The application of Fourier transform near infrared (FT-NIR) spectroscopy in the wine industry of South Africa

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Fourier transform near infrared (FT-NIR) spectroscopy was used as a rapid method to measure the °Brix content and to discriminate between different must samples in terms of their free amino nitrogen (FAN) values. FT-NIR spectroscopy was also used as a rapid method to discriminate between Chardonnay wine samples in terms of the status of the malo-lactic fermentation (MLF). This was done by monitoring the conversion of malic to lactic acid and thereby determining whether MLF has started, is underway or has been completed followed by classification of the samples. Furthermore, FT-NIR spectroscopy was applied as a rapid method to discriminate between table wine samples in terms of the ethyl carbamate (EC) content. EC in wine can pose a health threat and need to be monitored by determining the EC content in relation to the regulatory limits set by the authorities.

For each of the above mentioned parameters, QUANT+™ methods were built and calibrations derived and it was found that a very strong correlation existed in the sample set for the FT-NIR spectroscopic predictions of °Brix ($r = 0.99$, SECV = 0.306), but the correlations for the FAN ($r = 0.61$, SECV = 272.1), malic acid ($r = 0.58$, SECV = 1.06), lactic acid ($r = 0.51$, SECV = 1.14) and EC predictions ($r = 0.47$, SECV = 3.67) were not as good.

Soft Independent Modeling by Class Analogy (SIMCA) diagnostics and validation was applied as a sophisticated discrimination method. The must samples could be classified in terms of their FAN values when SIMCA was applied, obtaining results with recognition rates exceeding 80%. When SIMCA diagnostics and validation were applied to determine the progress of conversion of malic to lactic acid and the EC content, again results with recognition rates exceeding 80% were obtained.

The evaluation of the applicability of FT-NIR spectroscopy measurement of FAN, °Brix values, malic acid, lactic acid and EC content in must and wine shows considerable promise. FT-NIR spectroscopy has the potential to reduce the analytical times considerably in a range of measurements commonly used during the wine making process. Where conventional FT-NIR calibrations are not effective, SIMCA methods can be used as a discriminative method for rapid classification of samples. SIMCA can replace expensive, time-consuming, quantitative analytical methods, if not completely, at least to some extent, because in many processes it is only needed to know whether a specific cut off point has been reach or not or whether a sample belongs to a certain class or not.