

# ● Analysis Report Wine-Profiling™

Sample ID: 6183921

## Additional Sample Information

Variety: Sangiovese

Country: Italy

Vintage: 2009

Type of Wine: red

Measuring Date: 21-Nov-2014 03:11:06

Reporting Date: 19-Dec-2014 16:35:12, Version 3.0.1, 9 pages

## Results Summary

Type of Analysis	Analysis ID	Result	Status
<b>Classification Analysis</b>			
Red Wine Country	WI-1105-01/0681	In-Model	●
Italian Variety	WI-1103-01/0681	In-Model	●
<b>Targeted Analysis</b>			
Quantification	WI-Q/0583	–	●
Comparison with NMR Reference Database	WI-QC/0707	–	●
<b>Untargeted Verification Analysis</b>			
Univariate Verification	WI-2022-02/705	In-Model	●
Multivariate Verification	WI-2022-02/705	In-Model	●
Wine Content Analysis	WI-4022-01/706	In-Model	●

## Notification:

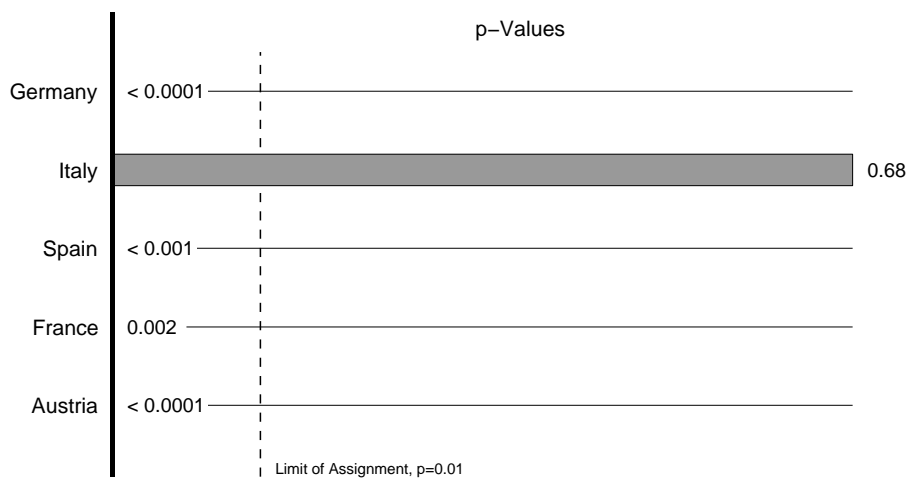
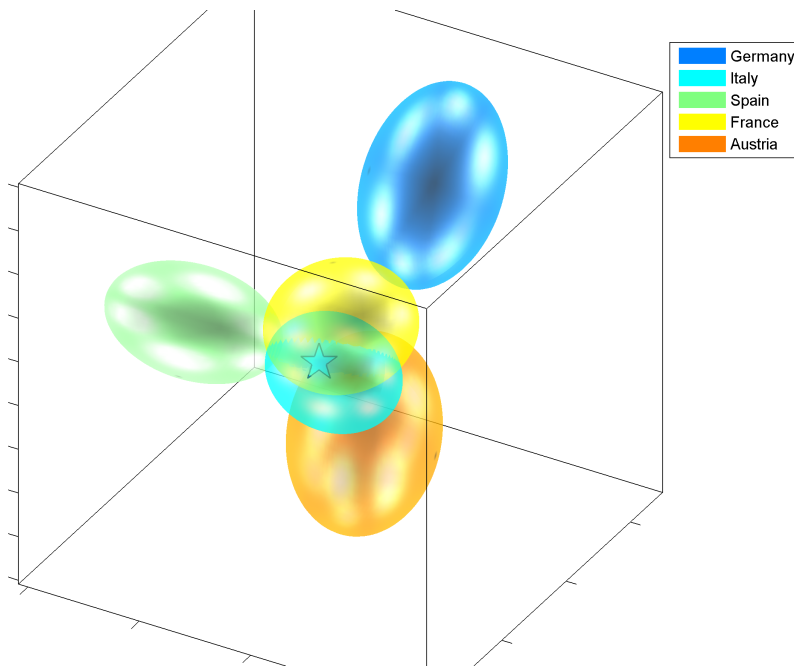
Quantitative analysis including traffic light rating indicates possible violations according to official reference values defined by the European Council Regulations – expert interpretation is needed in individual case. A special expert interpretation is needed regarding the dedicated area and/or country of production not underlying EU-regulations.

## Classification Analysis

**Model:** Red Wine Country

(Analysis-ID: WI-1105-01/0681)

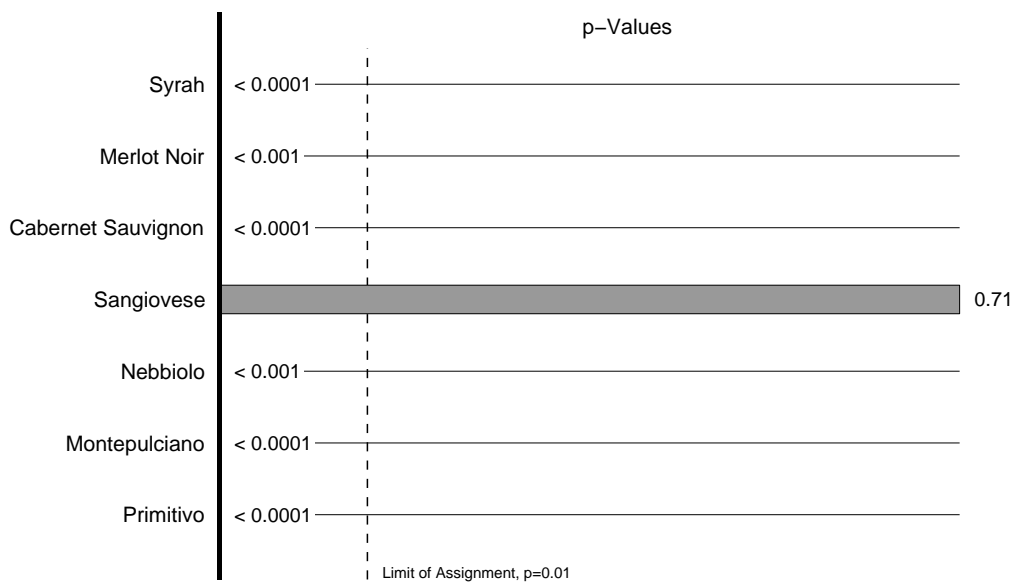
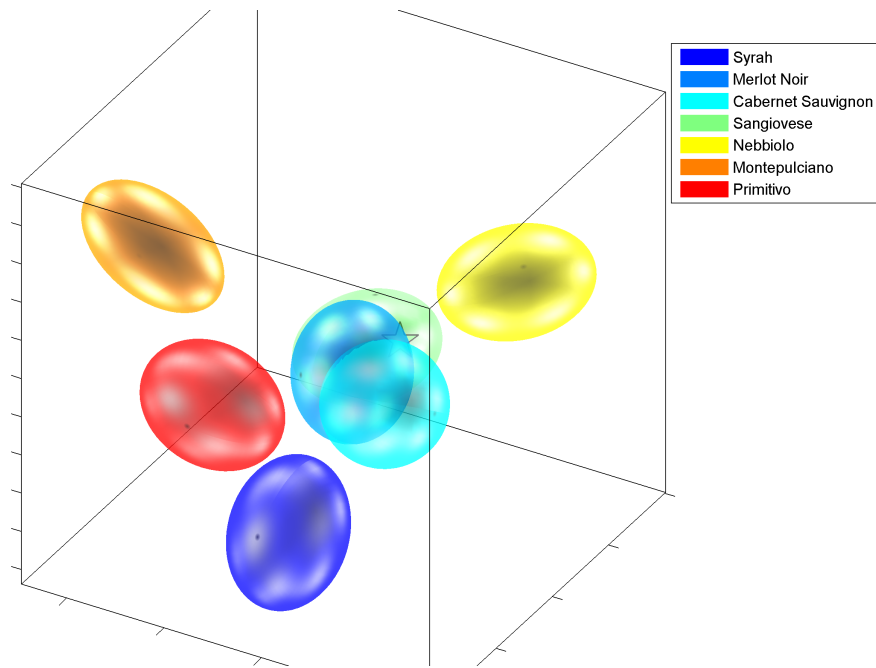
**Result:** Declared origin *Italy* is consistent with classification result.



**Model:** Italian Variety

(Analysis-ID: WI-1103-01/0681)







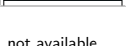






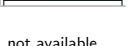
**Result:** Declared variety *Sangiovese* is consistent with classification result.







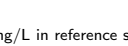
## Targeted Analysis

In the following tables the results of the quantitative analysis are given. Parameters labelled with \* are calculated parameters. Please refer to the additional remarks for quantified parameters, flags and reference values on page 9. The displayed distributions of the Wine-Profiling™ NMR reference database refer to group *Sangiovese*.






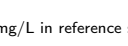



### Standard Parameters:

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™	
					min	max	NMR reference database	
total alcohol*	123.7	g/L	-	●↑	-	-	96.7	 124.1
total alcohol-v*	15.7	%vol	-	●↑	-	-	12.3	 15.7
ethanol	123.0	g/L	5.0	○	-	-	94.7	 123.6
ethanol-v*	15.6	%vol	-	○	-	-	12.0	 15.7
glycerol	11.3	g/L	0.5	○	-	-	7.3	 11.7
glucose	<0.5	g/L	0.5	○	-	-	<0.5	 5.3
fructose	1.2	g/L	0.5	○	-	-	<0.5	 6.2
glucose/fructose*	-	-	-	○	-	-	not available	
sucrose	<0.2	g/L	0.2	●	-	-	<200 mg/L in reference set	
arabinose	101	mg/L	100	○	-	-	<100	 412
total sugar (bef. inv.)*	1.4	g/L	1.0	○	-	-	<1.0	 11.4
total fermentable sugar*	1.4	g/L	1.0	○	-	-	<1.0	 11.4
tartaric acid	2.1	g/L	0.5	●	-	-	<0.5	 2.9
malic acid	0.2	g/L	0.2	○	-	-	<0.2	 1.6
lactic acid	754	mg/L	200	○	-	-	<200	 1561
citric acid	<200	mg/L	200	●	-	1000	<200	 360
energy value*	3890	kJ/L	-	○	-	-	not available	
bread units*	<0.2	1/L	0.2	○	-	-	not available	
carbohydrate units*	<0.2	1/L	0.2	○	-	-	not available	



**Degradation Parameters:**

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™
					min	max	NMR reference database
acetic acid	715	mg/L	100	○	-	-	334  1067
acetoine	10	mg/L	10	○	-	-	<10  72
ethylacetate	170	mg/L	50	○	-	-	<50  226
ethylactate	182	mg/L	150	○	-	-	<150  219
formic acid	11	mg/L	5	○	-	-	<5  12
fumaric acid	<5	mg/L	5	○	-	-	<5 mg/L in reference set
gluconic acid	<400	mg/L	400	●	-	-	<400 mg/L in reference set
putrescine	<50	mg/L	50	○	-	-	<50 mg/L in reference set
cadaverine	<50	mg/L	50	○	-	-	<50 mg/L in reference set
HMF	<5	mg/L	5	●	-	-	<5 mg/L in reference set
furfural	<2	mg/L	2	○	-	-	<2 mg/L in reference set






**Higher Alcohols / Fermentation Products:**

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™
					min	max	NMR reference database
methanol	127	mg/L	30	●	-	400	99  217
1,3-propanediol	<40	mg/L	40	○	-	-	<40 mg/L in reference set
2,3-butanediol	632	mg/L	100	○	-	-	277  1223
2-methyl-propanol	<70	mg/L	70	○	-	-	<70  94
2-phenylethanol	87	mg/L	25	○	-	-	<25  108
3-methyl-butanol	247	mg/L	100	○	-	-	162  322
acetaldehyde	23	mg/L	10	○	-	-	<10  58
pyruvic acid	<20	mg/L	20	○	-	-	<20 mg/L in reference set
galacturonic acid	771	mg/L	160	○	-	-	370  1475
succinic acid	950	mg/L	50	○	-	-	638  1155
glycerol/ethanol*	9.2	%	-	●	-	-	7.0  11.3

**Amino Acids:**

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™
					min	max	NMR reference database
4-aminobutanoic acid	<120	mg/L	120	○	-	-	<120 mg/L in reference set
alanine	36	mg/L	35	○	-	-	<35  57
arginine	<150	mg/L	150	○	-	-	<150 mg/L in reference set
proline	1.1	g/L	0.1	○	-	-	0.5  1.7

**(Poly-)phenols:**

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™
					min	max	NMR reference database
caftaric acid	21	mg/L	15	○	-	-	<15  84
epicatechin	<30	mg/L	30	○	-	-	<30  42
gallic acid	151	mg/L	25	○	-	-	<25  183
shikimic acid	23	mg/L	20	○	-	-	<20  39
trigonelline	15	mg/L	10	○	-	-	<10  19

**Stabilising Agents:**

Compound	Value	Unit	LOD	Flag	Official Ref.		Wine-Profiling™
					min	max	NMR reference database
benzoic acid	<10	mg/L	10	○	-	LOD	not available
sorbic acid	<10	mg/L	10	○	-	200	not available
salicylic acid	<20	mg/L	20	○	-	LOD	not available

## Untargeted Verification Analysis

Applied Model: Sangiovese

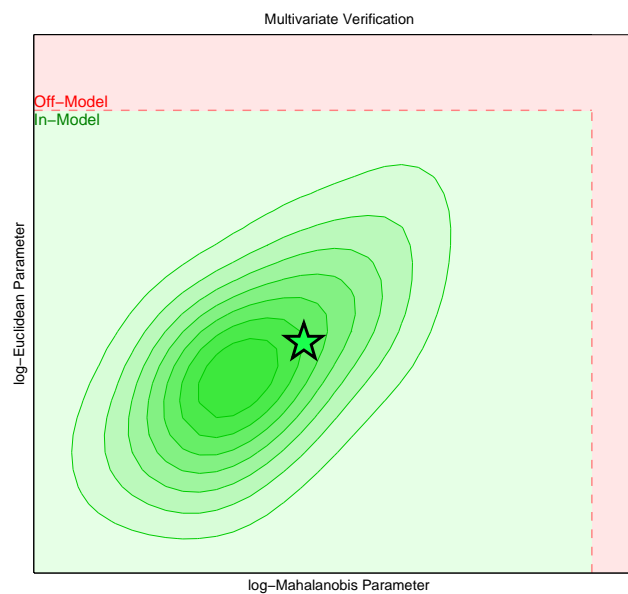
(Analysis-ID: WI-2022-02/705)

### Univariate Verification

**Result:** No deviation was detected in univariate verification (In-Model).

### Multivariate Verification

**Result:** No deviation was detected in multivariate verification (In-Model).



### Wine Content Analysis

**Result:** Based on the comparison with the reference database, there is **no indication for an addition of water**.

## General Remarks

### Classification Models

The aim of a classification model is to assign a specific sample to its most probable group. This assignment does not guarantee that the sample is exclusively a member of this group.

The 3D-discrimination diagram shows available groups (ellipsoids) in the projection space of the NMR-profiles with maximized discrimination. The star represents the actual sample.

In most cases these models are discriminating in multidimensional spaces. For such models human perceptibility and options for graphical representation are limited. Misperception is possible in certain cases. The mathematically correct probability for any group membership is represented by p-values which are calculated in the complete space. Typically values higher than 0.05 or 0.01 will accept the hypothesis of group membership. Expert interpretation is necessary before deducing any conclusions.

Only groups listed in the respective models can be considered. Therefore models are not applicable for blends, origins or varieties which are not listed in the corresponding model.

### Verification Models

Verification models are non-targeted analyses comparing the whole NMR-Profile of a specific sample with one corresponding group of reference spectra (database). All spectra data points are taken into account irrespective of whether the signals are caused by already identified molecules or not.

There are different possible reasons for any deviation from the group of reference spectra. If there are detected deviations, this does not automatically mean, that the sample is adulterated. Expert interpretation is necessary before deducing any conclusions.

In the univariate analysis, the NMR spectrum is checked for any unusual low or high signal intensities for a given sample, while taking into account the natural variability of a respective reference group. Multivariate models also take into account the relation between different signals in the NMR spectrum.

### Quantification Results

Obtained concentrations are compared to official reference values if available and consistency is indicated by an extra traffic light flag. Additionally, quantitative values are compared to the reference wine database (visualised by distribution). Expert interpretation is necessary before deducing any conclusions.



## General Remarks for Quantified Parameters

Following flags are used for comparison with (official) reference values:

- no reference values available
- value is consistent with reference range

Compound	Flag	Comment
total alcohol	●	for dedicated wine-producing regions (e.g. Germany and Austria), according to Council Regulation (EC) 479/2008, value must be between 67 g/L and 118.5 g/L
total alcohol-v	●	for dedicated wine-producing regions (e.g. Germany and Austria), according to Council Regulation (EC) 479/2008, value must be between 8.5 vol% and 15 vol%
ethanol	●↓	expert interpretation suggested, if value is lower than 58 g/L
ethanol-v	●↓	expert interpretation suggested, if value is lower than 7.3 vol%
sucrose	●↑	expert interpretation suggested, if value exceeds 500 mg/L
tartaric acid	●↓	expert interpretation suggested, if value is lower than 700 mg/L
lactic acid	●↑	expert interpretation suggested, if value exceeds 4.0 g/L
citric acid	●↑	expert interpretation suggested, if value exceeds 800 mg/L
citric acid	●↑	according to Council Regulation (EC) 606/2009, value must not exceed 1000 mg/L
acetic acid	●↑	expert interpretation suggested, if value exceeds 900 mg/L (red wine)
acetic acid	●↑	expert interpretation suggested, if value exceeds 700 mg/L (white wine)
gluconic acid	●↑	expert interpretation suggested, if value exceeds 600 mg/L
putrescine	●↑	expert interpretation suggested, if value exceeds 50 mg/L
cadaverine	●↑	expert interpretation suggested, if value exceeds 50 mg/L
HMF	●↑	expert interpretation suggested, if value exceeds 5 mg/L
methanol	●↑	expert interpretation suggested, if value exceeds 200 mg/L (white wine)
methanol	●↑	expert interpretation suggested, if value exceeds 350 mg/L (red wine)
methanol	●↑	according to OIV Resolution OENO 19/2004, value must not exceed 250 mg/L (white wine)
methanol	●↑	according to OIV Resolution OENO 19/2004, value must not exceed 400 mg/L (red wine)
acetaldehyde	●↑	expert interpretation suggested, if value exceeds 70 mg/L
pyruvic acid	●↑	expert interpretation suggested, if value exceeds 40 mg/L
glycerol/ethanol	●↑	expert interpretation suggested, if ratio exceeds 10
benzoic acid	●↑	according to Council Regulation (EC) 606/2009, value must not exceed detection limit
sorbic acid	●↑	expert interpretation suggested, if value exceeds 180 mg/L
sorbic acid	●↑	according to Council Regulation (EC) 606/2009, value must not exceed 200 mg/L
salicylic acid	●↑	according to Council Regulation (EC) 606/2009, value must not exceed detection limit