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Examination of the potential for using chemical analysis as a surrogate for sensory analysis

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ABSTRACT

The application of a multi-block statistical analysis method, known as Common Components and Specific Weight Analysis, to the determination of connections between sensory descriptors and analytical data for Hunter Valley Semillon is described. Sixteen wines were used in the data analysis with 15 sensory descriptors and 10 analytical measurements available for each wine. The multi-block analysis simplifies the comparison between the data sets and allows relationships between the sensory and analytical parameters to be readily ascertained, more effectively than a linear regression approach. A sweetness zone established the connections between several sensory descriptors and analytical measurements based on fructose. Glucose was not part of the sweetness connections, although glycerol was connected to the sensory sweetness descriptors. Sensory assessment of acidity was positively related to the titratable acidity and pH was negatively related. The malic acid concentration was also negatively related to sensory acidity and the possible reasons for this are described. Several sensory descriptors including toast, honey and kerosene were found to be in opposition to the sweetness sensory parameters and not connected to any analytical parameters. The outcomes of this multi-block treatment indicate the potential for using analytical measurements as a surrogate for sensory analysis.

1. Introduction

Sensory analysis involves the application of human senses to the description and/or evaluation of a product for consumer use. Rigorous sensory analysis involves a panel of assessors that have been trained for a specific evaluation. For example, the determination of descriptors to characterise a wine style or to assess the impact of a processing step on the wine style is now a routine practice. Each separate sensory exercise, however, requires an intensive training program for the assessors.

A full sensory analysis, particularly descriptive, texture and time-intensity analyses, are complex processes demanding considerable time with an associated high cost. A proper sensory analysis of a food or beverage, including wine, can take at least 3 months and possibly 6 months of training and application. Extensive training is necessary to ensure consistency in and between assessors. The time period demands commitment from panel members and this in turn implies a high cost of the operation [1]. The time and cost factors restrict the extent to which full sensory analysis can be routinely applied.

The generation of analytical measurements for a range of quality parameters related to aroma, flavour and texture is faster, generally less expensive and more objective than sensory analysis. That is analytical measurements, when properly collected, do not suffer from bias due to personal preference [2]. The application of chemometrics to the interpretation of analytical data has opened up many interesting possibilities in food and beverage studies, particularly with respect to process monitoring, determination of geographical origin, authentication, adulteration and substitution [3–6].

The possibility of using analytical data as a surrogate for sensory data is less well examined, although Lesschaeve [personal communication] argues that this has been a sought after goal in many studies over the last 20 or more years. This position is supported by Piggott [7], who argues that flavour cannot be measured directly by instruments. That is only individual chemical compounds can be measured quantitatively by instrumental analysis and not the interactions between them that give rise to flavour.

While there have been several studies examining the link between sensory properties and aroma compounds, the main focus has tended to be on validation of the product type or characterising

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its origin. For example, there have been studies examining the link between sensory properties and non-volatile and volatile parameters on dry-cured ham [8], drinking water [9], balsamic vinegar [10], broiler chicken cuts [11] and netted muskmelon [12]. Bakker and Arnold [13] have described the positive relationship between sensory perception and chemical data for colour in port wines, while Kennedy et al. have examined the relationship between several methods of tannin analysis in red wines and perceived astringency [14]. Neural networks have been applied to modelling the sensory characteristics in Scotch whiskey [2] and beer [15]. The potential of instrumental texture measurements as a substitute for the sensory assessment of grape berry ripening properties has been evaluated [16].

A predictive model for the characterisation of the aromas in coffee based on the correlation between descriptive sensory profiling and analytical measurement obtained by proton transfer reaction-mass spectrometry [17] opens up new possibilities for using chemical analysis as a surrogate for sensory analysis. Principal Component Analysis was used in this coffee study. The recent advances in chemometric methods for the interpretation of multi-block data have provided new methodologies for data treatment [18]. Multi-block methods facilitate the comparison of different blocks of variables describing the same samples, highlighting similarities and differences among the blocks and also among the variables within each block. The present study investigates the potential of using a multi-block technique known as Common Components and Specific Weight Analysis [19] to the comparison of sensory descriptors and chemical analysis of a white wine. Semillon wine from the Hunter Valley, Australia, was chosen for this study. This wine is characterised for its low alcohol concentration (about 10%, v/v), high acidity (pH 3.2 or less), low residual sugar and capacity for ageing [20,21].

2. Experimental

2.1. Wine samples

Sixteen Semillon wines from the Hunter Valley, Australia, were provided by wine companies supporting a major study entitled '*Matching Semillon characteristics to consumer expectations*'. All wines were in bottle and opened only for sensory and chemical analysis. The selected wines spanned 10 vintages.

2.2. Chemical analysis

Table 1 contains the analytical parameters for the 16 Semillon wines. Glucose and fructose concentrations were determined using a D-glucose/D-fructose enzymatic kit from Boehringer (Mannheim, Germany). The total glucose plus fructose concentration (Total (G + F) in Table 1) was obtained by summing the individual values, while the sugar sweetness response was calculated as (glucose + 2.382 fructose) concentration to allow for the enhanced sweetness of fructose with respect to glucose and to allow for its earlier perception [22]. Malic acid was determined enzymatically using a L-malic acid kit from Boehringer (Mannheim, Germany). Glycerol was also determined enzymatically using a Megazyme K-GCROL kit (Megazyme International Ireland Ltd.). The pH and titratable acidity (TA) were assessed using a Cyberscan 510 pH meter, with the TA being determined by titration to pH 8.2 with sodium hydroxide and quoted as gram tartaric acid equivalents per litre. The volatile acidity was determined using a Foss Winescan^{TM} analyser. An Anton Parr Alcolyser DMA 450 density meter was used to determine the alcohol concentration.

2.3. Sensory analysis

The sensory descriptors were determined by a panel composed of six females and nine males aged 21–45 years. An exhaustive list of descriptors was gradually refined during a 9-week period in May–July 2007 such that 15 common descriptors were included in the final testing. The inclusion criteria followed the international standard ISO 11035:94 [23], where consideration was given to the relevance to Hunter Valley Semillon, the discrimination between samples afforded and the panel's ability to detect and easily recognise each descriptor.

The descriptors, acidity and sweetness, could be considered to be taste parameters, while the remaining 13 descriptors characterise the aroma profile. Table 2 (taken from [24]) summarises the sensory data used in this analysis.

2.4. Data analysis

Simple linear regressions and multiple linear regressions were performed on the sensory and analytical parameters using Statistica 7.1 (StatSoft, Inc., 2005).

Table 1
Analytical parameters for the 16 Semillon wines. Values are in g L^{-1}, except alcohol (%, v/v).

	Analysis code									
	A1 Glucose	A2 Fructose	A3 Total (G + F)[a]	A4 Sugar sweetness response[b]	A5 Titratable acidity	A6 pH	A7 Alcohol	A8 Malic acid	A9 Volatile acidity	A10 Glycerol
Wine code										
A	0.61	5.93	6.54	14.74	6.7	3.25	10.48	2.3	0.2	4.96
B	0.32	0.31	0.63	1.06	6.5	3.15	10.32	1.7	0.3	3.97
C	ND	0.08	0.08	0.19	7.7	2.84	10.64	1.4	0.2	3.94
D	0.13	ND	0.13	0.13	6.3	3.09	10.43	3.2	0.3	4.93
E	0.16	0.27	0.43	0.80	8.2	2.92	11.33	1.7	0.3	5.11
F	0.24	2.04	2.28	5.10	7.5	2.89	10.37	1.7	0.2	4.08
G	0.93	0.97	1.9	3.24	7.3	3.05	10.71	2.7	0.2	5.49
H	0.43	0.78	1.21	2.29	6.2	3.09	10.50	2.6	0.3	4.45
1	0.23	3.39	3.62	8.30	6.9	2.93	10.68	1.9	0.2	5.88
J	0.49	3.48	3.97	8.78	7.6	2.89	10.09	1.6	0.1	4.04
K	1.49	1.73	3.22	5.61	7.1	3.16	11.37	2.9	0.2	4.86
L	0.13	1.25	1.38	3.11	6.8	3.08	11.87	1.5	0.2	5.91
M	0.17	0.03	0.2	0.24	7.5	2.89	10.12	1.3	0.1	3.99
N	1.41	1.56	2.97	5.13	7.7	3.09	10.13	2.5	0.3	3.77
O	0.05	0.16	0.21	0.43	6.5	3.24	11.57	2.3	0.2	4.01
P	1.55	2.11	3.66	6.58	6.9	2.97	10.64	2.4	0.3	4.50

[a] Total G + F, sum of the glucose (G) and fructose (F) concentration.
[b] Sugar sweetness response; see text for details of calculation.

Table 2
Sensory descriptors for the 16 Semillon wines. See Ref. [24] for details.

	Sensory code														
	SI LEMON/LIME	S2 FLORAL	S3 GRAPE FRUIT	S4 PINE APPLE	S5 HAY/STRAW	S6 ORANGE MARMALADE	S7 HONEY	S8 TOAST	S9 GRASSY	S10 ASPARAGUS	S11 LYCHEE	S12 KEROSENE	S13 CONFECTIONARY	S14 ACIDITY	S15 SWEET NESS
Wine code															
A	5.24	4.10	2.63	3.13	2.27	0.98	2.28	1.08	2.55	1.30	1.67	1.46	3.48	4.49	5.05
B	3.73	1.51	2.19	1.67	3.76	2.74	4.62	4.23	1.76	1.51	1.12	3.74	0.98	5.06	2.52
C	4.29	2.40	2.83	2.09	3.06	0.79	1.59	1.51	2.49	1.06	0.94	1.77	1.67	5.89	3.05
D	4.59	2.59	2.43	2.17	2.83	1.43	2.57	2.21	2.26	1.57	1.40	1.68	1.83	4.91	3.33
E	4.09	2.17	2.17	2.38	3.01	2.14	3.66	2.72	1.78	0.87	1.01	2.61	1.24	5.30	2.89
F	3.20	1.62	1.63	1.26	3.78	2.18	4.15	5.33	1.27	1.04	0.96	2.83	1.01	5.14	2.88
G	5.37	4.13	2.85	3.22	2.21	1.47	1.80	1.17	2.55	1.33	2.04	1.24	2.47	5.42	3.86
H	3.75	1.77	1.72	1.95	3.79	3.64	5.55	5.46	1.33	0.82	1.27	3.13	0.78	4.87	2.79
I	4.50	3.91	2.91	3.13	2.59	1.04	1.78	1.03	2.97	1.13	1.49	1.18	2.72	5.77	3.83
J	4.18	1.99	2.26	1.85	3.26	1.09	2.76	2.15	2.16	1.04	0.89	1.79	1.28	5.70	3.07
K	3.98	1.77	2.47	1.52	3.34	1.55	2.55	2.72	2.33	1.45	0.70	2.32	0.90	5.00	3.37
L	4.55	2.27	2.66	1.98	3.19	1.21	2.21	1.96	2.18	1.07	1.16	2.09	1.45	5.01	3.67
M	3.74	1.91	2.19	1.94	3.13	1.34	2.81	3.54	1.79	0.95	1.00	2.24	1.28	5.53	3.09
N	4.50	2.72	2.54	1.98	2.85	1.93	2.66	2.13	2.17	1.22	1.29	2.11	1.67	4.90	3.67
O	3.77	1.77	2.23	2.48	3.01	2.39	3.28	3.06	1.72	1.31	1.14	2.43	1.51	4.21	2.93
P	4.51	3.60	2.45	2.23	3.05	1.30	2.46	1.26	2.45	1.34	1.81	1.61	2.54	4.81	3.99

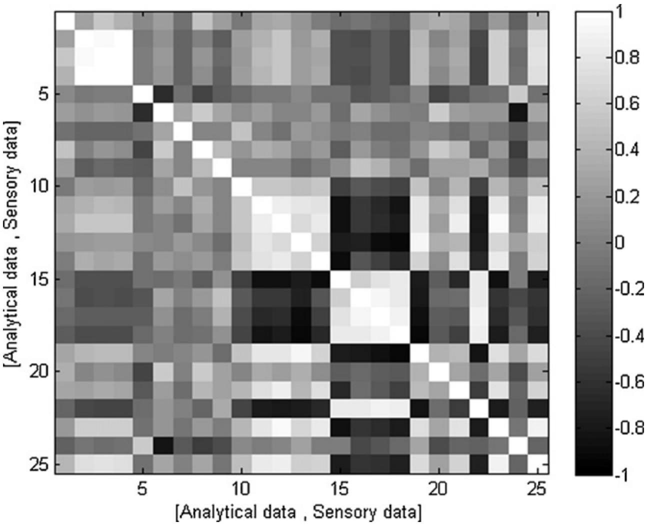

Fig. 1. Correlations between all pairs of sensory and analytical parameters.

The Common Components and Specific Weight Analysis multiblock approach, abbreviated as ComDim, was also applied to relate the sensory and analytical data. Qannari et al. [19] have described the statistical definition and interpretation of ‘common dimensions’ as well as demonstrating mathematically the equivalences and difference among several multi-block methods. The theory of ComDim multi-block analysis method is described in Scheme S1 (Supplementary Data). To avoid giving too much weight to variables with large values or large variability in the analysis used here, all data were column-centred and standardised, that is subtracting each column’s mean and then dividing each column by its standard deviation.

3. Results and discussion

The correlations among all the analytical variables (columns and rows 1–10) and sensory variables (11–25) are presented graphically in Fig. 1 (see also Supplementary Fig. S1) where it is clear that the positive and negative correlations are much stronger within the sensory variables block than between the analytical and the sensory variables blocks. Supplementary Figs. S2–S4 show the correlations between all pairs of analytical parameters, all pairs of sensory parameters and sensory and analytical parameters respectively.

The initial statistical analysis used simple linear regressions to determine if there were any potentially significant correlations between the sensory and analytical data that would suggest that there may be value in a more detailed analysis. Table 3 and also Fig. S4 present a summary of the correlations found by this approach.

The sensory SWEETNESS (S15) score is clearly significantly correlated with the analytical measures of residual sugar, that is with the total glucose plus fructose concentration (Total (G + F), Table 1) and the sugar sweetness response, the total sugar concentration adjusted for the enhanced sweetness of fructose (A2, A3, A4). Similarly, CONFECTIONARY (S13), a sensory descriptor also related to sweetness shows a positive correlation with the total residual sugar concentration, although not as strong as with the SWEETNESS score (Table 3).

The sensory score for ACIDITY (S14) is significantly correlated with titratable acidity (A5, Table 1) and shows significant, but negative, correlations with malic acid (A8) and pH (A6). Although a strong negative link between pH and sensory assessment of acidity is logical, it is somewhat unexpected here, given the narrow range

Table 3
Correlation parameters for linear regression analysis between sensory scores and analytical data. Data analysis performed using Statistica 7.1 (StatSoft, Inc., 2005).

Sensory descriptor	Analytical parameter[a]	Correlation, *r*	Probability	Standard error of estimate
SWEETNESS	Total (G + F)	0.756	0.0007	0.423
SWEETNESS	Sugar sweetness response	0.746	0.0009	0.430
CONFECTIONARY	Total (G + F)	0.594	0.0152	0.632
CONFECTIONARY	Sugar sweetness response	0.611	0.0120	0.623
ACIDITY	pH	−0.829	0.00007	0.265
ACIDITY	TA	0.563	0.0231	0.392
ACIDITY	Malic acid	−0.511	0.0430	0.395
FLORAL	Total (G + F)	0.561	0.0239	0.297
FLORAL	Sugar sweetness response	0.551	0.0271	0.792
FLORAL	Glycerol	0.536	0.0322	0.800
LEMON/LIME	Glycerol	0.553	0.0264	0.491
PINEAPPLE	Glycerol	0.553	0.0263	0.491
GRASSY	Glycerol	0.506	0.0453	0.417
ASPARAGUS	pH	0.572	0.0206	0.191
ASPARAGUS	Malic acid	0.577	0.0194	0.190
ORANGE MARMALADE	Volatile acidity	0.508	0.0448	0.677

[a] Total G + F, sum of the glucose (G) and fructose (F) concentration; sugar sweetness response: see text for details of calculation.

of pH values of these wines, from pH 2.84 to pH 3.16 (Table 1). The malic acid correlation is discussed in more detail below.

Intriguingly, positive and significant correlations were also found between some analytical measurements and aroma sensory scores (Table 3). For example, FLORAL sensory score (S2) is positively correlated with fructose (A2), the total residual sugar score (A3) and sugar sweetness response (A4) as well as with the glycerol concentration (A10). Glycerol also showed a relationship with LEMON/LIME, FLORAL, PINEAPPLE (S1–S4) and GRASSY (S9). There was a positive correlation between ASPARAGUS (S10) with pH (A6) and malic acid (A8) as well as between ORANGE MARMALADE (S6) and volatile acidity (A9), a reflection of acetic acid in the main.

This initial linear regression analysis implied that the potential for developing a model that used analytical data as a surrogate for sensory descriptors might be achievable. Several of the sweetness and acidity correlations are very significant when the probability values and standard errors (Table 3) are considered. Several of the other correlations in Table 3 are also moderately strong, implying that there may be a real relationship. This suggested that an in-depth analysis of the relation among sensory and analytical parameters using the more sophisticated multi-block ComDim analysis would be of value.

Several relations of proximity and opposition can be seen in the projection of the sensory and analytical parameters onto the CD1–CD2 plot (Fig. 2). It is clear that there are several regions of related descriptors in the CD1–CD2 plot. The region labelled *Sweetness* represents the commonality between the mouthfeel sensory parameter of SWEETNESS (S15), the aroma parameters of LEMON/LIME (S1), FLORAL (S2), GRAPEFRUIT (S3), PINEAPPLE (S4), GRASSY (S9), LYCHEE (S11) and CONFECTIONARY (S15) and the analytical parameters of fructose (A2) and glycerol (A10) and the calculated parameters of total glucose + fructose (A3) and sugar sweetness (A4). These groupings of descriptors are in general agreement with the linear regression analysis (Fig. 1 and Table 3), but of course the multi-block ComDim data are presented on a single map, rather than calculated individually as in linear regression.

Glucose (A1) is not part of the *Sweetness* region, but perhaps this is not surprising, given its zero to low concentrations in the wines examined here (Table 1). Ethanol (A7), which is sometimes considered to show sweetness [25], is not part of the *Sweetness* region. The ethanol concentration in the 16 wines is essentially invariant (Table 1), so it is reasonable to expect that it would not have any commonality with the common dimensions identified here.

The inclusion of glycerol (A10) in the *Sweetness* region is intriguing. Glycerol is known to affect various sensory attributes including sweetness, acidity, mouthfeel and viscosity. However, the actual concentration at which these attributes are expressed is the subject of considerable debate. Gawel et al. [26] found varying taster responses to different concentrations of glycerol. Noble and Bursick [27] suggested that additions of 26 g L^{-1} of glycerol were necessary before an increase in viscosity could be perceived, while Nurgel and Pickering [28] claimed a perceived increase in viscosity could be detected as the glycerol concentration increased from 10 to 25 g L^{-1} in a model wine. Intriguingly, the glycerol concentration in the wine studied here is much less than that for the levels examined by others. Clarification of these conflicting reports is outside the scope of this present work, but the ComDim analysis used here may well have the capacity to provide a better interpretation of published data and lead the way to a better understanding of the sensory aspects of glycerol in wine.

Two opposing relations of *Acidity* are identified in the ComDim variables plot for CD1 and CD2 (Fig. 2). One zone in the positive CD2 direction contains the sensory attribute ACIDITY (S14) and the analytical parameter titratable acidity (A5). Titratable acidity is a measure of the amount of acid present in the wine, so the commonality with the sensory acidity attribute is to be expected. The second *Acidity* zone in the negative CD2 direction contains only the analytical parameters of pH (A6) and malic acid (A8). The placement of pH opposed to sensory acidity is also as expected, given

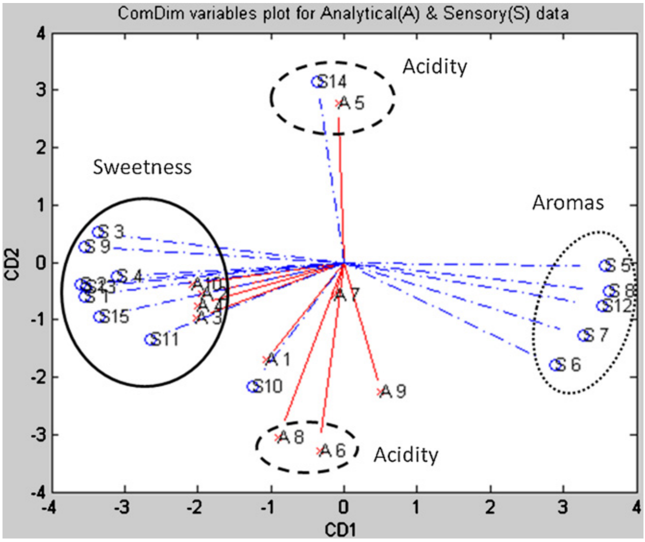

Fig. 2. Scatter plot of scores for analytical variables (stars) and sensory variables (circles) onto Common Dimension 2 vs. Common Dimension 1, calculated by ComDim.

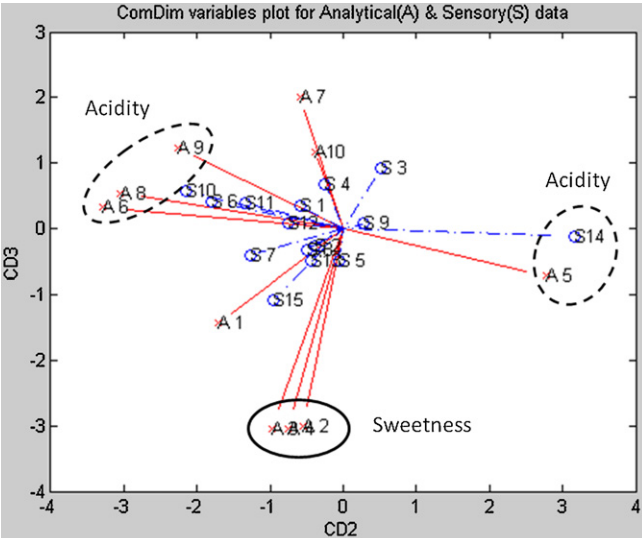

Fig. 3. Scatter plot of scores for analytical variables (stars) and sensory variables (circles) onto Common Dimension 3 vs. Common Dimension 2, calculated by ComDim.

its negative relationship with acid concentration, as noted above with the linear regression analysis. The placement of malic acid is unexpected, but also in accord with the linear regression analysis (Table 3 and Fig. S2).

Malic acid is sometimes regarded as 'green', while tartaric acid is considered to be 'hard' [29]. The relative acid taste of these two acids in white wine is still the subject of debate. Early work by Amerine et al. [30] on white wine showed that at the same titratable acidity, malic acid is perceived as more acidic, reflected as an increase in sourness. Relative sourness was also found to be higher for malic acid when the wines were adjusted to the same pH [30]. Noble et al. [31] focused on a comparison of sourness of organic acid anions at equal pH and equal titratable acidity in binary acid solutions. Only succinic acid (a minor component of wine) was found to be more sour than malic acid. Lugaz et al. [32] in a study of the time-intensity effects of organic acids on saliva suggested that it is the hydrogen ion that is the stimulus and not the neutral acid molecule or its monoanion.

In the Hunter Valley Semillon wines used here, the pH is generally around 3.2 or less and the malic acid concentration is only a small component of the titratable acidity (Table 1). The main acid is tartaric acid, a stronger acid than malic acid ($\mathrm{p}K_\mathrm{a}1$ (tartaric): 2.93; $\mathrm{p}K_\mathrm{a}1$ (malic): 3.46), suggesting that the hydrogen ion may well be the dominating factor in determining sensory acidity. Clearly more work is required, and the multi-block analysis approach used here may well provide greater insight into the competing effects than has been possible in earlier studies.

The sensory aromas fall into two categories: one group (labelled Aromas in Fig. 2) consists of HAY/STRAW (S5), ORANGE MARMALADE (S6), HONEY (S7), TOAST (S8) and KEROSENE (S12). There is no commonality between these sensory attributes and the analytical measurements used here. These same attributes are in opposition to the sweetness aroma attributes of LEMON/LIME (S1), FLORAL (S2), GRAPEFRUIT (S3), PINEAPPLE (S4), LYCHEE (S11) and CONFECTIONARY (S13) (Fig. 2). LEMON/LIME (S1), GRAPEFRUIT (S3) and PINEAPPLE (S4) are orthogonal to the acidity parameters (Fig. 2), despite the strong association of acidity with the taste of these fruits.

Interestingly, the sensory attribute ASPARAGUS (S10) is midway between the *Sweetness* region and the *Acidity* region that is in opposition to titratable acidity (Fig. 2). There is no proximity between ORANGE MARMALADE (S6) and volatile acidity (A9) in the CD1–CD2 plot, despite the correlation observed using linear regression (Table 3 and Fig. S4). This confirms the weakness of that correlation.

The CD2–CD3 plot (Fig. 3) confirms the strong connection among the analytical sweetness parameters A2, A3, A4. The unexpected proximity of pH (A6), malic acid (A8) and volatile acidity (A9) with titratable acidity (A5) and ACIDITY (S14) in opposition, is also confirmed in this plot. HONEY (S7) and SWEETNESS (S15) are this time in the same quadrant as glucose (A1).

4. Conclusion

In summary, the multi-block analysis, ComDim, has provided considerable insight into the connections between analytical data and sensory descriptors for Hunter Valley Semillon. Zones for *Sweetness* and *Acidity* describing the connections between various analytical and sensory parameters were readily identified. The orthogonal relationship between the analytical measurement for malic acid and the sensory score for acidity opens up the possibility of further research on the factors contributing to acid taste. One group of aroma sensory attributes did not show any connection with the analytical data used in this analysis. A GC–MS study of the aroma compounds in these Semillon wines is presently underway. The future inclusion of these data in the multi-block analysis may provide information on connections in addition to those already identified.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.aca.2009.10.062.

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