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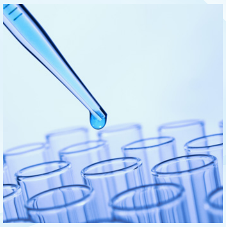
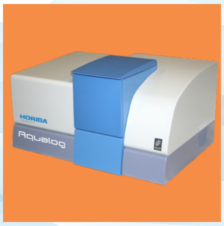
Classification and Phenolics Analysis of Red Wines with A-TEEM Molecular Fingerprinting

ELEMENTAL ANALYSIS
FLUORESCENCE
GRATINGS & OEM SPECTROMETERS
OPTICAL COMPONENTS
FORENSICS
PARTICLE CHARACTERIZATION
RAMAN
SPECTROSCOPIC ELLIPSOMETRY
SPR IMAGING





Simultaneous measurement of Absorbance, Transmission, Fluorescence Excitation and Emission Matrix

Introduction

HORIBA Scientific has developed Aqualog®, an analytical instrument based on the simultaneous measurement of Absorbance, Transmission, Fluorescence Excitation and Emission Matrix (A-TEEM™).

Aqualog reports NIST-traceable A-TEEM fingerprints which can be evaluated using multivariate statistics such as PARAFAC (Parallel Factor Analysis), PCA (Principal Components Analysis), CLS (Classical least Squares) and PLS (Partial least Squares Analysis). Importantly A-TEEM fingerprints yield qualitative and quantitative composition of key flavor and color determinants in wine and spirits that are not discernible with simple Absorbance or Transmission data analysis.

Of the hundreds of different compounds that have been identified in grapes, it is the phenolic content of ripening grape berries that fundamentally determines the quality of a wine. The different classes of phenolics (anthocyanins, tannins, flavonols, catechins) affect the color, the mouthfeel, flavor and aroma to various extent[1].

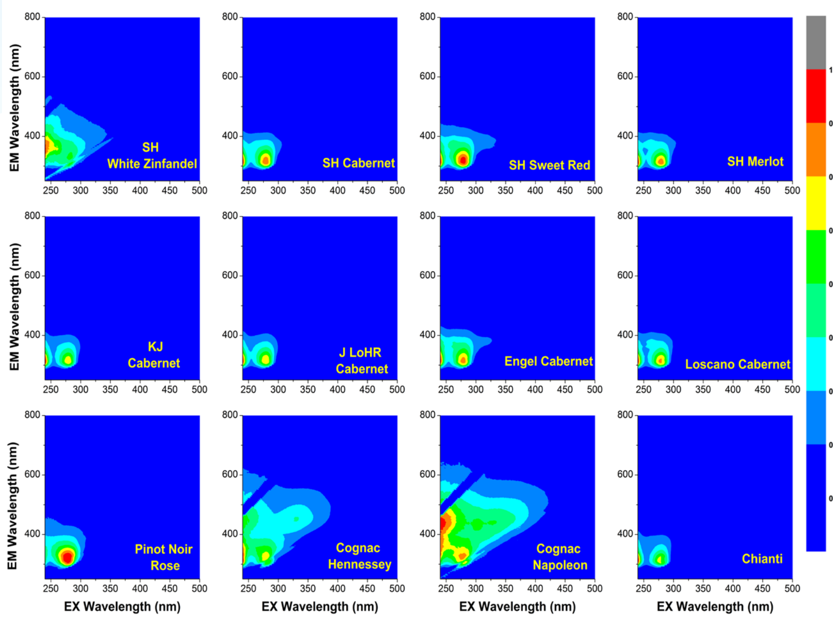
The individual compounds comprising these classes of phenolics contribute in concert to give the wines their unique character.

The simultaneously acquired Absorbance, Transmission and IFE-corrected EEM data can be used to evaluate lot-to-lot, regional, and varietal characteristics. (See Figure 1.)

The samples were measured at room temperature and diluted 1:100 with 50% deionized water 50% ETOH in a 1-cm path quartz fluorescence cell. Spectral A-TEEMs were automatically corrected for the influence of Inner Filter Effects (IFE), and Rayleigh masking was applied prior to PARAFAC and CLS analysis using the Eigenvector Inc. SOLO™ package.

The phenolics in Table 1 are just some of the most prevalent compounds known to affect wine characteristics like flavor, long term stability and color.

Figure 1: An array of A-TEEM molecular fingerprints of various wines and spirits displaying perceptible differences.



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Molecular Groups	Main Contribution	Examples of individual molecules
Anthocyanins	Color	cyanidin-, petunidin-, delphinidin-, malvidin (-3-glucosides)
Catechins	Bitterness	monomeric flavon-3-ols catechin, epicatechin, epicatechin-gallate
Tannins	Astringency	polymers of flavon-3-ols catechin, epicatechin
Non-flavonols	Antioxidants, sun screen	coumaric,caffeic, ferru-lic,gallic acids, resveratrol
Flavonols	Photoprotection	quercetin, myricetin, kae-mpferol, isorhamnetin, syringetin

Table 1.

CLS analysis of the wines and spirits in Fig. 2 based upon a library of 9 phenolic compounds for illustrative purposes yields their relative contribution to the total phenolic fingerprint normalized to 100%. Significant differences between wines are reflected visibly in their phenolic compound fingerprints.

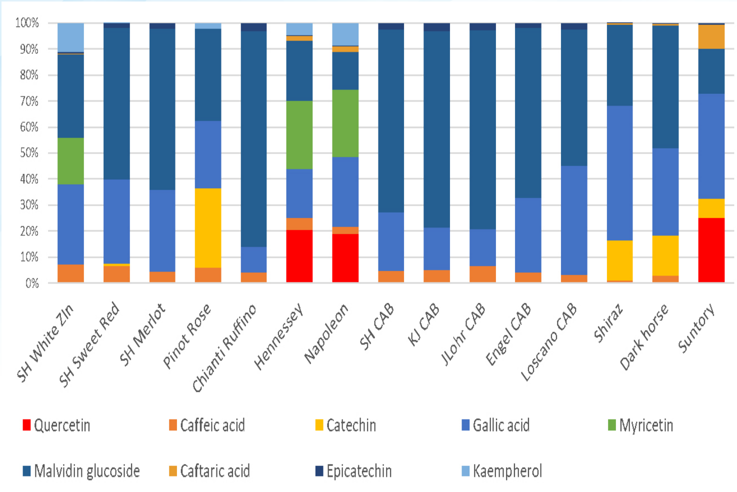

Figure 2.

CLS analysis of spirits only, as seen in Figure 3 (cognacs and scotches) yields a different distribution, consistent with their being prevalently matured in oak casks that impart Quercetin and Myricetin compounds to them.

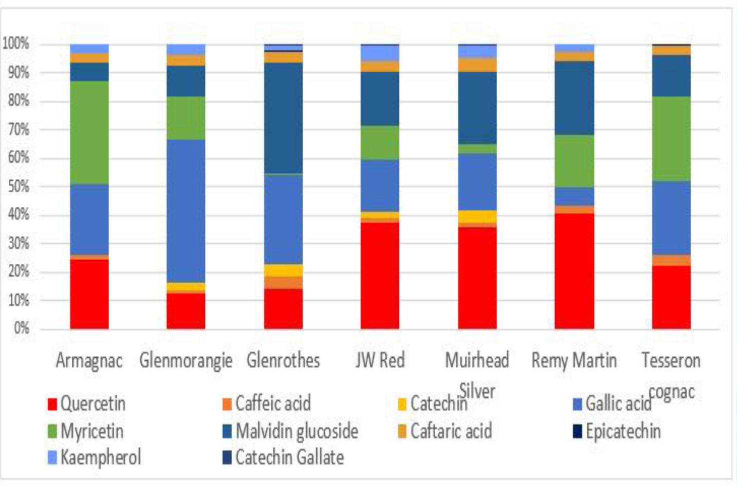

Figure 3.

Monitoring the phenolics content in grapes and in grape juice after harvest allows the winemaker to determine the optimal period of fermentation and consequent extraction of these compounds from the skin and seeds of the berries. Adjustment of these values in the finished product by deciding on a course of blending, contributes to flexibility in producing wine with the desired characteristics, and also corrects for color or aroma shortcomings.

Traditional analysis relies on the use of HPLC, GC / MS techniques that require sophisticated laboratory equipment and expert preparation by trained personnel. UV/VIS optical density measurements are being used to provide bulk assessment of component molecules, but lack specificity.

In contrast, the A-TEEM technique with IFE provided by Aqualog requires only a single scan of a diluted sample lasting a few seconds. Subsequent application of a predetermined multivariate model, calibrated using a library of reference compounds, is the fastest and simplest technique to classify and compare wines, detect adulteration, spoilage, quantify SO_2 treatment[2], etc.

1. (Waterhouse et al. Understanding Wine Chemistry ed. Wiley and Sons 2016)
2. Coelho, C. et al. Anal. Chem. 2015, 87, 8132–8137

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