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Non-destructive methods for assessing smoke-derived compounds

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Wildfires are an increasing occurrence throughout the world. Grapevine smoke exposure can result in wines characterized by unpalatable smoke aromas. Current chromatographic techniques to assess levels of smoke-derived compounds in berries and wine are destructive, expensive to operate and time-consuming. This research assessed the use of near-infrared technology along with artificial neural network modelling as rapid, non-destructive, and cost-effective tools to assess smoke-derived compounds in berries, must and wine.

Field trials, winemaking, and volatile phenols and glycoconjugates analysis

Three smoke treatments were applied for one hour to Cabernet Sauvignon grapevines at around seven days post veraison using a purpose-built tent[1, 2]. These treatments consisted of high- and low-density smoke exposure from burning ~5 and 1.5 kg of barley straw, respectively, high-density smoke exposure coupled with a fine mist of water applied at canopy level, besides, a control treatment with no smoke exposure or mist of water, and a control treatment with misting and no smoke exposure. The grapes were then used to produce wine on a small-scale using 5 kg bunches per fermentation batch and performed triplicates for each treatment. Levels of volatile phenols (VPs) and their glycoconjugates were determined in grape juice/homogenate (must) from berries harvested one day after smoke exposure and at harvest, and the final wine using already described stable isotope dilution analysis (SIDA) methods[2, 3].

Near-infrared absorbance patterns

The chemical fingerprinting of berries was obtained 24 hours after applying smoke treatments using a portable near-infrared (NIR) spectroscopy device (microPHAZIR™ RX Analyzer; Thermo Fisher Scientific, Waltham, MA, USA), which can measure within the 1596-2396 nm range[1, 4]. A total of 36 berries per treatment were measured in triplicates at ambient temperature. Evaluation of must and wine samples was performed via a previously reported procedure that used a Whatman® filter paper soaked in the desired sample[5]. Each sample was measured three times using three samples per treatment.

Machine learning modelling

Five artificial neural network (ANN) regression models were developed using a customized MATLAB® R2020b (Mathworks, Inc., Natick, MA, USA; Figure 1) code[5]. Models 1-3 used NIR grape berry spectra (1596-2396 nm) measured 24 hours after smoke exposure as inputs to predict levels of 10 VPs and 18 different glycoconjugates in grapes 24 hours after smoke exposure (Model 1) and at harvest (Model 2), and six VPs and 17 glycoconjugates in the final wine (Model 3). On the other hand, Models 4 and 5 were created using the NIR absorbance values (1596-2396 nm) from must and wine, respectively, to predict the levels of six VPs and 17 glycoconjugates in wine.

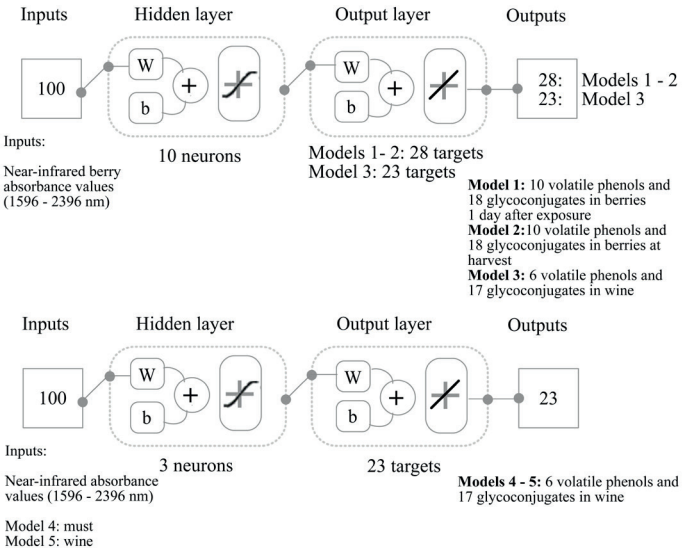


FIGURE 1. Two-layer feedforward networks for the five artificial neural network models developed.

Results and discussion

The five models were able to predict levels of VPs and glycoconjugates in berry and wine samples with high levels of accuracy according to the correlation coefficient ($R \geq 0.98$) and with no signs of overfitting according to their performance based on means squared error (MSE; Figure 2). Models 1–3 may therefore provide an in-field, non-destructive and rapid method to assess levels of smoke compounds in berries and the potential wine, providing growers on-time decision-making to avoid heavily contaminated berries and saving money by selecting smaller samples for further chemical analysis. Besides, Models 4 and 5 can be used by winemakers to assess in near-real-time the levels of VPs and glycoconjugates in wine to decide whether to apply amelioration treatments such as activated carbon to reduce or eliminate smoke taint. Furthermore, as this technique is non-destructive, repeated assessments can be conducted, allowing winemakers to assess changes in VP and glycoconjugate levels over time. However, further research needs to be conducted to deploy the models in natural smoke contaminated grapevines and to develop other grape and wine varieties models[5].

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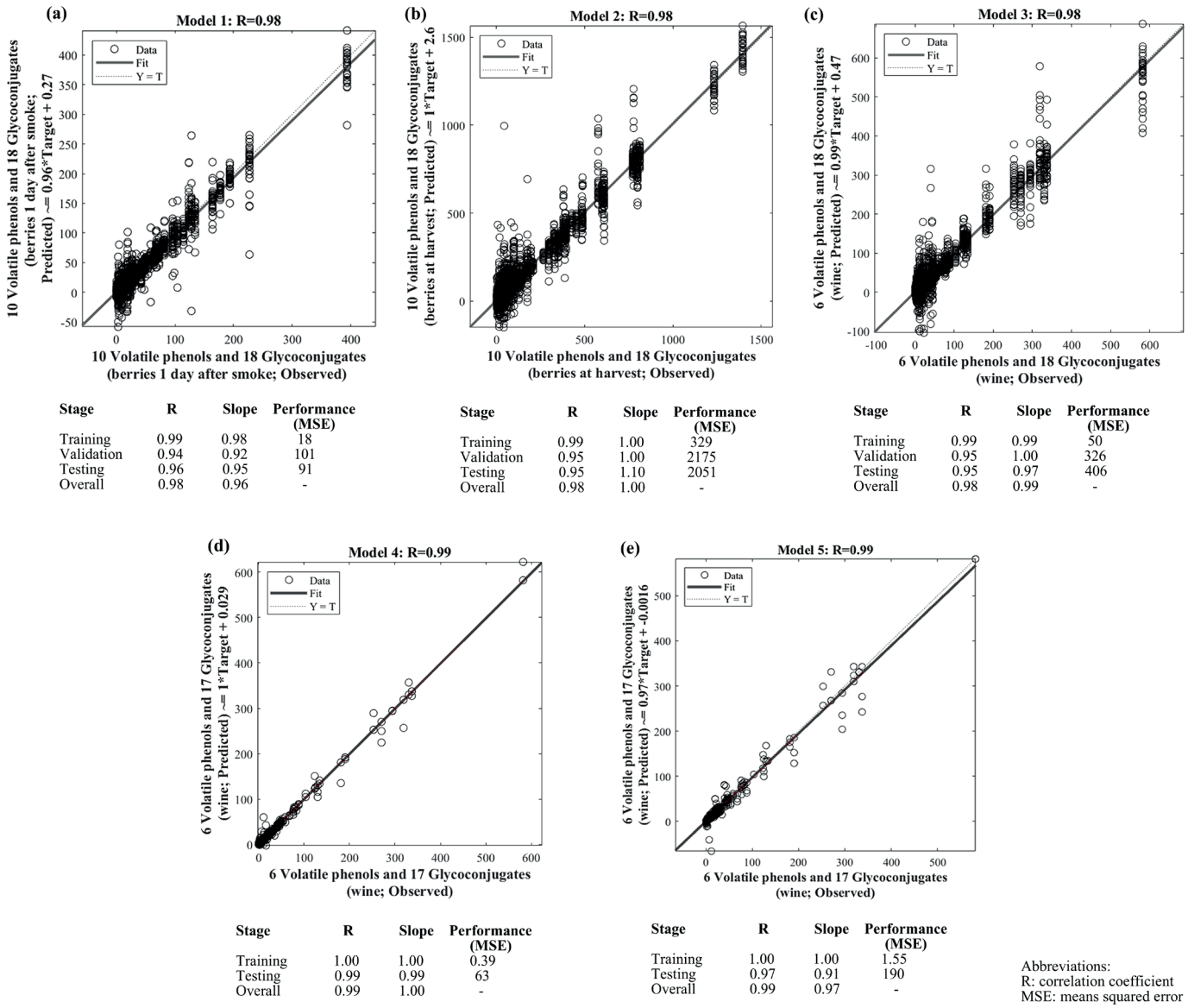


FIGURE 2. Overall artificial neural network regression models to predict volatile phenols and glycoconjugates (a) in berries one day after smoke, (b) in berries at harvest, (c) in wine using near-infrared (NIR) absorbance values from berries, and to predict volatile phenols and glycoconjugates (d) in wine using NIR absorbance values from must, and (e) in wine using NIR absorbance values from wine.

Conclusions

Near-infrared spectroscopy, together with machine learning, may provide rapid, non-destructive tools for assessing the levels of VPs and their glycoconjugates in grapes and wine, allowing winemakers and grape growers to make rapid and cost-effective decisions regarding the contaminated grapes and wine. The proposed method is also low-cost considering the availability of affordable NIR devices that range within US $2,000 - $5,000. The models may be integrated and automated using digital twins, which may aid in the availability of predicted smoke taint scenarios for producers to assess the best smoke-taint mitigation techniques in a timely manner if bushfires occur. ■

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