- Comparison of Pivot Profile[®] to Frequency of Attribute Citation: analysis of complex 1
- products with trained assessors. 2
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Abstract 15

Pivot[®] profile (PP), a method which compares samples to a reference (pivot), has shown 16 profiling potential for complex matrices. However, various aspects require further 17 18 investigation. This study's aim was to compare PP to frequency of attribute citation (FC) 19 considering individual judges' data and sample set complexity. A trained panel analysed 20 three wine sets with different within-set product similarity levels. The stability of the PP 21 sensory space was tested by changing the pivot. PP and FC results were compared using 22 RV coefficients. Confidence ellipses on correspondence analysis (CA) plots were constructed to consider individual judges' data. CA plots constructed from different pivot PP 23 24 data sets, were less similar to each other, than to CA plots of FC data, for the set with 25 medium and the set with high within-set variation. The most profound differences were 26 observed for the set with the high within-set variation. PP configurations of the set with low within-set variation, were more similar to each other than to FC configurations. Higher 27 explained variance was obtained with PP than FC, but confidence ellipses overlapped more 28 29 frequently indicating fewer significant differences between samples. PP and FC data were

comparable for the set with medium within-set variation. From this study's results PP is
recommended for wine profiling if medium within-set variation between samples exist but not
when sample sets with low or high within-set variation are profiled. PP is recommended over
FC for comparative studies where a reference sample is required for example during
benchmarking or for aging and shelf-life studies.

Keywords: Pivot profile, frequency of attribute citation, CATA, trained panel, correspondenceanalysis

37 **1. Introduction**

Describing the intrinsic properties of food products to obtain sensory profiles is a primary need within the food industry. It plays an important role during product development, production, quality control, advertising and marketing. Due to increased pressure from the food and beverage industry to profile products faster, new sensory methods and optimised statistical tools are continuously being developed. These include rapid sensory methods whereby product experts or naïve consumers can do the evaluation without training (Valentin et al., 2012; Varela & Ares, 2012).

One of the recent additions to rapid sensory methods is Pivot Profile[©] (PP), a frequency-45 based method proposed by Thuillier et al. (2015). When PP is performed, each sample is 46 47 compared to a reference sample, also referred to as the pivot. Sensory judges are required to list those attributes that they perceive as, respectively, less or more intense in the sample 48 than in the pivot. PP, therefore, provides an estimation of the intensity of attributes in the 49 50 samples relative to the pivot. Check-all-that-apply (CATA), (Adams et al., 2007; Lancaster & 51 Foley, 2007) can also provide an estimate of attribute intensities through the assumption that those attributes mentioned by more judges are more intense than those mentioned by fewer 52 judges (Campo et al., 2010). PP could, therefore, potentially be more suitable than CATA for 53 54 benchmarking applications of complex matrices such as wine (Thuillier et al., 2015) since; (1) relative intensity is captured during the tasting, while with CATA an assumption is made 55

56 about intensity, and (2) PP involves direct sample comparison and CATA monadic

57 presentation.

58 Several studies showed that PP is a valuable asset in the rapid sensory method toolbox. Thuillier et al. (2015) profiled champagne, using product experts as sensory judges when the 59 method was introduced. Subsequent research on a set of beer samples showed that the 60 choice of the pivot did not have a significant effect on the product positioning in 61 62 correspondence analysis (CA) plots (Lelièvre-Desmas et al., 2017). In the field of dairy research, Fonseca et al. (2016) compared PP to comment analysis (Symoneaux et al., 63 2012) and demonstrated that consumers could profile chocolate ice cream products 64 efficiently with both methods. PP was compared to CATA and projective mapping (PM) 65 66 (Risvik et al., 1994) in a study on Greek yoghurt samples (Esmerino et al., 2017). The results showed that PP, CATA and PM provided similar results of sufficient quality. Recently, 67 Deneulin et al. (2018) used PP to profile a large number of honey samples from all over the 68 69 world.

70 As with all new methods, further studies are needed to investigate and understand the appropriate use and performance of PP when applied to different products. Aspects 71 identified in earlier studies are related to possible effects of the choice of the pivot on the 72 73 stability of the sensory space (Thuillier et al., 2015) and the performance of the method when applied to sample sets with various degrees of within-set similarity (Lelièvre-Desmas 74 et al., 2017). Lelièvre-Desmas et al. (2017) reported that within-set similarity had a more 75 pronounced impact on the results than the choice of the pivot. However, in that study, the 76 77 between-sample discrimination power of PP, which is important for benchmarking of wine, 78 was not studied.

Yet another aspect that requires further investigation is the measurement of panel performance. In the studies by Deneulin et al. (2018) and Fonseca et al. (2016), panel performance was not measured. Deneulin et al. (2018) concluded that the vocabulary used required more attention and that calculating panel repeatability and consensus could shed light on these matters. Since Fonseca et al. (2016) used consumers as sensory judges, 84 repeatability could not be measured. However, investigating segmentation could be

interesting and could contribute to understanding the sensitivity of PP as a sensory method.

Thuillier et al. (2015) suggested that descriptive analysis (DA) might be more suitable than PP if the objective is to obtain a detailed description of products. In terms of comparing PP to other methods, no study has been conducted to test PP against traditional sensory methods that involve training of a panel to profile complex products such as beer and wine. DA has the limitation that, when assessing complex matrices, sensory judges could experience difficulty in differentiating between different odours by using a line scale (Lawless, 1999).

93 Frequency of attribute citation (FC) is a method that does not entail rating on a line scale 94 (Campo et al. 2008). FC refers to a profiling method whereby sensory judges are trained using a pre-determined list of attributes and reference standards. Judges are required to 95 96 select attributes from the list to describe the products under evaluation. FC is an adapted 97 CATA procedure with specific changes and restrictions where: (1) the list contains only sensory attributes: no phrases emotional or hedonic terms are allowed; (2) the sensory 98 attributes are organised into categories such as odour or aroma families; (3) judges are 99 trained with reference standards to use the CATA list; (4) judges can reorganise the CATA 100 101 list during training through panel consensus; and (5) panel repeatability is measured to ensure quality data. FC was used to analyse wine (Campo et al., 2008) and was compared 102 to DA in a later study in which similar results were obtained with DA and FC (Campo et al., 103 2010). 104

The aim of this study was to gain a better understanding of the appropriate application of PP when applied to wine profiling taking sample set complexity, defined as within-set variation, into account. A trained panel was used in this study for both PP and FC to eliminate the panel effect when comparing the two methods and to limit heterogeneity through training. FC, as opposed to DA, was used as reference method, to minimise difficulty experienced by judges in differentiating between odours, particularly experienced when rating intensities on a line scale (Lawless, 1999). Furthermore, comparing continuous DA data obtained from using a line scale to the categorical data obtained from PP might addextra variation.

Three objectives were formulated: (1) to evaluate the ability of PP to discriminate between different wines using confidence ellipses calculated by bootstrapping; (2) to test the robustness of PP by changing both the pivot sample and the sensory complexity, referred to in this paper as within-set variation; and (3) to compare panel performance for PP and FC in terms of repeatability, consensus and the perceived difficulty of the task. Three sets of wines, one red and two white cultivars, of varying within-set variation, were designed for the investigation.

121 2. Materials and methods

122 2.1 Samples

123 The wines used in this study were selected based on the knowledge acquired in previous 124 research on similar wines (Bester, 2011; Hanekom, 2012; Van Antwerpen, 2012), the 125 knowledge of expert tasters, wine industry professionals and sensory professionals. The 126 following three sets (six wines each) with different within-set sensory variation were 127 subjected to sensory analysis: (1) wooded Pinotage wines with similar characteristics; (2) 128 wooded Chenin Blanc wines of medium within-set variation; and (3) Sauvignon Blanc wines with extreme style differences. For this study, wines were selected in such a way that 129 130 specific cultivars represented sets with different levels of within-set variation. It is important to note that cultivar per se cannot be used as an indication of complexity. 131

The wines from the set with low within-set variation (Pinotage) had "oaky", "red berry", "blackberry", "spicy", "caramel" and "dried fruit" notes amongst other. The Chenin Blanc wines, with medium within-set variation, had "citrus", "tropical fruit", "yellow apple", "dried fruit", "honey", "caramel" and "woody" aromas. "Tropical" aromas including "guava", "passion fruit" and "pineapple", "green" aromas including "green pepper", "asparagus" and "tomato leaf" as well as "mineral", "flinty" and "oaky" nuances were used to describe the set with high within-set variation (Sauvignon Blanc wines). Each set was analysed by FC and PP using the same sensory methodology and workflow, resulting in six separate data sets. Three PP experiments were conducted for each set using different pivot samples, P1, P2 and P3. P1 and P2 were selected to show high sensory characteristics, as described below. P3 was a blend of equal volumes of all the samples in a cultivar set. The assumption was made that P3 of each set was "the average" sample (Thuillier et al., 2015); representative of the set and having no extreme sensory characteristics.

For the set with low within-set variation (Pinotage), P1 was chosen as a predominantly "fruity" sample with "red berries" and "black berries" as the main aroma contributors. P2 had prominent "oaky", "caramel" and "vanilla" notes.

The dominating aromas characteristics of P1 selected for the set with medium within-set variation (Chenin Blanc), were "fresh green", "grapefruit" and "citrus". P2 was characterised by intense "oaky", "vanilla" and "caramel" aromas, with subtle notes of "dried fruit", "marmalade" and "honey".

For the set with high within-set variation (Sauvignon Blanc), P1 was characterised by dominant "mineral" with subtle "tropical" and "green" notes. P2 was predominantly "oaky" with "fruity" attributes.

All wines were commercially available, produced in South Africa and certified by theSouth African Wine and Spirits Board (Table 1).

158 /Insert TABLE 1/

159 2.2 Panel

The panel of sensory judges consisted of three males and 12 females between 24 and 65 years of age (average age: 32). All judges were trained sensory assessors with more than two years of experience in wine sensory analysis and were paid for their participation. The same panel participated in the PP and FC experiments.

164

165 2.3 Sensory Methodology

166 2.3.1 FC and PP methodology

2.3.1.1 Training. Panel training consisted of 15 sessions of one hour each over six weeks. 167 Ballot training on 134 wine aroma attributes using reference standards (Table 2) was 168 conducted according to the frequency of attribute citation training procedure (Campo et al., 169 170 2008 and Campo et al., 2010). The list of terms given to the panel was subdivided into 171 aroma categories according to literature (Noble et al., 1987; Campo et al., 2010; Bester, 2011; Hanekom, 2012; Van Antwerpen, 2012). During each training session, judges were 172 presented with 10 to 15 aroma standards to familiarise themselves with the terms on the list 173 174 (ballot). Two to three wines were presented per session. Attributes used by the panel to describe the wines were discussed and the most frequently cited attributes were highlighted 175 176 by the panel leader.

The training consisted of two phases; a general phase in which the judges were trained 177 on the initial list of terms, followed by a specific training phase where judges were trained to 178 179 profile wines similar to those presented during the evaluation. During the specific training, 180 judges could add terms to the initial list and change their categorisation in the separate 181 aroma families to describe the wines accurately. The final aroma attribute list with aroma standards is shown in Table 2 and consisted of 103 attributes. Two specific training 182 sessions, discussing wines from the relevant cultivar and vintages, were performed per 183 cultivar sample set. For this study, judges were trained since detailed descriptions of the 184 wines were required, and panel heterogeneity had to be limited. However, PP could also be 185 performed by industry professional or consumers without training the sensory judges if less 186 detailed profiles are required. 187

188 /Insert TABLE 2/

Procedures. Judges had to provide three to five terms from the list to describe the most prominent aromas of each wine. Campo et al. (2010) suggested that the required number of attributes that each judge should use to describe products should be specified with FC to avoid the use of too few or too many descriptors. People have a limited capacity to discriminate between and describe odours in complex samples and using too few descriptors can lead to incomplete descriptions of samples (Laing & Glemarec, 1992). On
the other hand, when large numbers of attributes, including many synonyms, are used to
describe wines, noise could be added to the data, complicating and adding biases during the
statistical analysis of the data.

During PP sessions, judges were asked to write down the attributes that they perceived 198 "less intense" and "more intense" in the sample than the pivot from the list of attributes (Fig. 199 200 1). The same list as provided for FC was used. Judges were limited in terms of the number of attributes that they could use during PP to achieve a degree of standardisation between 201 the instructions for PP and FC. No more than the five most prominent attributes per sample 202 203 were allowed to describe the aromas that they perceived "less intense" in the sample than 204 the pivot. The same rule applied to the attributes perceived "more intense" than the pivot. 205 Finally, judges had to provide at least three attributes in total per sample.

The final task of the sensory evaluation session was to rate the difficulty of performing the sensory methods. Judges were asked to give a score out of 9 on an easiness scale that was derived from the nine-point hedonic liking scale (Peryam & Pilgrim, 1957). The specific words used were: "extremely easy (1); very easy (2); moderately easy (3); slightly easy (4); neither easy nor difficult (5); slightly difficult (6); moderately difficult (7); very difficult (8); and extremely difficult (9)".

To minimise panel learning effects, and matrix change due to wine aging, several 212 measures were taken and followed for all three sample sets. Sensory evaluation sessions of 213 214 a specific set of wines and one pivot, for example P1, were conducted in duplicate by 15 assessors on the same day. The panel did not receive information on the nature of the wines 215 in terms of style, vintage or cultivar and did not know that they evaluated the same wines 216 twice. The same cultivar set with P2 as pivot was only evaluated two to three weeks later. 217 The order in which evaluations, PP-P1, PP-P2, PP-P3 and PP-FC, were performed was 218 randomised within the different sets. The entire set PP-P1, PP-P2, PP-P3 and PP-FC, for 219 example, all the Chenin Blanc evaluations, were done within two and a half months, to 220 221 ensure that wine ageing did not change sensory characteristics. Since the latter aspect is of

particular importance for the white wines, the sets were analysed consecutively. The set with
medium within-set variation was analysed first, the set with high within-set variation second
and the set with low within-set variation last. The sets were, therefore, not analysed from the
lowest to highest, or from highest to lowest within-set variation.

226 2.3.1.3 *Wine evaluation.* Wines were evaluated in a well-ventilated, temperature controlled 227 ($20 \pm 2^{\circ}$ C), odour free sensory lab secluded from extraneous noise. The laboratory was 228 equipped with separate off-white individual tasting booths with controlled lighting conditions.

Black (ISO NORM 3591, 1977) tasting glasses labelled with random 3-digit codes were used. Samples were randomised across judges according to a Williams Latin-square design (MacFie et al., 1988). Monadic sample presentation was applied for FC. For PP, samples were presented in pairs. Each pair consisted of a sample and a fresh pivot. Each glass contained 25 mL of wine and was covered with a Petri-dish lid. Wines were poured 20 to 30 minutes before the sensory evaluation session to allow volatile compounds to reach equilibrium in the headspace of the glasses.

Wines were evaluated orthonasally in duplicate for both methods. Duplicates were evaluated on the same day with an enforced 10-minute break in between to limit sensory fatigue. Data were collected using Compusense cloud software (<u>www.compusense.com</u>, Compusense).

240 2.4 Data analysis

241 2.4.1 Panel performance

Repeatability. Panel repeatability was calculated for the individual judges using the
reproducibility index (R_i) proposed by Campo et al. (2008). Two times the number of
common descriptors used in the first and second repeat was divided by the total number of
descriptors used in both repeats. This ratio was calculated for every wine and summed over
all the wines tasted by one judge to calculate the R_i value for that judge. In addition, a global
reproducibility index (R_i) was calculated by computing the average across all judges' R_i
values. This measure ranges from 0 to 1. If all the attributes cited during the first and second

repeat are the same, then the R_i value will be 1. If entirely different attributes were cited, 249 then the R_i value will be 0. A minimum R_i of 0.2 was proposed by Campo et al. (2008) to 250 deem a sensory judge repeatable enough to record the response as data. 251

252
$$R_i = \frac{1}{n} \sum \frac{2 \times des_{com}}{\left(des_{rep1} + des_{rep2}\right)}$$

253 Where: n = number of wines

 $des_{com} = number of identical descriptors chosen by the judge in both replicates$ 254 $des_{rep1} = number of descriptors chosen by the judge in replicate 1$ 255

 $des_{rep2} = number of descriptors chosen by the judge in replicate 2$ 256

257 R_i values were calculated for the FC and PP methods for all the data sets. For PP data the following rule was applied: if a descriptor was cited as "more intense" in one repeat and "less 258 intense" in the other repeat it was not counted as an identical descriptor occurring in both 259 repeats and that descriptor did not contribute to the R_i value. Each PP set obtained from 260 261 using a different pivot sample was treated as a separate data set.

262 A three-way mixed model ANOVA with cultivar, method and the cultivar*method interaction as fixed factors and sensory judges as random factors was computed. The 263 264 ANOVA was used to study the differences between repeatability of the panel in terms of Ri values computed when (1) sample sets with different within-set variation was evaluated and 265 (2) different sensory methods (PP and FC) and pivot samples were used. Sample sets from 266 different cultivars represented sets with different within-set variation, as explained before. 267 268 Pinotage represented low, Chenin Blanc medium and Sauvignon Blanc large within-set sample variation. The methods used were FC and PP using different pivot samples, P1, P2 269 and P3. The REML estimation method was used. When significant ANOVA results were 270 found, pairwise comparisons were calculated using the Fisher's LSD post hoc test with α set 271 at 5%. 272

Consensus. Panel consensus was measured calculating Cohen's kappa coefficients for 273 274 each pair of judges. Cohen's kappa coefficient is a measure of the similarity or agreement between the ratings provided by two individuals. It is commonly used on nominal data as an 275

- interrater reliability measure in the field of medical and educational surveying (Cohen, 1960;
- Altman 1991; McHugh, 2012; Gisev et al., 2013). In this study, Cohen's kappa coefficients
- (κ) were calculated using the mathematical equation below:

$$\kappa = \frac{p_0 - p_e}{1 - p_e}$$

- 280 Where:
- 281 $p_0 =$ the relative observed agreement among raters (sensory judges in this case)
- 282 $p_e = the hypothetical probability of chance agreement$

283 In addition, the average panel consensus was calculated for each data set by computing the average of all the Cohen's kappa coefficients across all the judges. Individual data 284 285 obtained from PP were handled by means of the following rule: if a descriptor was cited as "more intense" by one sensory judge and "less intense" by another the agreement among 286 those two judges for that descriptor was noted as zero as if two different descriptors were 287 used. Each PP sample set obtained from using a different sample as pivot was treated as a 288 289 separate data set. A three-way mixed model ANOVA similar to the ANOVA computed on the 290 R_i values was computed on the Cohen's kappa coefficients.

291 Difficulty of the sensory task. A three-way mixed model ANOVA, similar to the ANOVA's

applied to assess panel consensus and repeatability, was performed to investigate

significant differences between the perceived difficulty of the different FC and PP data sets.

294 2.4.2 Product characterisation

The descriptors generated to describe each group of wines in the verbalisation phase were captured by constructing a contingency table. The number of attributes used was reduced before statistical analysis. Attributes cited by less than 20% of the panel were combined with similar terms or discarded. Three sensory experts combined similar terms independently by employing lemmatisation and semantic categorisation. Attributes combined differently by the sensory experts were discussed and consensus was reached before the final attribute reduction step. Fig. 1a shows the scheme used for data organisation andanalysis.

Correspondence analysis (CA) with confidence ellipses, calculated using bootstrapping 303 (Cadoret et al., 2013; Dehlholm et al., 2012), was performed on the contingency tables and 304 305 used to visualise the sensory space spanned by the different wines within a data set. 306 Contingency tables were constructed from FC and PP data in different ways. For FC data, the total number of citations over all the judges for each descriptor per wine was 307 tabulated with the attributes as variables in the columns and the wines as objects in the 308 309 rows. The number of judges who cited an attribute for a specific wine was tabulated at the intersection of the corresponding column (representing the attribute) and row (representing 310 the wine). This procedure is the same as for standard CATA (Valentin et al., 2012). 311

PP data sets were compiled by subtracting the citation frequency of "less" from "more" for 312 313 each attribute for each wine. The pivot sample was added as centre point by including zeros 314 for all the descriptors for the pivot wine. This procedure was followed when P1 and P2 was used as pivot. When P3, the blend, was used as pivot sample this procedure was not 315 followed. The absolute value of the minimum was added to all the values as a translation 316 317 step. This procedure produced both positive and negative values. Since CA cannot be conducted on a table containing negative values, translation had to be performed to obtain a 318 contingency table consisting of positive values. Through this procedure the relative intensity 319 of the pivot (P1 or P2) relative to the other samples was determined during translation of the 320 321 data and was reflected in the contingency table on which CA was performed. Consequently, 322 CA plots obtained for P1, P2 and P3 were comparable containing the same samples, which included P1 and P2 but not P3. This procedure is described in detail by Thuillier et al. (2015) 323 and summarised in Fig.1. In order to apply bootstrapping on the PP data, the contingency 324 325 table was converted into an appropriate data set for CA by repeating each combination of wine and descriptor n_{ii} times where n_{ii} is the frequency of the *i*-th wine and the *i*-th descriptor 326 327 in the contingency table.

328 /Insert Fig. 1/

329 2.4.3 Comparison of methods and testing the stability of the sensory space for PP

The similarities between multivariate plots were assessed by calculating RV coefficients 330 on the first two dimensions. RV coefficients are used to measure the similarity between two 331 matrices or data sets by measuring the amount of variance shared (Robert & Escouffier, 332 333 1976; Abdi et al., 2013; Abdi et al., 2014). CA plots generated from PP data sets where 334 different samples were used as the pivot were compared to each other and to the CA plot constructed from FC data (Fig. 1b). This procedure was followed for the set with the low 335 within-set variation (Pinotage), the set with medium within-set variation (Chenin Blanc) and 336 337 the set with large within-set variation (Sauvignon Blanc) separately. In addition, the repeatability, panel consensus and difficulty perceived by the panellists when performing PP 338 and FC were compared using ANOVA, as described above. 339 All data organisation and analyses were conducted using Microsoft Excel 2016 340 (www.microsoft.com, Microsoft), XLSTAT (www.XLSTAT.com, Addinsoft SARL.), Statistica 341

13 (<u>www.statsoft.com</u>, Statsoft Inc.) and R version 3.4.0, packages "car" and "cabootcrs"

343 (www.R-project.org).

344

345 **3. Results**

346 3.1 Panel performance

The individual R_i values for all the sensory judges were above 0.2 for both FC and PP, irrespective of which samples were used as the pivot. The highest R_i value was 0.86 and the lowest 0.26. All the judges produced repeatable results, considering that R_i values can range from 0 to 1, and Campo et al. (2008) proposed 0.2 as the lowest acceptable value.

It is clear from the three-way mixed model ANOVA results (Fig. 2a) performed on panel repeatability, with method and cultivar (representing different levels of within-set variation) as fixed factors, that the method*cultivar effect was significant (p < 0.001). Therefore, the method*cultivar interaction effect was interpreted using Fisher's LSD *post hoc* test since the same trend could not be seen for all cultivars or sample sets. Thus, the panel repeatability was influenced by the complexity of the data set analysed. Sensory judges were less

repeatable when conducting FC than PP for the data set with medium within-set variation 357 (Chenin Blanc wines). A significant difference between FC and PP with P2 and P3 was 358 seen. In addition, judges were less repeatable when P1 was used than when P2 was used. 359 No significant difference in repeatability was seen when P1 and P3 (the blend of all the 360 361 samples) and P2 and P3 were used. A significant difference between using P2 and P1 as pivot sample could be seen for the data set with high within-set variation (Sauvignon Blanc 362 wines). In addition, no significant differences between PP when changing the pivot or 363 between PP and FC was observed for the data sets with low within-set variation (Pinotage 364 wines). 365

In summary, the average panel repeatability was the lowest for the Pinotage wines, which
had the least within-set variation and differed significantly from the Sauvignon Blanc wines,
(which had high within-set variation).

369 /Insert Fig. 2/

Panel consensus, measured by Cohen's kappa coefficients, ranged from 0.02 to 0.55. Values below 0.2 are considered poor, 0.4 fair and between 0.4 and 0.6 moderate (Altman, 1991). As with the panel repeatability, the method*cultivar effect was significant with p < 0.001. Therefore, the method*cultivar interaction effect's Fisher's LSD *post hoc* test was interpreted since the same trend could not be seen for all cultivar sample sets for all the methods in terms of significant differences between panel consensus.

The ANOVA results (Fig. 2b) clearly show that different trends were observed for the sample sets with different within-sample variation in terms of average panel consensus. The panel consensus for the set with the low (Pinotage) and the set with medium (Chenin Blanc) within-set variation was poor with the average Cohen's kappa coefficient of the panel below 0.2. Interpreting significant differences with such low values would be unwise.

It is interesting to note that the only data set with acceptable average panel consensus
coefficients, above 0.2, was the set with high within-set variation (Sauvignon Blanc). Cohen's
kappa coefficients above 0.2 were observed for FC and PP except when the blend of the

samples was used as a pivot for which a significantly lower value of 0.17 was observed. The
best consensus was achieved when P1 was used and was significantly higher than when FC
was performed and when other pivot samples were used.

For easiness/difficulty of the task, as with the panel repeatability and consensus, the method*cultivar effect was significant with p < 0.001. Therefore, the method*cultivar interaction effect's Fisher's LSD *post hoc* test was interpreted since the same trend could not be seen for all cultivars for all the methods in terms of significant differences in the difficulty of the task. The sensory judges experienced PP as significantly more difficult to perform when compared to FC, irrespective of the within-set variation of the data set and the pivot sample used (Fig. 2c).

394 Product description and comparison of methods

395 The RV coefficients calculated between the PP CA configurations when the pivot sample 396 was changed for the set with the lowest within-set variation (Pinotage wines) ranged from 0.52 to 0.83 (Table 3). Since all the RV coefficients were above 0.5, the configurations could 397 be regarded as similar (Louw et al., 2013). However, the similarity between the FC 398 configuration and PP configurations, corresponding to P1 (Fig. 3a) and P2 (Fig. 3b) as pivot 399 samples, indicated low similarity with RV coefficients below 0.35 (Table 3). When a blend of 400 all the samples was used as pivot sample, namely P3 (Fig. 3c), better similarity was 401 observed with an RV coefficient of 0.60. 402

403 /Insert TABLE 3/

Furthermore, overlapping confidence ellipses indicated that no significant difference between samples could be observed when PP was conducted on this sample set although the explained variance for the first two factors was well above 60%. The cumulative explained variance for the first two factors was 68% when P1 (Fig. 3a), 75.7% when P2 (Fig. 3b), 69% when P3 (Fig. 3c) and 68.2 when FC (Fig. 3d) was used. Confidence ellipses on the CA plot of the FC configuration indicated that two of the samples were perceived as significantly different from the other four samples (Fig. 3d). It is interesting to note that the cumulative explained variance of factor one and two of the CA plot of PP when P2 was used
as pivot sample was higher for PP (Fig. 3b) than for FC (Fig. 3d). This was, however, not the
case when P1 and P3 were used as pivot samples.

414 Descriptors belonging to the same aroma families appeared more scattered on the CA plot and showed less positive correlation with each other for PP data than FC data. The 415 most obvious and prominent cases occurred when extreme samples, P1 and P2, were used 416 417 as pivot samples (Fig. 3a and b). When the blend P3 (Fig. 3c) was used as pivot, aroma attributes belonging to the same aroma family grouped well together indicating acceptable 418 positive correlation. Examples were: (1) "oaky", "wooded", "pencil shavings", "toasted" and 419 "burnt wood", belonging to the "wooded" aroma family, and (2) "blackberry", "blackcurrant", 420 421 "black fruit" (including all dark berries except blackberry and blackcurrant), "cherry", "raspberry" and "strawberry", belonging to the "berry" aroma family. 422

423 /Insert Fig. 3/

424 The data set with medium within-sample set variation (Chenin Blanc) produced CA plots 425 (Fig. 4) with cumulative explained variances of the first two dimensions above 65%. When 426 P1 was used, the cumulative explained variance of dimension one and two was 71.3%, 427 when P2 was used 68.6%, when P3 was used 84.2% and when FC was conducted it was 66.7%. Furthermore, similar configurations for the PP and FC data sets with RV coefficients 428 429 ranging from 0.66 to 0.88 (Table 3) were observed. In general, the differences between CA plots from PP data when different pivot samples were used, were more pronounced, with 430 lower RV coefficients, than the differences between PP and FC. The similarity between P1 431 and P3 with an RV coefficient of 0.75 was an exception and showed good similarity. The RV 432 coefficient between the CA plots constructed using P1 and P2 was 0.44, indicating 433 434 dissimilarity. P2 had aroma characteristics that could overshadow other aroma nuances since aroma was described by words such as "vanilla", "wooded", "oaky", "buttery" and 435 "caramel" by many of the judges (Fig. 4b). The confidence ellipses on this CA showed 436 frequent overlap between samples. A possible explanation could be that it was difficult for 437 438 the sensory judges to detect differences between the other samples when comparing

samples to P2, which had intense and extreme sensory characteristics. Confidence ellipses 439 overlapped less frequently when a blend between the samples was used as pivot (P3), 440 indicating clearer significant differences between samples (Fig. 4c). It is interesting to note 441 that descriptors from the same aroma family were grouped well together on all CA plots 442 obtained for this set. Examples were: (1) "sweet associated" characteristics such as "vanilla", 443 "caramel", "honey" and "toffee" and (2) "oaky", "wooded" and "planky", which were positively 444 correlated. Furthermore, higher explained variance could be observed when P3 was used as 445 pivot sample when compared to FC and to the other PP evaluations when P1 and P2 were 446 447 used.

448 /Insert Fig. 4/

449 From the CA plots constructed for the data set with high within-sample set variation (Sauvignon Blanc), the variation explained by dimension 1 and 2 was above 70% (Fig. 5), 450 which is regarded as high for sensory data. When P1 was used, it was 79.9%, when P2 was 451 452 used 87.1%, when P3 was used 82.4% and when FC was used it was 71.5%. Clear separation between the confidence ellipse of the pivot sample and the other samples was 453 visible, but the overlapping confidence ellipses of the other samples indicated similarity and 454 an inability of the panel to discriminate between those samples. It is possible that the 455 uniqueness of the pivot sample caused the high explained variance and overshadowed the 456 variation between other samples, causing a loss of separation between them. 457

The RV coefficients between the different sample sets varied from 0.28 to 0.95. Even though the effect of the pivot was overshadowing sensory characteristics, the RV coefficients between the CA maps when the extreme samples were used as pivots, P1 (Fig. 5a) and P2 (Fig. 5b), and the FC CA map were above 0.86 (Table 3). The low RV coefficient of 0.28 between CA maps constructed from P3 and P2, 0.51 between P1 and P3 and 0.36 between FC and P3, originated from the fact that one of the samples, TSL, was profiled differently when P3 was used as pivot sample.

465 /Insert Fig. 5/

466 **4. Discussion**

PP can be a useful technique to use for the profiling of complex products such as wine 467 (Thuillier et al., 2015) and beer (Lelièvre-Desmas et al., 2017). The objective of this study 468 was to evaluate PP critically for the profiling of complex matrices, comparing PP to FC, a 469 well-established descriptive method (Campo et al., 2008). More specifically, the objective 470 was to determine whether one of these techniques offered better discrimination between 471 472 samples than the other one. To investigate these aspects thoroughly, three wine sample sets with different levels of within-sample set variation were analysed using a trained panel 473 and CA was performed to obtain multivariate sensory maps. 474

475 Inspecting these CA plots, the following conclusions were reached. The variance explained by the first two factors when PP was used, regardless of the within-set variation 476 complexity of the data set or the choice of pivot, was higher than 60%, indicating that the 477 478 differences between samples were described well with PP. Confidence ellipses, calculated 479 with bootstrapping, were added to the CA results as suggested by Lelièvre-Desmas et al. (2017) to understand the significance of product differences described by PP and FC. The 480 confidence ellipses overlapped more frequently for PP than FC, showing that fewer samples 481 were perceived to be significantly different when PP was performed than when FC was 482 483 performed.

In addition, confidence ellipses shed light on perceived product differences when within-484 set product variation was varied. It is clear that the lower the within-set variation between 485 samples was, the more frequent the overlap of confidence ellipses of different samples was. 486 Due to the severe overlap of confidence ellipses for the data set with low within-set variation, 487 it is not recommended to use PP to analyse such a set of products, even though it was 488 suggested by Lelièvre-Desmas et al. (2017) that PP might be better suited to more 489 490 homogenous spaces. However, for the sets with medium and large within-set variation, the confidence ellipses overlapped less frequently when a blend of the samples, rather than a 491 492 sample with extreme characteristics, was used as pivot sample. It can, therefore, be

493 concluded that more samples were perceived as significantly different when the blend was494 used as the pivot and the within-set variation was medium or high.

The similarity between sample configurations on the CA plots was tested by means of RV 495 coefficients. Similarity between the different PP configurations, when the pivot sample was 496 changed, and FC configurations differed for data sets with different degrees of within-set 497 variation. Similar product configurations were obtained when the pivot was changed for the 498 499 data set with low within-set variation, indicating that the choice of the pivot was not crucial. This observation was in line with observations made by Thuillier et al. (2015) when PP was 500 proposed and Lelièvre-Desmas et al. (2017) when the stability of the product space was 501 tested by varying the pivot sample used as well as the within-sample set variation. However, 502 503 the similarity between PP configurations and the FC configuration was poor, except when a blend of all the samples was used as pivot. Thuillier et al. (2015) proposed using the blend 504 as the pivot to create a centre sample, containing a wide range of sensory properties that 505 506 spanned the sensory space, to which other samples were compared. Lelièvre-Desmas et al. 507 (2017) noted that the idea of using a blend as pivot might be well suited to profiling of 508 homogeneous spaces, which was confirmed in this study.

It is important to keep in mind that few significant differences between samples were 509 510 observed for this set when PP was conducted. Even though Lelièvre-Desmas et al. (2017) found that PP might be more suited to homogenous spaces than heterogeneous spaces, this 511 set was probably too homogeneous for profiling using PP. Lelièvre-Desmas et al. (2017), 512 however, did not compute confidence ellipses by means of bootstrapping to validate product 513 514 discrimination. Furthermore, the lack of quantification of the degree of similarity within a 515 sample set causes subjective interpretation of what low, medium and high within-sample set 516 variation is. Measures to quantitatively determine sample set complexity needs to be 517 developed and can shed light on the performance of many other rapid methods.

If the set, regarded by Lelièvre-Desmas et al. (2017) as the set with low within-sample set variation was compared to the set defined in this study as the set with medium within-sample set variation, remarkably similar results were obtained.

The similarity between FC and PP data sets was good, with RV coefficients above or 521 close to 0.7, regardless of the pivot used for the sample set with medium within-set variation. 522 It is interesting to note that higher RV coefficients, indicating better similarity, were observed 523 between the different PP data sets when different pivot samples were used and FC data 524 525 than when these PP data sets were compared to each other. This was observed for the data 526 set with large within-set variation as well with an exception when a blend of all the samples was used as pivot. In that case, poor similarity, with low RV coefficients was observed with 527 the FC CA configuration and the PP CA configurations, originating from different pivot 528 529 samples. Visual inspecting of the CA plots revealed that one sample was described differently and was consequently located differently relative to the other samples. It was 530 noted by El Ghaziri and Qannari (2015) that RV coefficients would not provide a good 531 estimate of the similarity of two spaces if one sample was not in the same position on both 532 maps. In other words, if one sample was perceived differently, the RV coefficient would be 533 low even though all the other samples were perceived similarly and would not provide a 534 reasonable estimate of the overall similarity between two configurations, in this case, 535 sensory spaces. 536

The question, however, remains why this sample was perceived differently. Two factors 537 could play a role here: a physiological perception factor and a methodological limitation to 538 use vocabulary that would distinguish wines from each other. It was noted by Lelièvre-539 Desmas et al. (2017) that the vocabulary might change when a different pivot is used. 540 541 Therefore, they suggested that PP might not always be the best method to obtain a detailed sensory characterisation of samples but should rather be used to compare samples. In order 542 543 to answer this question, a study could be designed in which sample sets with different complexities are created by substituting some samples with less and more complex wines 544 but keeping to the same wine style and cultivar. Analysing these wines with DA and PP 545 could then shed light on perceived differences due to a change of the pivot sample relative 546 547 to the DA profile obtained.

The suggestion by Thuillier et al. (2015) to add the pivot sample as centre point by 548 including zeros for all the descriptors in the table of citation frequencies containing +1 for a 549 citation of more intense and -1 for a citation of less intense for individual judges was followed 550 when P1 and P2 was used. The intensity of the pivot relative to the other samples was then 551 552 determined during translation of the data and was reflected in the contingency table on 553 which CA was performed. When P3, the blend, was used as pivot sample, this procedure was not followed and only the samples evaluated were represented in the CA plots. This 554 should not affect the data, particularly the CA plots, if the assumption that P3 was an 555 556 average centre sample representing the characteristics of all the samples equally held since all the samples were evaluated relative to the pivot. It, however, cannot be ruled out that the 557 data was affected and, therefore, the RV coefficients describing the similarities between P1, 558 P2 and P3 configurations. It should be noted then that it might be worthwhile testing, by 559 statistically including P3 in the CA plot and comparing the configuration to a CA plot with P3 560 561 excluded. Furthermore, a sensory experiment including the pivot as a sample as well and not just a theoretical centre point during the statistical analysis could be insightful. 562

563 In the light of what has been discussed, it has to be said that the total number of descriptors allowed for product description was three to five when FC was performed and 564 three to 10 when PP was performed, if the number of descriptors allowed to describe 565 sensory characteristics perceived as less and more intense for PP was taken into account. 566 567 This could contribute to sensory judges focussing less on the most prominent characteristics 568 of the sample causing more noise, therefore more overlap between confidence ellipses. Furthermore, the chance of choosing the same attribute for more than one sample could 569 also increase the overlap of confidence ellipses around samples on the CA plots. In contrast, 570 571 richer data might have been obtained since more descriptors per wine were generated, which could explain the higher explained variance observed for PP in comparison to FC. 572 Even though these restrictions might have influenced results, it was considered as the most 573 practical choice for the method when using a trained panel. The choice of the number of 574 allowed attributes was made based on recommendations from the literature but mainly on 575

feedback from the panel during training sessions. These limits were set to ensure that all thepanellists used the protocol and a similar approach.

An aspect of PP that still requires attention is the testing of panel performance. In 578 579 previous studies in which PP was used as a profiling technique, the measurement of panel performance did not receive enough attention. Thuillier et al. (2015) proposed the method 580 but did not propose a strategy to measure panel performance since the focus of that study 581 was on a simulation in which panel heterogeneity was set as a parameter. It would, 582 583 therefore, not make sense to test panel performance on the simulation data. Fonseca et al. (2016) and Esmerino et al. (2017) performed PP using consumers as panellists without 584 investigating possible segmentation or testing the performance of individuals. Testing panel 585 repeatability was not possible with the data obtained during the consumer studies as judges 586 587 did not repeat the test. Testing consumers' performance is not common and is deemed irrelevant due to the large number of participants that increases the statistical power of the 588 experiment. However, investigating panel segmentation and individual differences could 589 590 provide valuable insights into how consumers profile the product when performing PP. 591 Lelièvre-Desmas et al. (2017) proposed a strategy to evaluate global panel consensus and repeatability when performing PP, but the authors also acknowledged that more work 592 needed to be done in this field. 593

594 In this study, panel repeatability was measured using the Ri value and consensus using 595 Cohen's kappa coefficients. Both these measures provide useful insights into panel 596 performance but are probably too strict since they only take exact matches of attributes as good consensus between two judges. It could make sense to penalise judges less or not at 597 all when two judges use slightly different attributes that still belong to the same odour family. 598 599 Weighing contributions to the Ri value could be applied by assigning, for example, 0.5 instead of zero if an attribute from the same aroma family is sited in both the first and second 600 601 repeat. In order to incorporate this idea into panel performance testing, more work is required in the field of sensometrics. 602

603 Critical investigations of panel performance measurements and a proposed workflow to 604 measure consensus and repeatability for PP and FC, similar to the work published by Tomic 605 et al. (2007) and Tomic et al. (2010) for DA, could be valuable additions to the methodology 606 development of rapid methods.

607 It would be interesting to evaluate the performance of PP when performed by industry professionals or naïve consumers when judges are not trained, and less detailed results 608 609 might be captured. Industry professionals' sensory perception responses generally reflect the lexicon that they developed during their years of experience taking part in 610 quality/competition-type tastings, keeping the production process in mind. PP was originally 611 proposed by Thuillier et al. (2015) as an alternative to free description when capturing 612 industry professionals' sensory perceptions. Capturing consumers' less detailed descriptions 613 related to styles in general, preferences and emotion could be a new application for PP. 614

615 In this study, a single modality, aroma, was assessed. This modality can easily be 616 assessed by methods such as FC and CATA. Mouthfeel and taste might be difficult or unpractical to asses with FC since it often means little if the relative intensity of the attribute 617 in terms of the products cannot be assessed by the individual judges. The assumption that 618 the number of citations will indicate the intensity is not always true when a trained panel 619 620 profiles wine. From unpublished data, it was found that most wines in a sample set could, for example, be sour and alcoholic but some wines are more sour or less sour than other wines 621 (Brand and O'Kennedy, unpublished research on white wines). Although it was not 622 specifically stated that FC was less suitable for taste attributes than aromas, Campo et al. 623 624 (2008) only proposed the technique and compared it to DA (Campo et al., 2010) for aroma 625 evaluation of wine. In this case, FC will not be able to detect differences between wines in 626 terms of taste attributes and PP might offer a solution and could be a more suitable option 627 than FC for profiling the taste and mouthfeel properties of wines.

628 **5. Conclusions**

PP could be a useful wine sensory evaluation technique when a comparison between products is required either through profiling of individual wines or direct comparison, for example during benchmarking. As a profiling technique, PP could be a viable alternative for FC. However, the results obtained clearly showed that the nature of the samples analysed and particularly the level of variation between samples needs to be considered and that the results could be influenced by the choice of the pivot sample.

From this study, it was clear that when sample sets with very low within-sample set
variation were tested, FC was a more sensitive technique to use than PP.

The sensory space generated using PP for a wine sample set with medium within-set variation and using a central sample as the pivot was comparable to results obtained with FC. The most reliable results were obtained from this type of sample set when a blend of all the samples was used as the pivot.

Sample sets with large within-set variation might be less suitable for analysis by PP and
FC results will probably be more stable. However, with these sets, good similarity between
FC and PP results was obtained when extreme samples were used a pivot samples,
whereas poor similarity between PP and FC was observed when a blend of the samples was
used as pivot.

The panel repeatability was comparable and good for both PP and FC. PP was experienced by judges as significantly more difficult to perform compared to FC, irrespective of the complexity of the data set and the pivot sample used. Cohen's kappa coefficients indicated reasonable to moderate consensus for both PP and FC when the sample set with large within-sample variation was analysed, but low values were obtained when a blend of all the samples was used as pivot.

A workflow to test panel consensus and repeatability will add value to the PP
methodology. Panel performance testing is currently a shortcoming of the methodology
available for PP in the literature. Testing the ability of Cohen's kappa and related kappa
coefficients, for example Fleiss' kappa, on data sets varying in terms of within-set variation

for PP analysis to assess both repeatability and consensus could be a first step in designingsuch a workflow.

To conclude, for sensory studies where simultaneous sample presentation is required to 658 get an overview of the sample set during profiling, PP could be preferred over FC. This could 659 be the case when product experts, producers or consumers evaluate samples since these 660 judges are generally not trained and might be inconsistent when evaluating samples in a 661 662 monadic manner. These types of panels are generally not required to evaluate sample sets with small with-in set variation. When FC is used the assumption is made that the larger the 663 number of citations the more intense that attribute might be. In the case of wine fault 664 analysis this assumption might not hold. A method where relative intensity is captured, such 665 666 as with PP, could be more informative than FC measuring how many judges perceived attributes related to the fault. Another application where PP could be more relevant to use 667 than FC is when a one-to-one comparison between two products is required. The stability of 668 the sensory space will not play a role here since only two products are evaluated directly 669 670 with each other and not in relation to a common reference. Examples of such cases include 671 benchmarking and shelf-life studies. For these two applications it would be interesting to compare PP to other rapid sensory methods such as sorting and particularly reference-672 based rapid sensory methods such as polarised sensory positioning (Teillet et al., 2010) and 673 polarised projective mapping (Ares et al., 2013). 674

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