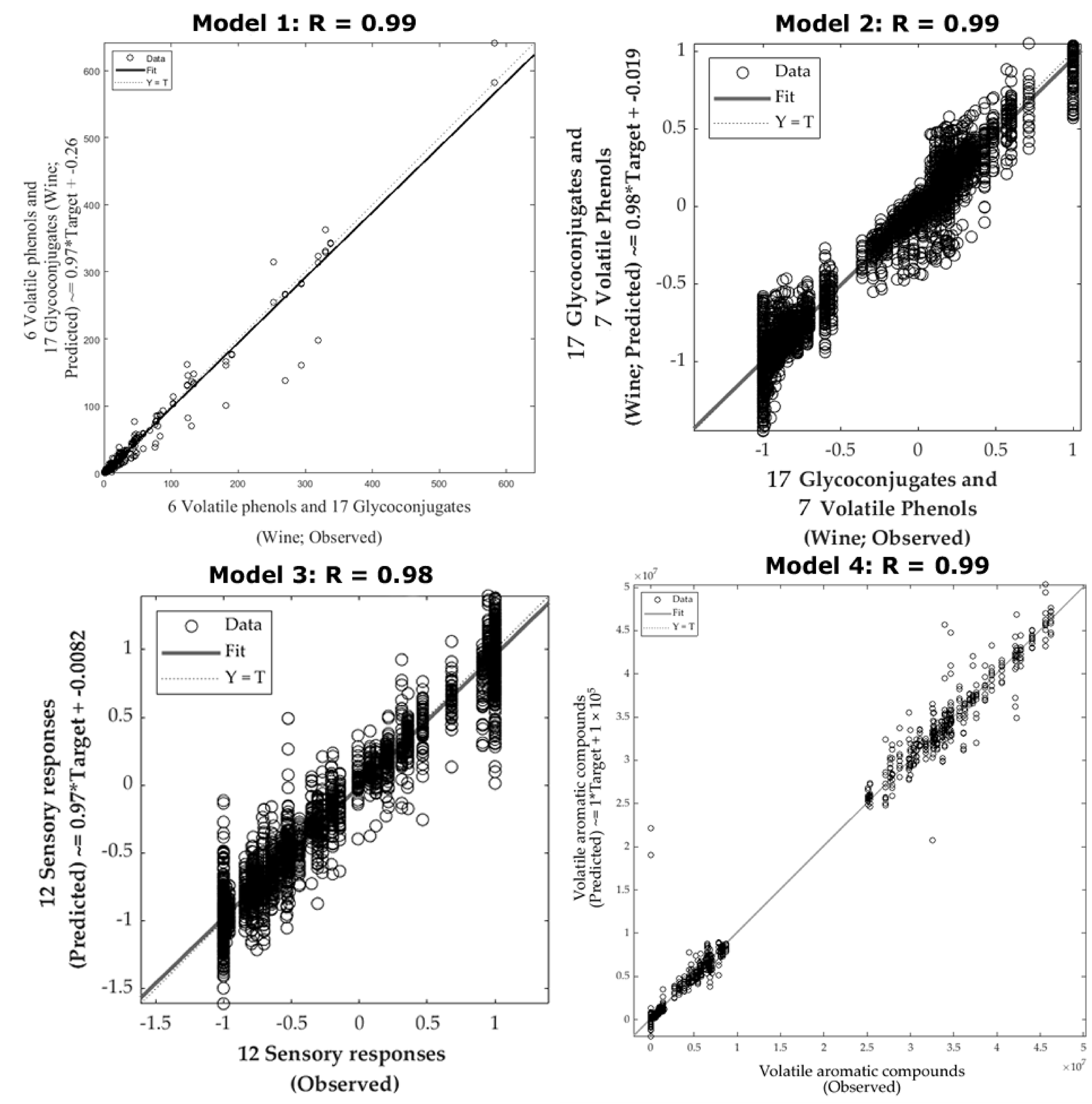

Figure 2. Overall regression models sowing the correlation coefficients (R) with the observed data in x-axis and predicted results in y-axis.

Table 1 shows the accuracies of Models 5 and 6, which were very high with 97% and 98%, respectively. Furthermore, from the performance data, it can be observed that there were no signs of overfitting (training value < testing value). For Model 6 (Study 2), data from the smoke-tainted treatments (v and vii) were used for deployment and obtained that the amelioration treatments were 90% successful by classifying them as non-smoked.

Table 1. Statistical data from the classification Models 5 and 6 showing the accuracy and performance based on means squared error (MSE) for each stage.

Stage	Samples	Accuracy	Error	Performance (MSE)
Model 5: Study 1: Inputs: e-nose outputs; Targets: smoke treatment				
Training	180	99%	1%	0.01
Validation	60	93%	7%	0.04
Testing	60	92%	8%	0.05
Overall	300	97%	3%	-
Model 6: Study 2: non-smoked treatments and smoke-tainted control treatment				
Training	90	100%	0%	<0.01
Testing	60	95%	5%	0.02
Overall	150	98%	2%	-

Conclusion

The methods and models presented in Study 1 resulted in cost-effective and accurate technologies with potential applications to the vineyard and wineries to assess levels of smoke taint and associated compounds for decision-making purposes. Furthermore, the amelioration treatments suggested in Study 2 along with the use of the low-cost e-nose and machine learning model showed to be accurate, reliable and effective to be applied to smoke-tainted wines.

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