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A CHEMOMETRIC APPROACH TO ANALYSIS OF GRAPE AROMA BY GC-MS: IDENTIFICATION OF COMPOUNDS RELATED TO 'PEPPER' AROMA IN AUSTRALIAN SHIRAZ BY COMBINING HS-GC-MS WITH MULTIVARIATE DATA ANALYSIS

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To measure and influence the level of 'black pepper' flavour in Australian Shiraz red wines, we started a project to identify the volatile compounds responsible for this sensory character. Based on advice from key industry collaborators, we have obtained sets of potentially 'peppery' grape samples from numerous vineyards in South Australia and Victoria. The important sensory attributes of the grapes, including the aroma descriptor 'pepper', were rated by a sensory panel. The sensory study revealed a strong correlation between the intensity of 'pepper' aroma and the intensity of 'pepper' flavour perceived on the palate. Gas chromatography-mass spectrometry-olfactometry (GC-MS-O) experiments revealed detectable analytical differentiation among grapes that showed differences in the intensity of 'black pepper' character.

The grape homogenates were analysed by static headspace GC-MS (HS-GC-MS) using a Cool Inlet System (CIS). Vectors obtained by analysis of over 132 000 individual mass spectra (selected from > 13 000 per analysis) were then subjected to multivariate analyses. Both principal component analysis (PCA) and partial least squares (PLS) were used to develop multivariate models (x = mass spectra; y = aroma descriptor) to explain the intensity of the rating of the 'peppery' character. This allowed us to narrow our focus to several compounds, which might be related to the 'pepper' characteristic in the grape homogenates. Furthermore, differences were observed among vineyards, and from the same vineyards in different years. Additional optimisation of the methodology enabled a single region of the GC-MS chromatogram to predict 'pepperiness' with a correlation > 0.98 and led to the identification of a terpenoid compound that acts as a marker for this sensory characteristic. Currently quantitative measurements are being optimised, further investigations are underway, and the results arising shall be presented.