

## **Analytical and Chemometric Investigation of Phenolic Content of South African Red Wines**

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Phenolic compounds have been the focus of a lot of research in recent years for their important contribution to sensory characteristics of wine, their beneficial health effects, as well as the possibility they offer of characterising wines. In this contribution, a method is developed that allows the direct injection of wine samples followed by liquid chromatography-diode array-electrospray ionisation-ion trap mass spectroscopy (MS) for the quantitative and qualitative analysis of a wide range of non-coloured phenolics. Diode array detection was found to be more suitable for quantitative purposes, while on-line UV spectra in combination with mass spectra greatly facilitate the identification of phenolics. Although MS detection was characterised by relatively poor sensitivity (full scan mode) and linear response, this form of detection proved to be an exceedingly powerful identification tool, allowing identification of 20 non-standard compounds in wine. These include procyanidins, epigallocatechin, prodelfinidins (only the second time these compounds are identified in wine), tartaric acid esters of p-coumaric acid and caffeic acid, 3 resveratrol derivatives, myricetin and flavonol-glucosides. It is concluded LC-UV-MS currently represents the state-of-the art in analysis methods for wine polyphenols, combining quantitative and identification capabilities.

The LC-diode array method was subsequently used to quantify 16 phenolic compounds in 55 South African red wines. Values are compared to those reported in the literature for these compounds in wines from other countries. These data were used together with chemometric methods for the characterisation of these wines according to variety. Discriminant analysis allowed a 100% correct recognition of the 5 cultivars studied, independent of the vintage or geographical origin, based on non-coloured phenolic content.