

Interactions between Grape Maturity Indices and Quality for Pinotage and Cabernet Sauvignon Wines from Four Localities¹⁾

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Three grape maturity indices viz. degrees Balling ($^{\circ}\text{B}$), $^{\circ}\text{B}$ total titratable acid (TTA) ratio and the $^{\circ}\text{B}\cdot\text{pH}$ product of musts were compared regarding their ability to predict optimum quality for Cabernet Sauvignon and Pinotage wines. Comprehensive analytical data from 128 musts and corresponding wines for the 1979 and 1980 vintages from the Stellenbosch, Durbanville, Lutzville and Robertson areas were subjected to principal component analysis using variables and variable ratios selected by correlation to quality weighting. The results indicated that $^{\circ}\text{B}$ alone could not perform the function of a grape maturity index for predicting optimum quality. In the case of the $^{\circ}\text{B}/\text{TTA}$ index, the range wherein maximum wine quality occurred was too wide to be of practical value in this instance. The $^{\circ}\text{B}\cdot\text{pH}$ index gave a narrower optimum range, and in contrast to the two other indices gave similar results for both cultivars.

INTRODUCTION

Many scientific studies have been performed with the aim of finding grape maturity indices for the prediction of optimum quality other than sugar (Amerine & Winkler, 1941; Berg, 1958; Sinton, Ough, Kissler & Kasimatis, 1978; Coombe, Dundon & Short, 1980). It was frequently found that single parameters like $^{\circ}\text{Balling}$ ($^{\circ}\text{B}$) or acidity did not give satisfactory results (Berg, 1958; Du Plessis, 1976; Coombe *et al.*, 1980). More recently Du Plessis & Van Rooyen (1982) studied curvilinear relationships between several multi-parameter indices and wine quality determined by sensory evaluation, and found promising results for indices like the $^{\circ}\text{B}/\text{total titratable acidity}$ (TTA) ratio and the $^{\circ}\text{B}\cdot\text{pH}$ product of grape must. In the latter publication, however, no attention was paid to wine composition, especially flavour compounds, in relation to these indices. The purpose of this study was to relate wine composition to three maturity indices and to evaluate the latter in terms of their relationship to high quality wines within a set of data comprising two red wine cultivars from four distinct wine of origin regions. In contrast to previous studies wine quality was not used as a dependent variable in the final analysis in this instance, but as a guide to select independent variables and to identify a spectrum of high quality wines for the interpretation of the final results.

MATERIALS AND METHODS

Grape sampling and vinification procedures: Two wine grape cultivars viz. Pinotage and Cabernet Sauvignon from the Stellenbosch, Durbanville, Robertson and Elephants River areas (1979 & 1980 vintages) were studied. Sampling at various degrees of maturity (19-29 $^{\circ}\text{B}$) and vinification procedures were as described by

Du Plessis & Van Rooyen (1982). A total of 128 wines was used in the study.

Must analysis: Total titratable acidity (TTA) was determined on centrifuged juice samples (750 g x 5 min) by titrating with c.0,1 N NaOH solution to pH 8,2. Total soluble solids ($^{\circ}\text{B}$) were determined on the centrifuged samples by refractometer and corrected for grape sugars as reported by Cooke (1964).

Wine analysis and sensory evaluation: A total of 37 parameters was analysed by methods as set out in Table 1. Overall wine quality, as well as odour quality, was evaluated by a panel of 14 experienced judges using the system described by Tromp & Conradie (1979), and expressed as a percentage.

TABLE 1
Methods of analysis used in the study

Parameter	Method used
Alcohol (Vol. %)	Pycnometer
Total titratable acid (mg. ℓ^{-1})	Titration with NaOH to pH 8,2
pH	pH-meter
Phosphate (mg. ℓ^{-1})	Technicon Autoanalyser methodology (Anon)
Acetaldehyde (mg. ℓ^{-1})	Amerine & Ough (1975)
Total phenols (mg. ℓ^{-1})	Singleton & Rossi (1965)
Mg, Ca, Na, K, Cu, Mn, Fe, Zn, (mg. ℓ^{-1})	Atomic Absorption
Reducing sugars (g. ℓ^{-1})	Amerine & Ough (1975)
Tartaric acid (g. ℓ^{-1})	Rebelein (1973)
Total Higher alcohols (mg. ℓ^{-1})	Le Roux (1972)
Individual ester and higher alcohols	Marais & Houtman (1979)

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Categorization of certain parameters: To facilitate data processing and the interpretation of results, grape maturity indices were classified into distinct categories (Table 2), in such a way that the full range was accommodated for each index, with more or less equal numbers of wines in each category.

TABLE 2
Categories used for different grape maturity indices

Category* Number	Degrees Balling (°B)	°Balling/ Total titra- table acids (°B/TTA)	°Balling pH (°B.pH)
1	<20,6	<2,5	<68,0
2	20,6 — 21,5	2,5 — 2,80	68,00 — 73,99
3	21,6 — 22,5	2,81 — 3,09	74,00 — 79,99
4	22,6 — 23,5	3,10 — 3,39	80,00 — 85,99
5	23,6 — 24,5	3,40 — 3,69	86,00 — 91,99
6	24,6 — 25,5	3,70 — 3,99	92,00 — 97,99
7	25,6 — 26,5	4,00 — 4,29	98,00 — 103,99
8	26,6 — 27,5	4,30 — 4,50	104,00 — 109,99
9	>27,5	>4,50	>109,99

* Applicable to each index separately.

Raw variables, added features and preprocessing of data:

Each individual wine analysed was regarded as an "object" and each variable measured on every object defined as a "feature". The resulting data matrix was analysed using a batch process version of "ARTHUR" (Harper *et al.*, 1977) and executed on a UNIVAC 1110 computer at the University of Stellenbosch. Preprocessing was done using the programmes TUNE, autoscale and SELECT as set out by Van Rooyen *et al.*, (1982).

Variable reduction procedure: The programme SELECT was set to select 10 final features, using correlation to property weighting, the latter being either overall or odour quality, depending on the analysis. The application of principal component analysis (PCA) further reduced the actual number of variables to three or four eigenvectors with factor loadings for each of the 10 selected features, using the programmes, KAPRIN, KATRAN and KAVARI as explained by Van Rooyen *et al.*, (1982). Scatter diagrams of feature-property and feature-feature plots were generated by the programme VARVAR, coding objects according to the specific grape maturity index, wine quality and object number to facilitate interpretation of results.

RESULTS AND DISCUSSION

Overall quality as dependent variable: Because both aroma and taste contribute towards overall quality rating, all measured variables (and their ratios) were subjected to the variable selection procedure, the latter employing the programme SELECT with correlation to quality weighting as basis for selection. The features thus selected are listed in Table 3.

TABLE 3
Features selected from all variable ratios using overall quality weighting.

No.	Feature	Weight
1	Octanoic acid/2-Phenylethanol	0,530
2	Ethyl caprylate/i-Butanol	0,100
3	Total titratable acid (must)/ Acetaldehyde	0,041
4	Magnesium/ Potassium	0,035
5	i-Amyl acetate/ Hexyl acetate	0,022
6	pH (wine) Alcohol	0,023
7	Tartaric acid/ Ethyl caprylate	0,015
8	Hexanol/ Magnesium	0,013
9	Copper/ Octanoic acid	0,011
10	Total titratable acid (wine)/ Ethyl caprate	0,014

PCA variable reduction: After eigenvector rotation (VARIMAX procedure) the first five eigenvectors explained 77,8% of the total variance. The factor loadings for the features set out in Table 3 are listed in Table 4.

It can be deduced from Tables 3 and 4 that Factor 1 concerns mainly volatiles and TTA, Factor 2 is heavily weighted with pH and ethanol, Factor 3 with the Cu/Octanoic acid ratio and Factors 4 and 5 are weighted strongly with an ester ratio and the Hexanol/Mg ratio respectively. When these factors are plotted against overall wine quality some interesting results come to light. In the case of °B as grape maturity index, high quality wines (sensory scores above 70%) fall in a very wide category, viz. between categories 3 and 9 (°B from 21,6 to 28,8) as depicted in Figure 1, a plot of Factor 1 scores against quality. Similar results were obtained on plotting the other factors. A plot of Factor 1 against Factor 2 demonstrates the marked difference in behaviour of the two cultivars Cabernet Sauvignon and Pinotage (Figure 2) especially with factors heavily weighted with wine volatiles, a phenomenon noted throughout the study.

TABLE 4
Factor loadings for first five eigenvectors after Varimax rotation, with percentages explained variation.

Feature number	Factor 1 (28,1%)	Factor 2 (13,9%)	Factor 3 (12,7%)	Factor 4 (11,9%)	Factor 5 (11,2%)
1	-0,56	0,07	0,23	0,00	0,08
2	-0,43	0,11	0,37	0,05	0,02
3	-0,52	-0,31	0,01	-0,04	-0,04
4	0,02	0,09	-0,05	0,04	-0,03
5	-0,05	0,14	0,13	-0,88	0,12
6	-0,05	-0,78	-0,14	0,13	-0,02
7	0,19	-0,18	-0,22	0,25	-0,11
8	0,04	-0,04	-0,06	0,11	-0,96
9	0,12	-0,11	-0,85	0,14	-0,08
10	-0,42	0,45	-0,04	-0,32	0,20

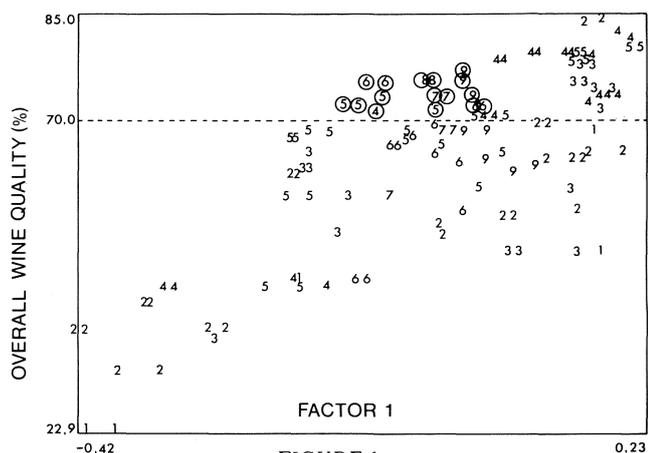


FIGURE 1

Plot of factor 1 (PCA analysis) against overall wine quality rating for Cabernet Sauvignon and Pinotage wines. Wines are coded according to °B category (Table 2), Pinotage wines with quality ratings above 70% circled.

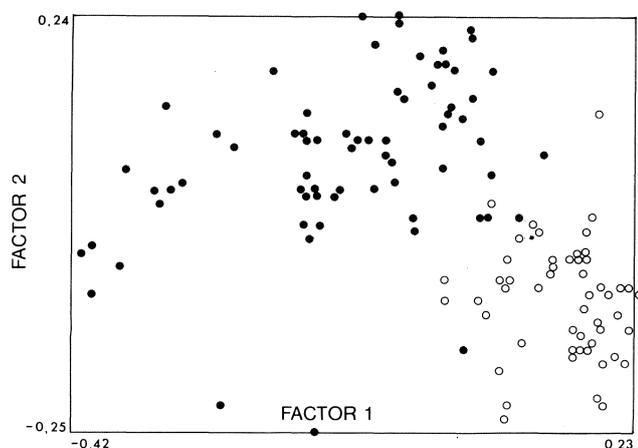


FIGURE 2

Plot of factor 1 against factor 2 (PCA analysis) for Cabernet Sauvignon (○) and Pinotage (●) wines.

In the case of the °B/TTA parameter, highest quality coincided with categories 3-8 for Pinotage (actual values: 2,9-4,4; mean 3,6) and 3-9 for Cabernet Sauvignon (actual values: 3,1-5,2; mean 4,2) (Figure 3). In this experiment the latter cultivar seems in this instance to attain optimum maturity at much higher °B/TTA values than Pinotage.

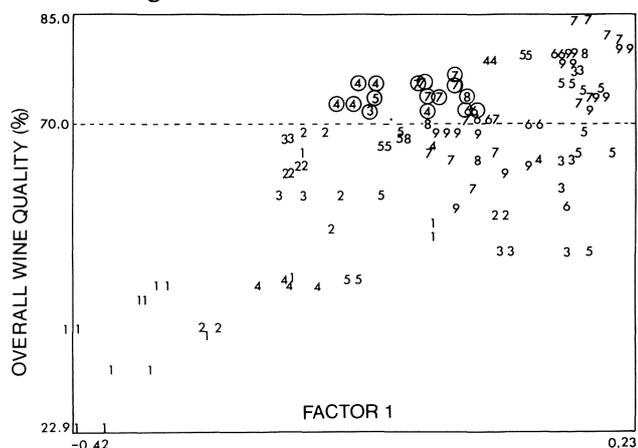


FIGURE 3

Plot of factor 1 (PCA analysis) against overall wine quality rating for Cabernet Sauvignon and Pinotage wines. Wines are coded according to °B/TTA category (Table 2), Pinotage wines with quality ratings above 70% circled.

The °B.pH maturity index indicated a range from 3-9 (actual values 78-106; mean 93) for Pinotage and 3-6 (actual values 79-95; mean 87) for Cabernet Sauvignon, in this analysis the only parameter giving more or less the same range for both cultivars, in terms of actual values. A plot of Factor 1 against overall wine quality illustrates the results (Fig. 4).

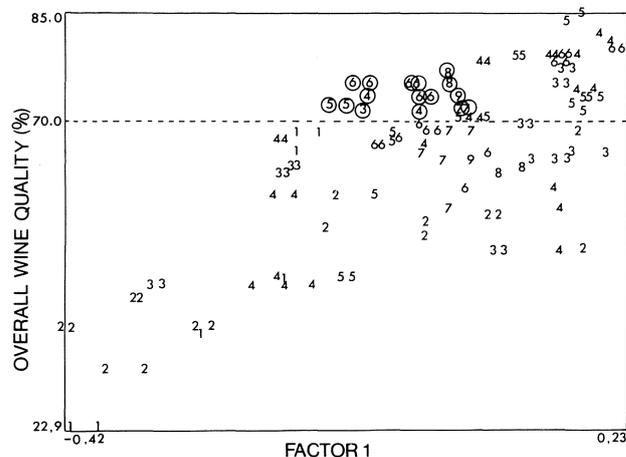


FIGURE 4

Plot of factor 1 (PCA analysis) against overall wine quality rating for Cabernet Sauvignon and Pinotage wines. Wines are coded according to °B.pH category (Table 2), Pinotage wine with quality ratings above 70% circled.

Aroma quality as dependent variable: In addition to data processing using the complete data base (the procedure followed above), an additional analysis was executed using aroma quality as dependent variable.

PCA using the complete variable set: Following the same variable selection procedure as set out before, a total of 10 features was again selected (Table 5).

TABLE 5
Features selected from all variables plus ratios using aroma quality weighting.

No.	Feature	Weight
1	iso + active Amyl alcohol/i-Butanol	0,292
2	Hexyl acetate/Reducing sugar	0,135
3	Octanoic acid/Hexyl acetate	0,076
4	Magnesium/Potassium	0,081
5	Total phosphate/Ethyl caprate	0,046
6	Ethyl acetate/Hexanoic acid	0,038
7	Sodium/Ethyl caprylate	0,025
8	Ethyl lactate/Hexyl acetate	0,025
9	Ethyl butyrate/Sodium	0,019
10	i-Amyl acetate/Calcium	0,022

After eigenvector rotation the factor loadings for the first five eigenvectors, accounting for 78,1% of total variation, were as set out in Table 6.

It follows from Tables 5 and 6 that Factor 1 is concerned mainly with iso-amyl acetate (IAA) and amyl alcohol ratios, explaining its powerful discriminatory power in distinguishing between Cabernet Sauvignon and Pinotage wines (Figure 5), the latter being known for its powerful IAA odour. Factor 2 is heavily loaded with

TABLE 6
Factor loadings for first eigenvectors after Varimax rotation, with percentage explained variation.

Feature number	Factor 1 (19,3%)	Factor 2 (16,8%)	Factor 3 (15,5%)	Factor 4 (15,2%)	Factor 5 (11,2%)
1	-0,63	0,26	-0,15	0,04	0,07
2	-0,03	0,10	-0,04	0,80	0,08
3	0,13	-0,53	0,07	-0,52	0,15
4	-0,05	0,07	-0,16	0,07	-0,04
5	0,11	-0,02	-0,03	-0,08	-0,30
6	-0,02	0,02	-0,15	-0,03	-0,89
7	-0,33	0,22	-0,59	-0,16	-0,25
8	0,01	-0,74	0,17	-0,10	-0,02
9	0,23	-0,14	0,70	-0,20	0,10
10	0,64	0,17	0,25	-0,09	0,08

hexyl acetate (HAC) ratios, Factor 3 with sodium/ester ratios and Factors 4 and 5 with HAC and ethyl acetate (ETAC) ratios respectively. Scatter diagrams depicting plots of the above eigenvector scores against wine aroma quality gave inconclusive results regarding must quality parameters, in that high quality wines gave wide ranges i.e. $^{\circ}\text{B}$ (2-8); $^{\circ}\text{B}/\text{TTA}$ (3-9) and $^{\circ}\text{B.pH}$ (3-6).

PCA using wine volatiles only: Variables remaining after the same selection procedure as discussed above are listed in Table 7.

TABLE 7
Features selected from volatiles data base using aroma quality weighting.

No.	Feature	Weight
1	Octanoic acid/2-Phenyl ethanol	0,529
2	Ethyl caprylate/i-Butanol	0,100
3	Octanoic acid/Ethyl butyrate	0,039
4	i-Butanol/Ethyl caprate	0,058
5	Ethyl butyrate/2-Phenyl ethanol	0,018
6	2-Phenyl ethanol/Diethyl succinate	0,013
7	Ethyl lactate/Octanoic acid	0,017
8	2-Phenyl ethanol/i-Amyl acetate	0,016
9	Hexanoic acid/Ethyl lactate	0,010
10	i-Amyl acetate/Diethyl succinate	0,022

Principal component analysis using the 10 variables in Table 7 for the wines, and subsequent vector rotation procedure, resulted in the factor loadings for the first five of seven eigenvectors as set out in Table 8.

TABLE 8
Factor loadings and percentage explained variations for five eigenvectors using selected volatiles data.

Feature number	Factor 1 (24,5%)	Factor 2 (21,5%)	Factor 3 (19,2%)	Factor 4 (12,6%)	Factor 5 (10,9%)
1	-0,12	-0,15	-0,17	0,78	0,26
2	-0,12	-0,65	0,02	0,13	0,03
3	0,01	0,08	-0,09	-0,13	-0,05
4	0,30	0,10	0,58	-0,20	-0,16
5	0,53	0,17	0,30	-0,12	-0,12
6	0,17	-0,09	0,66	-0,12	-0,11
7	-0,43	-0,22	-0,20	0,43	0,21
8	-0,10	-0,04	-0,12	0,23	0,91
9	-0,14	-0,65	-0,01	0,13	0,06
10	-0,60	-0,14	-0,19	-0,19	0,08

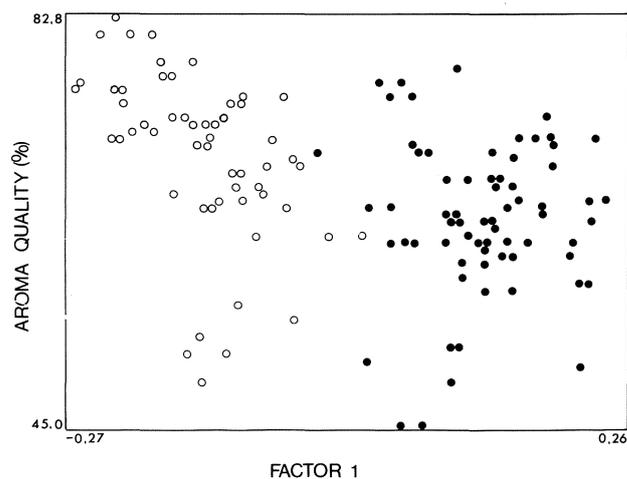


FIGURE 5
Plot of factor 1 (PCA analysis) against wine aroma quality for Cabernet Sauvignon (o) and Pinotage (●) wines.

A plot of Factor 1 scores against aroma quality illustrates clearly the difference in volatile flavour profiles of the two cultivars (Figure 6). In the case of $^{\circ}\text{B}$ as grape maturity parameter, the plots of Factors 1, 2 and 3 illustrated that top quality wines were obtained over a very wide range ($^{\circ}\text{B}$ categories from 2 to 8) with the data illustrated in Figure 7 as an example. In the case of $^{\circ}\text{B}/\text{TTA}$ the range was from categories 3 to 9. With $^{\circ}\text{B.pH}$ as maturity index, the range narrowed down somewhat (from 3-6 i.e. index values from 74-97), again as in previous cases giving the same range for both Cabernet Sauvignon and Pinotage (Figure 8).

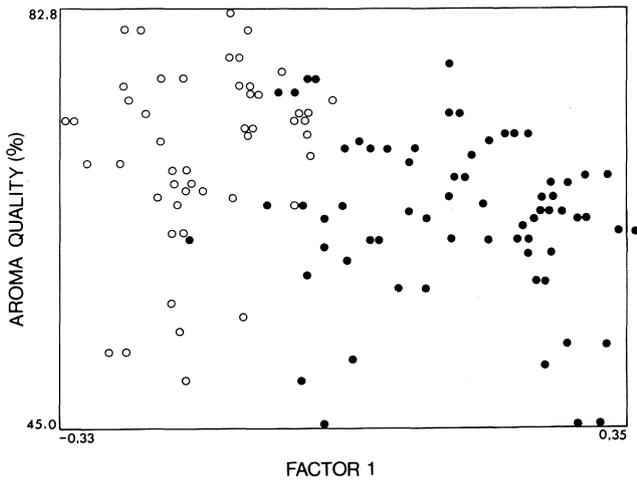


FIGURE 6

Plot of factor 1 (PCA analysis) against wine aroma quality for Cabernet Sauvignon (o) and Pinotage (●) wines with wine volatiles as independent variables.

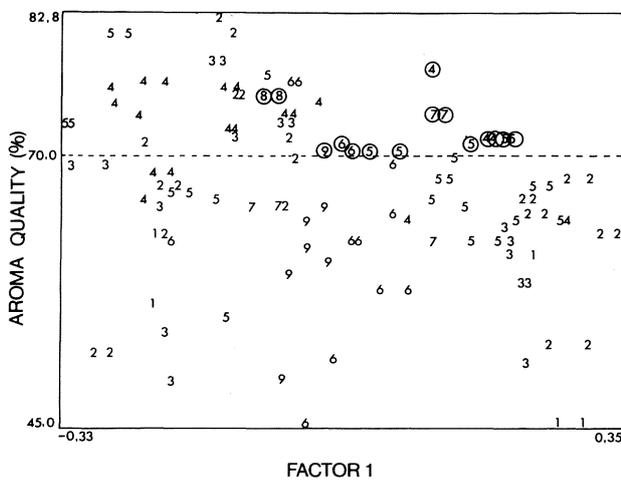


FIGURE 7

Plot of factor 1 (PCA analysis) against wine aroma quality for Cabernet Sauvignon and Pinotage wines. Wines are coded according to °B category (Table 2), Pinotage wines with quality ratings above 70% circled.

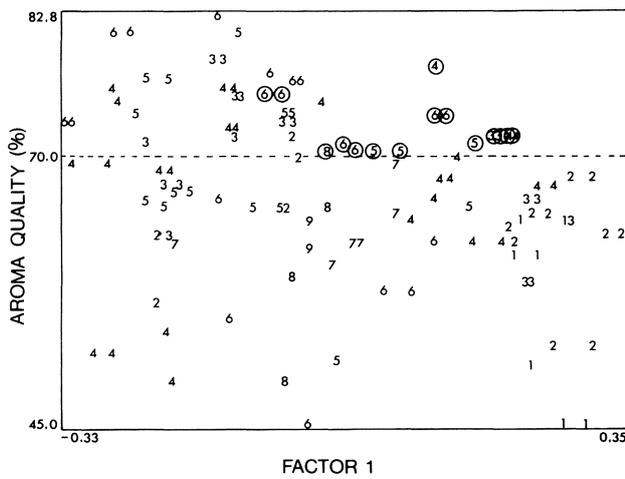


FIGURE 8

Plot of factor 1 (PCA analysis) against wine aroma quality for Cabernet Sauvignon and Pinotage wines. Wines are coded according to °B.pH category (Table 2), Pinotage wines with quality ratings above 70% circled.

SUMMARY AND CONCLUSIONS

The results obtained do not confirm the concept that °B alone is suited as a grape maturity index in relation to eventual high wine quality in South Africa. The two cultivars studied showed divergent behaviour with respect to both °B and °B/TTA indices, probably due to the fact that Cabernet Sauvignon wine quality depends to a large extent on cultivar character, while Pinotage wines rely heavily on fermentation products. Throughout the study the °B.pH index showed less erratic behaviour and a narrower range of values in the optimum wine quality category, especially in the case of Cabernet Sauvignon, for which extreme difficulty is usually experienced in finding a turning point for a grape maturity index. From the data at hand it seems that a °B.pH value of about 85-95 would satisfy the requirements for the two cultivars. In the case of °B/TTA, setting such a level would be at best a rough estimate. High correlation of certain inorganic element contents with wine quality needs further investigation, and the results also showed the utility of multivariable methods such as PCA to investigate the problem of finding a suitable grape maturity index.

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