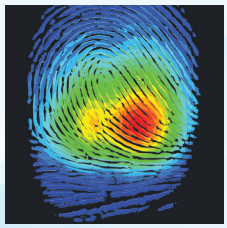
HORIBA

Fluorescence

A-TEEM™ Analysis of Wine Quality Compounds and Parameters with Machine Learning



Application Note
Agricultural Sciences
FL-2023-12-2

Doreen Schober, Adam Gilmore, Linxi Chen, Jorge Zincker, Alvaro Gonzalez

Summary

We introduce A-TEEM™ spectroscopy as a new and fast way to analyze 45 specific quality parameters in wine (ref. 1). A-TEEM, a fluorescence spectroscopy technique, simultaneously acquires transmission, absorbance, and fluorescence Excitation Emission Matrices, overcoming the inner filter effect on the fly (ref. 2).

No practical method currently exists to analyze these important compounds together for the wine industry. We designed the method to work within a certain range of concentrations, making it easy to measure absorbance and fluorescence. We tested the method on 126 wines and verified its accuracy with a prediction test-set of 13% and another independent validation set of 16 wines. We compared the individual and combined data of these components using two regression algorithms, namely, Partial Least Squares Regression and Extreme Gradient Boost Regression (XGBR). With various reference data measurements, we concluded that XGBR yielded more accurate results. Using a multi-block data approach to coordinate both the fluorescence and absorbance variable and analyzing with XGBR (Eigenvector Inc. Solo v8.9-9.21). We obtained accurate results, with respective average R^2 values of 0.941±0.041, 0.920±.040 and 0.971±0.017 for the anthocyanins and phenolic parameters (n=29), basic chemistry parameters (n=8) and the UV assay parameters (n=8).

Background

Grapes and wine quality have been studied for a long time to see if we can tell how good they are by looking at their chemical makeup. This matters because people care about how wine tastes and is made. Different chemicals and chemistry parameters can tell us about the quality of grapes and wine. We report data on a wide variety of key compounds and parameters known to reflect good quality in wine. These values are connected to several quality attributes, including things like color, strong taste, mouth-feel and even fruity flavors.

Some of these chemicals, namely the phenolic and anthocyanin compounds, play a big role in wine. They affect color, astringency, bitterness, and how the wine feels and ages. There are also other important chemicals like acids and sugars that affect the taste and feel of wine. We also know that the sugar level in grapes is related to how the wine will turn out.

Testing these chemicals to judge quality is not easy and can be expensive. People have used methods like chromatography and spectroscopy to do this. However, these methods can be slow, or not very practical. The wine industry has thus been looking for better ways to do this.

We tested a technique called A-TEEM on wine. It's good at picking up on certain chemicals that can tell us about wine quality. This technique is especially good for finding small amounts of these chemicals. Most of these chemicals emit light when we shine light on them, and A-TEEM can measure that light to tell us about the composition and concentration of these chemicals in wine. We used this technique to quickly measure how much of these chemicals are in wine. We wanted to see if it can help us.

Table 1 shows that Extreme Gradient Boost Regression analysis of A-TEEM data of wine extracts can be used to accurately predict quantification of a wide range anthocyanins and phenolic compounds, several basic chemistry parameters, and the results of commonly used UV assays for wine quality analysis from one A-TEEM scan.

Conclusion

Overall, this study aimed to develop a fast and reliable method to measure important chemicals in wine. We thought that the A-TEEM technique would be useful because it's good at detecting these chemical parameters. We also wanted to measure individual chemicals, not just general groups, because they each play a different role in wine quality. This study aimed to make the testing process better, including how we use the data we collect.

In this study, we showed that the A-TEEM method can measure different important chemicals in wine. We were able to estimate various compounds like tannins, pigments, and acids. This new method helps us understand different aspects of wine quality. By looking at both how light is absorbed and given off, we could

measure even the small amounts of these compounds. The XGBR algorithm helped make good predictions. Overall, we suggest using A-TEEM with machine learning algorithms to accurately predict the important chemical levels that affect wine quality.

Acknowledgements

We are very grateful to Professor Emeritus Dietrich von Baer and his coworkers at the University of Concepci´on for their support in the development of the HPLC analysis methods. Furthermore, we thank Veronica Weber, Camila Guti´errez and Monica Rodríguez for laboratory analyses, and Sergio Manzano and his coworkers for the production of the experimental wines. The project 17PIDE-80701 is supported by Corporaci´on de Fomento de la Producci´on (CORFO). None of this would have been possible without the participation of the Viña Concha y Toro Research Center in the development of this methodology and its team, Doreen Schober, Jorge Zinker, and Alvaro Gonzalez.

References

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#	Anthocyanins and Phenolics	XGBR R^2P	#	Basic Chemistry	XGBR R^2P	#	UN-Assays	XGBR R^2P
1	Delfinidin-3-glucoside	0.953	1	Alcohol %	0.923	1	Tannins (Microcellulose precipitated)	0.949
2	Cyanidin-3-glucoside	0.978	2	Total Acidity	0.897	2	Small Polymeric Pigments	0.993
3	Petunidin-3-glucoside	0.967	3	Volatile Acidity	0.897	3	Large Polymeric Pigments	0.955
4	Peonidin-3-glucoside	0.951	4	pH	0.965	4	Total Polymeric Pigments	0.988
5	Malvidin-3-glucoside	0.992	5	Color	0.979	5	Total Tannins	0.958
6	Peonidin-3-glucoside	0.988	6	SO2 Free	0.905	6	Total Phenolics	0.966
7	Malvidin-3-glucoside	0.989	7	SO2 Bound	0.947	7	Non-tannin Phenolics	0.970
8	Peonidin-3-glucoside	0.969	8	SO2 Total	0.874	8	Total Anthocyanins	0.990
9	Malvidin-3-glucoside	0.980						
10	Total Anthocyanins	0.991		**Mean**	**0.920**		**Mean**	**0.971**
				SD	**0.040**		**SD**	**0.017**
11	Carechin	0.961						
12	Epicatechin	0.797						
13	Flavan-3-Oles	0.914						
14	Caftaric acid	0.943						
15	Caffeic acid	0.888						
16	Cutaric acid	0.912						
17	Hydroxycinnamic acids	0.954						
18	Myricetin-3-O-galactoside	0.926						
19	Myricetin-3-O-galactoside	0.937						
20	Free Myricetin	0.926						
21	Hyperoside	0.929						
22	Quercetin-3-O-glucoside	0.909						
23	Quercetin	0.920						
24	Laricitrin (nex)	0.939						
25	Syringetin-3-galactoside	0.942						
26	Syringetin-3-glucoside	0.919						
27	Kaempferol	0.888						
28	Flavonoles	0.953						
29	Total Phenolics	0.977						
	Mean	**0.941**						
	SD	**0.041**						

Aqualog and Autosampler

Table 1: Comparison of the R2 values (R2P) for the test-set predictions of A-TEEM wine analyses using Extreme Gradient Boost Regression (XGBR) for a range of anthocyanins and phenolic compounds, basic chemistry parameters and UV-assays commonly used to evaluate wine quality. Mean and standard deviations values for each parameter column are shown in bold while compound summations are italicized.

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info.sci@horiba.com

horiba.com/fluorescence

USA: +1 732 494 8660
UK: +44 (0)1604 542 500
China: +86 (0)21 6289 6060
France: +33 (0)1 69 74 72 00
Italy: +39 06 51 59 22 1
Brazil: + 55 (0)11 2923 5400
Germany: +49 (0) 6251 8475 20
Japan: +81 (0)3 6206 4721
Other: +1 732 494 8660