

Analysis Report Wine-Profiling™

Sample ID: 2207075

Information/Declaration provided by customer:

Variety: Mencia
Country: Spain
Vintage: 2019
Type of Wine: red

Disclaimer: this information will affect the applicability and validity of analyses and results.

Measuring Date: 10-May-2022 23:38:24

Reporting Date: 12-May-2022 10:40:34, Version 4.0.6, 8 pages

Results Summary

Type of Analysis	Result	Status
Analysis of declared information		
Country Spain (red)	Consistent	●
Untargeted Verification Analysis		
Univariate Verification	Consistent	●
Multivariate Verification	Consistent	●
Wine Content Analysis	Consistent	●
Targeted Analysis		
Quantification	–	○
Comparison with NMR Reference Database	Typical concentrations	●

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.

The data analysis is performed at Bruker BioSpin GmbH (Ettlingen, Germany) according to testing method AA-72-02-08 (Wine-Profiling 4.0.6), released on 08-Apr-2022 (DIN EN ISO/IEC 17025:2018 Accreditation Certificate D-PL-19229-01-00 of Bruker BioSpin GmbH). All results solely refer to the tested sample as provided by the customer.

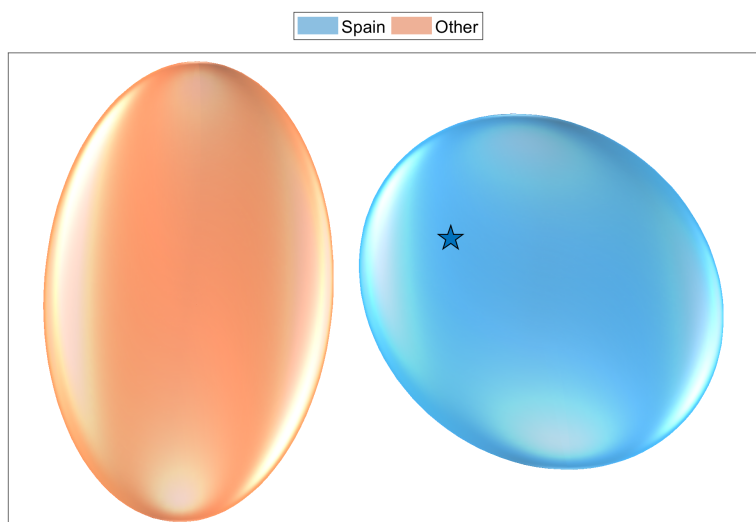
Analysis of declared Information

Statistical Model: Country Spain (red)

(Analysis-ID: WI-CC0006/0449)

This model is based on 11844 samples, thereof 3513 samples of reference group *Spain*. The true-positive rate of this model is 99.0%.

Result: Consistent with declared country Spain. The probability of consistency is 100.0%.



Untargeted Verification Analysis

Applied Model: Country Spain (red)

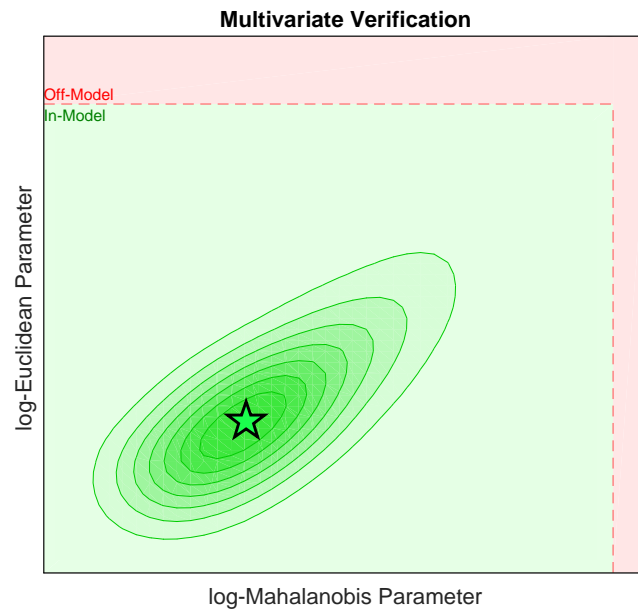
(Analysis-ID: WI-NT006/0450)

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

(Analysis-ID: WI-WC0006/0451)

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









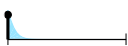





Targeted Analysis

(Analysis-ID: WI-Q/1001)

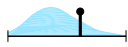




In the following tables the results of the quantitative analysis are given. Parameters labelled with * are calculated parameters. Please refer to the additional remarks for quantified parameters, flags and reference values on page 8. The displayed distributions of the Wine-Profiling™ NMR reference database refer to group *Country Spain (red)* (based on 3374 samples).

LOQ = Limit of Quantification, LOD = Limit of Detection




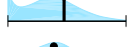






Standard Parameters:

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™	
					min	max	NMR reference database	
total alcohol*	111.7	g/L	-	○	-	-	94.4	 125.7
total alcohol-v*	14.1	%vol	-	○	-	-	12.1	 15.8
ethanol	111.2	g/L	5.0	○	-	-	91.4	 124.8
ethanol-v*	14.1	%vol	-	○	-	-	11.7	 15.7
glycerol	9.1	g/L	0.5	○	-	-	6.7	 11.1
glucose	0.8	g/L	0.5	○	-	-	<0.5	 6.5
fructose	<0.5	g/L	0.5	○	-	-	<0.5	 6.8
glucose/fructose*	-	-	-	○	-	-	not available	
sucrose	<0.2	g/L	0.2	●	-	-	<200 mg/L in reference set	
arabinose	457	mg/L	100	○	-	-	<100	 503
total sugar (bef. inv.)*	<1.3	g/L	1.3	○	-	-	<1.3	 13.1
total fermentable sugar*	<1.5	g/L	1.5	○	-	-	<1.5	 13.1
tartaric acid	1.3	g/L	0.5	●	-	-	<0.5	 2.9
malic acid	<0.2	g/L	0.2	○	-	-	<0.2	 0.4
lactic acid	1.4	g/L	0.2	○	-	-	<0.2	 3.0
citric acid	<200	mg/L	200	●	-	1000	<200	 302
energy value*	3490	kJ/L	-	○	-	-	not available	
bread units*	<0.2	1/L	0.2	○	-	-	not available	
carbohydrate units*	<0.2	1/L	0.2	○	-	-	not available	



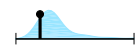
Degradation Parameters:

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™ NMR reference database
					min	max	
acetic acid	720	mg/L	100	○	-	-	334  964
acetoine	62	mg/L	10	○	-	-	<10  86
ethylacetate	93	mg/L	50	○	-	-	<50  173
ethyl lactate	<150	mg/L	150	○	-	-	<150  345
formic acid	<5	mg/L	5	○	-	-	<5  14
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

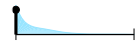
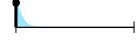



Higher Alcohols / Fermentation Products:

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™ NMR reference database
					min	max	
methanol	184	mg/L	30	●	-	400	<30  272
1,3-propanediol	<40	mg/L	40	○	-	-	<40 mg/L in reference set
2,3-butanediol	685	mg/L	100	○	-	-	<100  997
2-methyl-propanol	<70	mg/L	70	○	-	-	<70  88
2-phenylethanol	54	mg/L	25	○	-	-	<25  86
3-methyl-butanol	206	mg/L	100	○	-	-	148  297
acetaldehyde	32	mg/L	10	○	-	-	<10  59
pyruvic acid	<20	mg/L	20	○	-	-	<20  22
galacturonic acid	845	mg/L	160	○	-	-	<160  1500
succinic acid	843	mg/L	50	○	-	-	541  1000
glycerol/ethanol*	8.2	%	-	●	-	-	6.4  9.9

Amino Acids:

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™ NMR reference database
					min	max	
4-aminobutanoic acid	<120	mg/L	120	○	-	-	<120  134
alanine	<35	mg/L	35	○	-	-	<35  79
arginine	<150	mg/L	150	○	-	-	<150 mg/L in reference set
proline	610	mg/L	150	○	-	-	<150  2400

(Poly-)phenols:

Compound	Value	Unit	LOQ	Flag	Official Ref.		Wine-Profiling™ NMR reference database
					min	max	
caftaric acid	<15	mg/L	15	○	-	-	<15  107
epicatechin	<30	mg/L	30	○	-	-	<30  37
gallic acid	36	mg/L	25	○	-	-	<25  116
shikimic acid	<20	mg/L	20	○	-	-	<20  57
trigonelline	11	mg/L	10	○	-	-	<10  23

Stabilising Agents:

Compound	Value	Unit	LOD	Flag	Official Ref.		Wine-Profiling™ NMR reference database
					min	max	
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

General Remarks

Analysis of declared Information

The test applied is a classification analysis with the aim to check the consistency of the declared meta-information of the sample (geographical origin or botanical variety). The consistency with a group is expressed as posterior probability in the range from 0% to 100%. A posterior probability exceeding 50% is being regarded as consistent with the respective group. The underlying statistical models are based on Linear Discriminant Analysis for dimension reduction followed by a Linear (or Quadratic) Discriminant Analysis for final classification.

Within the discrimination space figure, the ellipsoids are representing the modeling samples and the star represents the actual sample under investigation.

Expert interpretation is necessary before deducing any conclusions.

All conformity statements in this section are based on the "Binary Statement for Simple Acceptance Rule" according to ILAC-G8:09/2019.

Non-Targeted Verification Analysis

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.

All conformity statements in this section are based on the "Binary Statement for Simple Acceptance Rule" according to ILAC-G8:09/2019.

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. The uncertainty of ethanol-vol% is expected to be in the range of 0.1 vol% to 0.2 vol%.

All conformity statements in this section are based on the "Binary Statement for Simple Acceptance Rule" according to ILAC-G8:09/2019.

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) 1308/2013, 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) 1308/2013, 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) 934/2019, 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) 934/2019, value must not exceed detection limit
sorbic acid	●↑	expert interpretation suggested, if value exceeds 180 mg/L
sorbic acid	●↑	according to Council Regulation (EC) 934/2019, value must not exceed 200 mg/L
salicylic acid	●↑	according to Council Regulation (EC) 934/2019, value must not exceed detection limit