Assessment of relationships between grape chemical composition and grape allocation grade for Cabernet Sauvignon

Introduction

A wide range of compounds that contribute to wine's appearance, aroma, flavour and texture are derived from grapes. Many of these compounds are known and measurable, and can be manipulated through viticultural and/or winemaking practices. Around the world, many wine companies use grape chemical measures to assess grape value or style; for example, E. and J. Gallo Winery in the USA applies an index of the concentration of multiple compounds primarily for fruit streaming (Smith 2013). Grower cooperatives in Germany are currently trialling measurements of aroma released from the glycoside precursors in grapes as a style indicator and companies in USA, NZ, Italy, Portugal and South Africa use grape tannin and colour measures to support winemaking decisions.

By contrast, measurement of compounds in grapes to objectively assess their value or style is not something that has been implemented widely in Australia, with only one or two measures used by just a handful of companies. Instead, in Australia the value of grapes is usually determined through visual and tasting assessments, often conducted by a single individual. Growers can be paid based on a subjective assessment of the condition of the vines, the flavour of the fruit and the presence of disease, as well as some simple chemical measures of grapes such as colour, total soluble solids, pH or TA. Other growers are paid based on the final value of the wine that is made from their grapes. Many growers and winemakers would like to support decision-making processes by using objective chemical measures that are directly related to attributes that confer value to wine. For both growers and winemakers, such measures could provide specifications that would allow the most value to be achieved from grapes.

A new project

To address this gap, a new project was developed in 2013 with Accolade Wines and FABAL vineyard managers as partners, funded by the Australian Grape and Wine Authority. The project aimed to measure a range of chemical compounds in multiple grape batches of different grades and determine which compounds, independently or in combination, could differentiate between grape grades. The objectives were to determine how variable the chemical measures are across a wide range of fruit grades, if there is a relationship to fruit grade and if the fruit can be clustered based on similarity of chemical composition. A further aim was to assess the practical application of grape grading measurements and to support wine producers who intend to apply these measures in their systems.

This article focuses on work investigating whether current fruit grading allocations can be predicted using chemical measurements, looking at data from Cabernet Sauvignon grape lots from the 2013 and 2014 vintages.

Grape sampling and analysis

Grapes from a range of quality grades were sourced by representative sampling of vineyards from multiple regions, and a wide range of chemical analyses were performed to determine the concentration of compounds known to affect wine style and key sensory properties. These included basic berry chemical composition such as average berry weight, pH, TA, TSS, moisture, malic acid, α-amino nitrogen, ammonia and YAN. Possible negative markers of style included laccase activity and chloride. In addition, data acquired using spectral measures included total phenolics (A280), red colour (A520), A420 and MCP tannin. Full spectral fingerprints in the UV-Vis, mid infrared (MIR) and near infrared (NIR) regions were also acquired. Aroma compounds quantified included the 'grassy, green' C-6 compounds, 'green capsicum' methoxypyrazines, free β-damascenone ('fruity'), and the broad flavour measure phenol-free glycosyl-glucose. For a summary of the functions of these compounds in grapes and wines, please refer to Smith (2013).

The grading data were supplied by the grower or winery contracted to make wine from those grapes. Accolade Wines grades grapes and wines on a scale from 1 (highest value) to 9. Forty-six samples of Cabernet Sauvignon grapes were studied in 2013 across grades 2–7 and 51 samples across grades 3–9 were studied in 2014. Grapes were sourced from eight geographical areas for both vintages (Swan Valley, Riverland, McLaren Vale, Langhorne Creek, Clare Valley, Padthaway, Coonawarra and Wrattonbully).

Which chemical compounds were associated with higher value fruit?

In 2013, a statistical discriminant analysis yielded a model capable of correctly predicting the grade of 39 of the 46 fruit samples. Almost half of incorrect predictions were less than two classes away. Using an alternative partial least squares (PLS) regression approach gave a model with moderate ability to predict grade with an overall R^2= 0.49 (that is, 49% of the variance in the grade is explained by the chemical measures), and the standard error of prediction was 0.79 grade points, which was a very promising result.

The results from this regression model are shown in Figure 1. Only one of the factors used for prediction is shown so that loadings can be examined more easily. Coefficients can be positive or negative depending on whether higher concentrations increase value (better grade) or decrease value (poorer grade) and only significant variables are shown.

In the 2013 dataset, YAN, total phenolics, A420 and A520 and β-damascenone were all positively associated (i.e. there are higher amounts) with better grade. These measures have been indicated as positively associated with grape and wine quality in Australia, and this dataset reinforces those observations. In addition, they are all in use internationally (with varying levels of sophistication) as objective measures of quality. By contrast, TA, cysteine, glutamate and glutathione were all negatively associated with grade (i.e. grade was lower with higher levels of these measures).

In the 2014 season, discriminant analysis yielded a model that was capable of correctly predicting the grade of 46 out of the 51 samples. Three of the five incorrect predictions were only one class away. Using the PLS approach gave a model with a good ability to predict grade, with R^2= 0.65 and standard error of prediction of 1.41 grade points. An uncertainty test was then used to identify the significant chemical compounds contributing to the prediction of grade, shown in Figure 2.

A larger number of chemical measures was identified in the 2014 dataset. Compounds that were positively associated (i.e. there are higher amounts) with higher value grade included TSS, A280 (total phenolics), A320 (hydroxycinnamic acids), A370 (flavonols, sun exposure markers), A420 and A520 (red colour), a range of amino acids (some of which may be precursors to aroma compounds), glycosyl glucose (GG, aroma precursors), tannin (MCPT) and chloride. Compounds that were negatively associated with grade included nitrogen measures (YAN, AAN), 2-aminobutyric acid, asparagine, glutamic acid and the two C6 'green', 'grassy' compounds Z-3-hexenol and E-2-hexenol. Tannin, GG, TSS, A280 (total phenolics) and A520 (red) have all been previously demonstrated to be generally positively

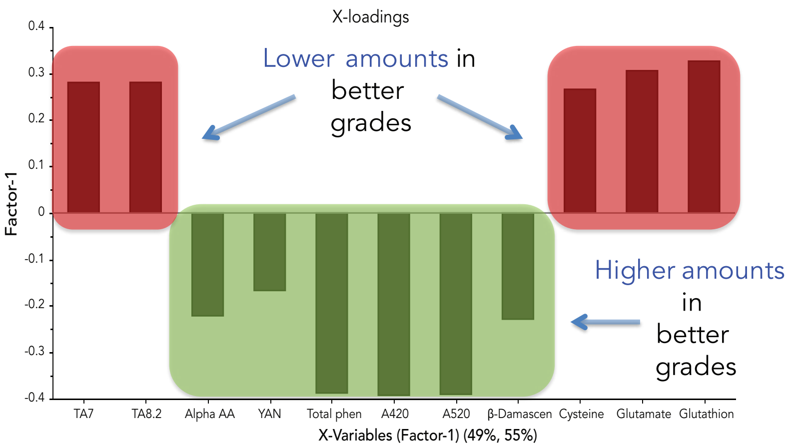

Figure 1. PLS regression model predicting grade, with loadings for significant chemical measures for 2013 Cabernet Sauvignon grape samples.

associated with grape and wine quality in Australia, and this dataset once again reinforces this observation.

The switch of YAN and AAN from positive to negative from 2013 to 2014 was unexpected, but the explanation may be related to a change in the amount of YAN in Riverland fruit relative to all other regional samples – from low in 2013 to high in 2014. Across both seasons studied, total phenolics (A280) and colour (A520) were consistently positively associated with grade. It is unclear why TA and damascenone turned up strongly in 2013 but did not show any relationship with grade in 2014.

The project has also studied Chardonnay and Shiraz in a similar approach, and wines have also been made from the grape samples under standardised conditions to allow the assessment of wine sensory properties and relate these to the grape compositional measures.

Conclusion

Developing an understanding of the relationships of available objective measures to well established subjective grading systems has the potential to significantly reduce production costs and increase value, by ensuring that fruit is used in the most efficient production stream and that maximum value is returned from the end-product. It also may lead to significant savings in the costs of assessing vineyards through more effective application of resources and clearer understandings of geographical, viticultural and climatic drivers. The maintenance of strong relationships along the value chain, and especially between grapegrowers and winemakers, is central to a sustainable Australian wine sector. Objective measures of quality

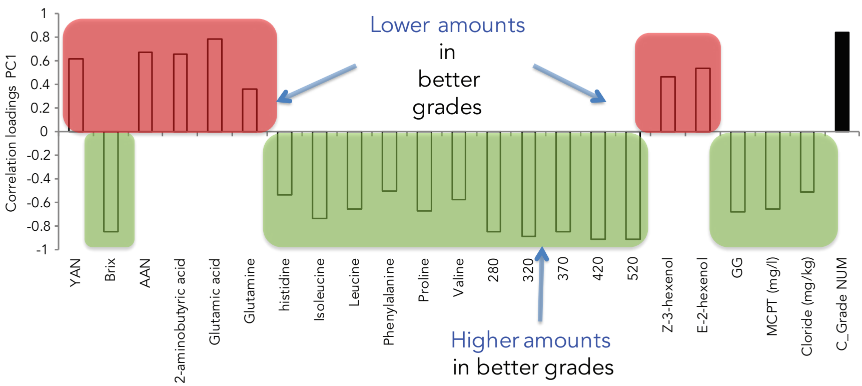

Figure 2. PLS model predicting grade with loadings for significant chemical measures for 2014 Cabernet Sauvignon grape samples.

may contribute significantly to ensuring that transparency, trust and the maximisation of value are achieved, by providing an objective framework within which all parties understand what is expected, to achieve the highest value and most effective use of available resources.

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