Analysis Report Wine-Profiling™

Sample ID: Delheim_Cab_Mer_2019

Information/Declaration provided by customer:

Customer:	Woolworths
Variety:	Cabernet Sauvignon
Country:	South Africa
Vintage:	2019
Type of Wine:	red

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

Measuring Date:	19-Nov-2021 18:05:08
Reporting Date:	06-Dec-2021 14:53:03, Version 4.0.4, 8 pages

Results Summary

Type of Analysis	Result	Status
Analysis of declared information		
Variety Cabernet Sauvignon (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 (Rheinstetten, Germany) according to testing method AA-72-02-06 (Wine-Profiling 4.0.4), released on 06-Nov-2020 (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.

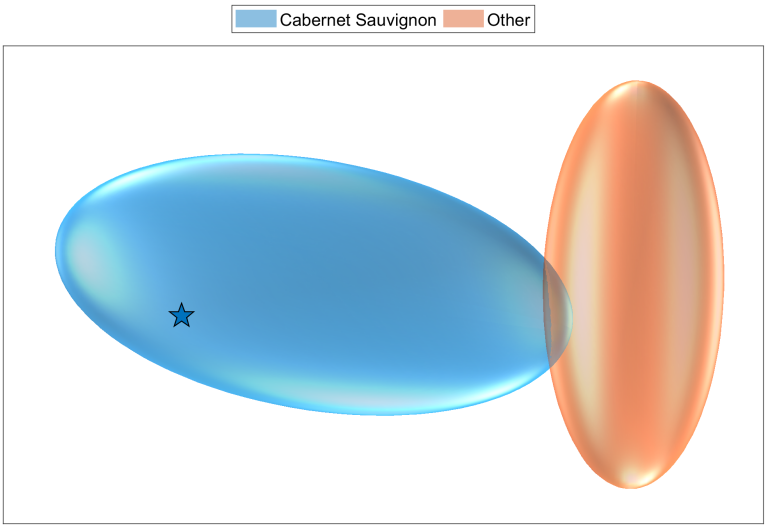
Analysis of declared Information

Statistical Model: Variety Cabernet Sauvignon (red)

(Analysis-ID: WI-CC0043/0450)

This model is based on 6744 samples, thereof 468 samples of reference group *Cabernet Sauvignon*. The true-positive rate of this model is 98.9%.

Result: Consistent with declared variety Cabernet Sauvignon. The probability of consistency is 100.0%.



Untargeted Verification Analysis

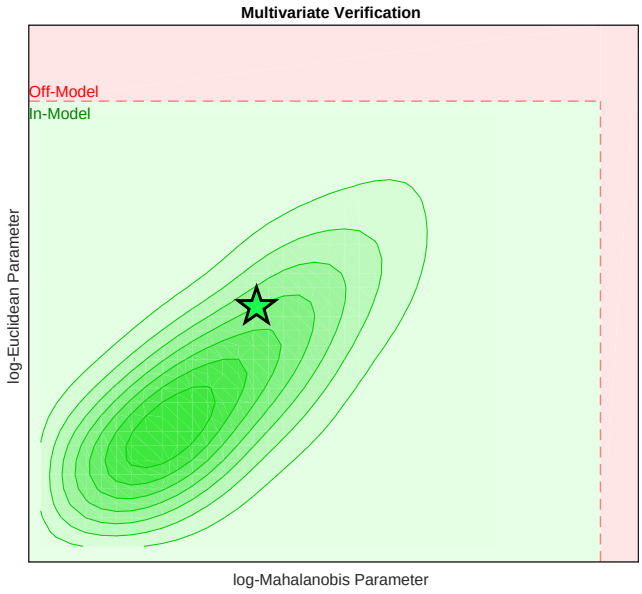
Applied Model: Variety Cabernet Sauvignon (red) (Analysis-ID: WI-NT043/0450)

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-WC0043/0451)

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 *Variety Cabernet Sauvignon (red)* (based on 451 samples).

LOQ = Limit of Quantification, LOD = Limit of Detection

Standard Parameters:

Compound	Value	Unit	LOQ	Flag	Official Ref. min	Official Ref. max	Wine-Profiling™ NMR reference database
total alcohol*	109.6	g/L	-	○	-	-	96.2 … 122.4
total alcohol-v*	13.9	%vol	-	○	-	-	12.3 … 15.4
ethanol	108.3	g/L	5.0	○	-	-	95.4 … 121.7
ethanol-v*	13.7	%vol	-	○	-	-	12.1 … 15.3
glycerol	10.5	g/L	0.5	○	-	-	6.7 … 12.2
glucose	<0.5	g/L	0.5	○	-	-	<0.5 … 6.8
fructose	2.2	g/L	0.5	○	-	-	<0.5 … 8.0
glucose/fructose*	-	-	-	○	-	-	not available
sucrose	<0.2	g/L	0.2	●	-	-	<200 mg/L in reference set
arabinose	<100	mg/L	100	○	-	-	<100 … 585
total sugar (bef. inv.)*	<2.7	g/L	2.7	○	-	-	<2.7 … 13.7
total fermentable sugar*	<2.9	g/L	2.9	○	-	-	<2.9 … 13.7
tartaric acid	1.2	g/L	0.5	●	-	-	<0.5 … 2.8
malic acid	<0.2	g/L	0.2	○	-	-	<0.2 … 0.8
lactic acid	1.4	g/L	0.2	○	-	-	<0.2 … 2.8
citric acid	<200	mg/L	200	●	-	1000	<200 … 349
energy value*	3460	kJ/L	-	○	-	-	not available
bread units*	<0.2	1/L	0.2	○	-	-	not available
carbohydrate units*	<0.3	1/L	0.3	○	-	-	not available

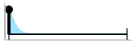
Degradation Parameters:

Compound	Value	Unit	LOQ	Flag	Official Ref. min	Official Ref. max	Wine-Profiling™ NMR reference database
acetic acid	624	mg/L	100	○	-	-	313 – 995
acetoine	26	mg/L	10	○	-	-	<10 – 84
ethylacetate	122	mg/L	50	○	-	-	<50 – 235
ethyllactate	223	mg/L	150	○	-	-	<150 – 268
formic acid	<5	mg/L	5	○	-	-	<5 – 15
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

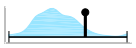
Higher Alcohols / Fermentation Products:

Compound	Value	Unit	LOQ	Flag	Official Ref. min	Official Ref. max	Wine-Profiling™ NMR reference database
methanol	161	mg/L	30	●	-	400	82 – 282
1,3-propanediol	<40	mg/L	40	○	-	-	<40 mg/L in reference set
2,3-butanediol	797	mg/L	100	○	-	-	<100 – 910
2-methyl-propanol	<70	mg/L	70	○	-	-	<70 – 135
2-phenylethanol	78	mg/L	25	○	-	-	<25 – 115
3-methyl-butanol	271	mg/L	100	○	-	-	170 – 384
acetaldehyde	39	mg/L	10	○	-	-	<10 – 54
pyruvic acid	25	mg/L	20	○	-	-	<20 – 36
galacturonic acid	679	mg/L	160	○	-	-	308 – 1700
succinic acid	1.0	g/L	0.1	○	-	-	0.6 – 1.4
glycerol/ethanol*	9.7	%	-	●	-	-	6.5 – 11.2

Amino Acids:

Compound	Value	Unit	LOQ	Flag	Official Ref. min	Official Ref. max	Wine-Profiling™ NMR reference database
4-aminobutanoic acid	<120	mg/L	120	◯	-	-	<120  129
alanine	38	mg/L	35	◯	-	-	<35  64
arginine	<150	mg/L	150	◯	-	-	<150 mg/L in reference set
proline	3.2	g/L	0.1	◯	-	-	0.7  4.2

(Poly-)phenols:

Compound	Value	Unit	LOQ	Flag	Official Ref. min	Official Ref. max	Wine-Profiling™ NMR reference database
caftaric acid	23	mg/L	15	◯	-	-	<15  88
epicatechin	<30	mg/L	30	◯	-	-	<30  49
gallic acid	77	mg/L	25	◯	-	-	<25  142
shikimic acid	49	mg/L	20	◯	-	-	<20  158
trigonelline	21	mg/L	10	◯	-	-	<10  27

Stabilising Agents:

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

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.

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.

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%.

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