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Discrimination of Juice Press Fractions for Sparkling Base Wines by a UV-Vis Spectral Phenolic Fingerprint and Chemometrics

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Received: 18 April 2018; Accepted: 8 June 2018; Published: 12 June 2018

Abstract: The feasibility of an ultraviolet-visible (UV-Vis) spectral phenolic fingerprint (SPF), combined with principal component analysis (PCA), is evaluated as a rapid, simple, and reliable technique for the discrimination of grape juice press fractions destined for the production of sparkling white wines. Juice press fractions of *Vitis vinifera* L. Chardonnay and Pinot noir grapes comprising free-run (i.e., juice released during the loading of press), *cuvée* (i.e., first press fraction), and *taille* (i.e., subsequent press fraction), were analyzed by SPF combined with multivariate data analysis. Two trials were carried out, a laboratory and a commercial scale trial. In both trials, *cuvée* and *taille* of Chardonnay and Pinot noir grapes were clearly separated in their corresponding PCA plots based on their SPF. The proposed method enables a rapid and objective discrimination of juice press fractions, which can be obtained using relatively inexpensive UV-Vis spectrophotometric equipment. Insights arising from this research suggest a future possibility of objective, real-time discrimination of juice quality that could liberate the winemaker from tasting juice at the press.

Keywords: press fractioning; sparkling wine; ultra violet-visible spectroscopy; spectral phenolic fingerprints; hydroxycinnamates; caffeic acid; ferulic acid

1. Introduction

Over the last decade, the Tasmanian wine industry has grown significantly, primarily due to an escalation in sparkling white wine production (*Méthode Traditionelle*), with Pinot noir and Chardonnay being the main *Vitis vinifera* varieties used [1]. Flavor is of primary importance for understanding consumer preference of sparkling white wines and, in general, intense aged/developed and complexity attributes are currently favored [2,3]. A number of viticultural and oenological decisions can affect a sparkling wine's flavor, such as grape variety selected, origin of grapes, and winemaking procedures adopted (e.g., juice extraction, oxygen management, fining, and length of lees aging) [4–7].

Particularly for sparkling white wines, the separation of grape juice during a pressing cycle is important, as many blending fractions with varying chemical (e.g., total acidity, pH, phenolic, polysaccharide, and oligosaccharide content) and sensory characteristics (e.g., color, green-grassy aroma, bitterness, astringency) can result from the pomace break-up [6,8,9]. Juice press fractions for sparkling wines are typically classified as free-run, *cuvée* and *taille* [6,10,11]. Whereas the free-run is the juice released during the loading of press (in case of whole bunch press), *cuvée* (i.e., first press fraction) and *tailles* (i.e., subsequent press fractions) represent the best and lesser quality juice, respectively. These fractions can vary in volume depending on production rules and/or winemaking style. For example, in Champagne, grape juice has to be separated into two tanks according to volumes

imposed by law: namely *cuvée*, consisting of 20.5 hL (after settling) per 4000 kg marc, and *tailles*, consisting generally of the last 5 hL extracted and corresponding to the first and second *taille* [6].

The separation of different juice press fractions, for sparkling white wines particularly, has to be carefully monitored, since an excessive extraction of phenolic substances (e.g., flavanols, hydroxycinnamates) may negatively affect the color, taste, and/or mouthfeel attributes of final wines [8,12]. For instance, an excess of hydroxycinnamates (non-flavonoid phenolics) and their derivates, such as caffeic acid and its *trans*-ester of tartaric acid i.e., caftaric acid (*trans*-caffeoyl tartaric) in both juice and wine matrices, can lead to the formation of an undesirable oxidative browning [13].

Apart from legislated volumetric requirements that regulate the press fractioning for certain sparkling wines, such as Champagne, typically winemakers discriminate juice press fractions by sensorial assessments for 'phenolic pick-up' (i.e., perception of drying, coarse in-mouth sensations). Although this is probably the best option for discriminating a small number of samples, it is limiting when dealing with large batches of juice in part because of inter-individual variability in tolerance thresholds and unreliability of human senses, health condition, and environmental interferences [14,15]. High volume juice production typically relies on empirical methods, such as volume or conductivity, and the opportunity arises to develop an algorithm for an objective method calibrated against sensory data. A rapid and reproducible tool for quality assurance purposes is needed for wine producers to discriminate juice press fractions, in order to ensure the quality and consistency of the final product delivered to the consumer.

Ultraviolet-visible (UV-Vis) spectral fingerprinting is an easy to adopt, inexpensive, and rapid way to discriminate and classify the characteristics and quality of food products including wine [16–19]. However, it is not well recognized as a technique to discriminate grape juice quality during pressing. Spectral fingerprints are the sum of instrumental signals for each significant compound present in the sample matrix and are normally acquired using detectors that generate high dimensional data (many variables per sample), such as infrared (IR), near-infrared (NIR), mid-infrared (MIR), mass (MS) and nuclear magnetic resonance (NMR) spectrometry [20–24]. The use of a spectrophotometric technique for discriminating juice press fractions could be of particular interest to the wine industry, since most laboratories are equipped with a UV-Vis spectrophotometer for other routine analyses. In addition, UV-Vis spectroscopy relies on π bonding and conjugated double bonds, so phenolics have distinct UV fingerprints, while the most abundant wine components, such as water, alcohol, organic acids, and sugars, have no absorbance in the UV wavelength range used (200–600 nm) [25].

Principal component analysis (PCA) is one of several multivariate methods, applied to convert correlated data (e.g., spectral measures) into linearly uncorrelated variables that describe or predict meaningful patterns from complex spectral fingerprints [26].

In the present study, UV-Vis spectrometry was used to provide a spectral phenolic fingerprint (SPF) that enables the discrimination of Chardonnay and Pinot noir press fractions destined to the production of sparkling white wines. Chardonnay and Pinot noir grapes were used as test material because of their significance to the Australian sparkling wine production and also to that of other regions around the world. PCA was employed to test the hypothesis that differences between juice press fractions produced from a single batch of Chardonnay or Pinot noir grapes can be discriminated based on their SPF that is detectable in UV-Vis spectroscopy.

2. Materials and Methods

2.1. Laboratory Scale Trial

2.1.1. Hydroxycinnamate Standards

Two low molecular weight phenolics, i.e., caffeic and ferulic acids, which are very abundant in Chardonnay and Pinot noir grape juices [27], were used as hydroxycinnamates standards for comparison of the spectral phenolic fingerprints. Standard solutions were prepared by dissolving 0.005 g of each compound in 50 mL of 50% ethanol aqueous solution (v/v), and diluted 1:2 in a stepwise

fashion, giving six solutions for each hydroxycinnamate. Each solution was then diluted 1:10 with 1 M HCl, as was the 50% ethanol solution, giving 13 solutions for UV-Vis analysis, which were read against 1 M HCl baseline.

2.1.2. Grape Juice Press Fractioning

The laboratory scale trial was carried out in the 2010/11 season, using Chardonnay and Pinot noir grapes sourced from a commercial vineyard located in the Tamar Valley winegrowing region of Northern Tasmania, Australia. A total of 15 kg of grapes was hand-harvested at a commercial ripeness of 10.5° Baumé. The titratable acidity of the Chardonnay fruit was 13.3 g L^{-1}, with pH 3.03. The titratable acidity of the Pinot noir fruit was 12.4 g L^{-1}, with pH 3.10. Fruit was pressed in a flatbed whole bunch press with rubber membrane pressurized with water at up to 1.0 bar (Solutions in Stainless, Launceston, Tasmania, Australia) with *cuvée* (i.e., first press fraction) and *taille* (i.e., subsequent press fraction) cut respectively at approximately 350 L ton^{-1} and 150 L ton^{-1} for Chardonnay and 400 L ton^{-1} and 150 L ton^{-1} for Pinot noir. These volumetric cut-offs were the average reported in a Tasmanian sparkling wine industry survey carried out by the research team in 2009. Four homogenous juice samples were collected from *cuvée* and *taille* respectively, for both Chardonnay and Pinot noir varieties. All samples were frozen at −18 °C for later analysis.

2.2. Commercial Scale Trial

The commercial scale trial was carried out in the 2011/12 season using for Chardonnay and Pinot noir grapes. Samples were supplied by a commercial winery located in the Tamar Valley winegrowing region of Northern Tasmania, Australia. Table 1 details the main processing characteristics of the 2011/12 vintage season, in which grapes were harvested at a commercial ripeness of 10.5° Baumé and pressed in a pneumatic press (RPX 80 model, Bucher Vaslin, Chalonnes-sur-Loire, France). *Cuvée* and *taille* cut-off were determined subjectively by an experienced winemaker tasting juice at the press, with particular attention to phenolic pick-up. *Cuvée* and *taille* were cut respectively at 481 L ton^{-1} and 228 L ton^{-1} for Chardonnay and 502 L ton^{-1} and 200 L ton^{-1} for Pinot noir. A juice sample at each pressure, for each press cycle, was collected at the press outflow (42 and 31 samples for Chardonnay and Pinot noir, respectively) and frozen at −18 °C for later analysis.

Table 1. Pressing operation parameters during the 2011/12 commercial scale trial.

Variety	Press Fraction	Number of Samples	Press Cycle	Pressure (Bar)
Chardonnay	*Cuvée* (481 L ton^{-1})	21	Free run	Free run
			1	0.2, 0.4, 0.6, 0.8, 1.1
			2	0.2, 0.4, 0.6, 0.8, 1.1
			3	0.2, 0.4, 0.6, 0.8, 1.1, 1.4
			4	0.4, 0.6, 0.8, 1.1
	Taille (228 L ton^{-1})	21	4	1.4
			5	0.6, 0.8, 1.1, 1.4, 1.7
			6	0.6, 0.8, 1.1, 1.4, 1.7
			7	0.6, 0.8, 1.1, 1.4, 1.7
			8	0.6, 0.8, 1.1, 1.4, 1.7
Pinot noir	*Cuvée* (502 L ton^{-1})	22	Free run	Free run
			1	0.2, 0.4, 0.6, 0.8, 1.1
			2	0.2, 0.4, 0.6, 0.8, 1.1
			3	0.4, 0.6, 0.8, 1.1, 1.4
			4	0.4, 0.6, 0.8, 1.1
			4	1.4, 1.7
	Taille (200 L ton^{-1})	9	5	0.6, 0.8, 1.1, 1.4
			6	0.6, 0.8, 1.1, 1.4, 1.7

2.3. UV-Vis Spectcroscopy

Frozen samples of Chardonnay and Pinot noir juices were thawed overnight at 4 °C prior to centrifugation using a 5804 Eppendorf (Hamburg, Germany) at 3350 radial centrifugal force (RCF) for 15 min for clarification. Samples were diluted 1:5 with 1 M HCl (Merck, Darmstadt, Germany) and dark incubated for one hour at ambient temperature (22 °C). Samples were then analyzed using a Genesys 10S UV-Vis scanning spectrophotometer (Thermo Scientific, Waltham, MA, USA) with an absorbance reading taken every 2 nm from 200 to 600 nm inclusive for the spectral phenolic fingerprint (SPF). Samples were analyzed using disposable 10 mm quartz cuvettes (Brand-GMHB, Wetheim, Germany), so wavelengths below 250 nm were discounted due to interferences.

2.4. Chemometrics

The raw spectral data were imported into the Unscrambler X software (ver. 10.2, Camo, Norway) and PCA was performed to discriminate treatment clustering and to determine important wavelengths that contributed to treatment discrimination. Data was evenly weighted and cross validated with 20 segments and 2 samples per segment. The Non-Linear Iterative Partial Least Squares (NIPALS) algorithm was used to perform the PCA.

3. Results and Discussion

3.1. Discrimination of Press Fractions in the Laboratory Scale Trial

The raw spectra of hydroxycinnamate ethanolic solutions and juice press fractions of Chardonnay and Pinot noir grapes are illustrated in Figure 1a,b, respectively. The spectral phenolic fingerprint (SPF) showed moderate to strong absorbance at around 330 nm, which gives an indication of the content of lower molecular weight phenolics, such as hydroxycinnamates, present in the samples [28]. There was also a shoulder at around 280 nm, likely arising from the contribution of total phenolics at this wavelength [29]. This information may be of sensory significance to sparkling wine producers, as total phenolics and hydroxycinnamates (i.e., summed concentration of free hydroxycinnamate acids and their tartaric acid and ethyl esters) have been reported to exert an effect of bitter taste on white wines [8]. However, total phenolics in combination with higher pH have also been shown to elicit perceived viscosity (i.e., overall perception of palate weight) [8], responsible for affecting the quality of some sparkling wines [2].

A comparison between the SPF of *cuvée* and *taille* obtained from Chardonnay and Pinot noir grapes at laboratory scale, indicates that most of the variation between these press fractions occurred within the 'fingerprint' region of interest; i.e., 230 and 450 nm (Figure 1b). For grape, juice, and wine samples, this region is known to contain absorbance bands attributable to phenolic compounds, and results from the electronic transition of π orbitals [19]. The hydroxycinnamate solutions had a distinct absorbance peak at 330 nm, with a shoulder at 290 nm, a trough at 260 nm and a peak at 238 nm (Figure 1a). Similar wavelengths feature in a comparison of press fractions from the laboratory trial (Figure 1b), with the *cuvée* fractions having higher absorbance values at 290 and 330 nm, suggesting that hydroxycinnamates may be more readily extracted than other phenolics. Spectra from the commercial trial feature greater separation between *cuvée* and *taille* (Figure 1c), with higher absorbances across all wavelengths for Pinot noir and an additional feature around 520 nm in the Pinot noir *taille*, are indicative of the contribution of anthocyanins from harder pressings (as indicated by press fraction volumes).

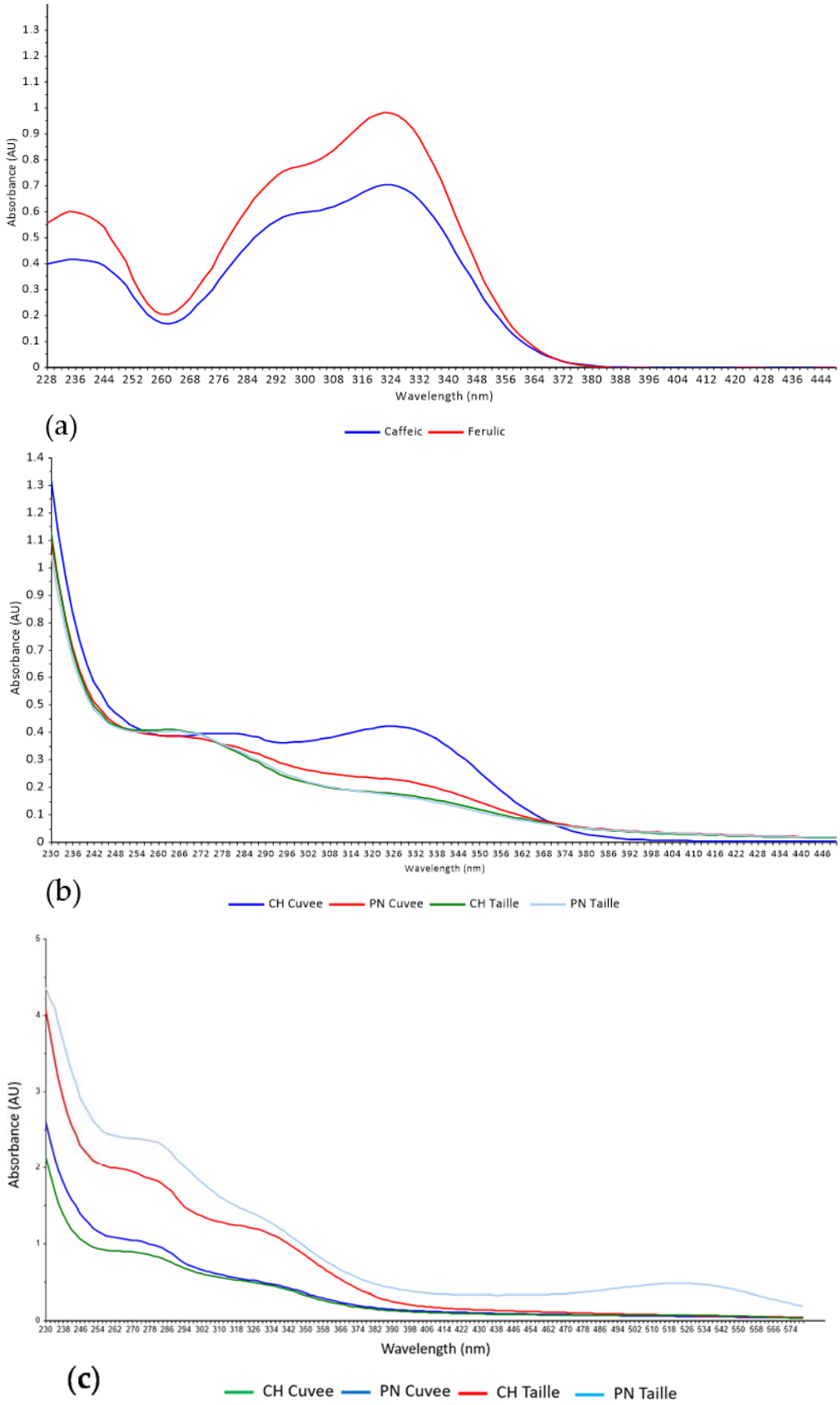

Figure 1. (**a**) Raw UV-Vis spectra of hydroxycinnamate ethanolic solutions, diluted in 1 M HCl; of (**b**) laboratory scale Chardonnay (CH) and Pinot noir (PN) *cuvee* and *taille* trials; and of (**c**) commercial scale Chardonnay (CH) and Pinot noir (PN) *cuvee* and *taille* trials.

The press conformation and mode of operation were different for the laboratory scale and the commercial press. The laboratory press was a flat-bed press with a faster operational cycle, so there was less skin contact time and less berry damage, more akin to a basket press often used for sparkling wine production. The commercial press was a pneumatic press that had long operational cycles with rolling of the press between cycles resulting in more damage and more skin contact, hence the phenolic profiles were different. It seems that gently pressing with minimal skin contact resulted in a different phenolic profile with less material that absorbed at 280 nm. With the more gentle pressing, fractions were best separated at wavelengths associated with hydroxycinnamates, which appeared to be easily extracted. The current data indicates that with both pressing methods, the fractions can be discriminated with spectral data, although the fractions will differ depending on the press type and mode of operation. Ultimately, the spectral data can be calibrated against a winemaker's preference for the fractions and used as an objective measure that correlates with that sensory data. This could be done using full spectra and chemometrics [30] or simple algorithms could be derived with a small number of critical wavelengths.

The PCA score plots of the first two principal components (PC), derived from the UV-Vis SPF of all grape juice press fractions obtained during the laboratory scale trial, are shown in Figures 2a and 3a for Chardonnay and Pinot noir, respectively. For Chardonnay samples, PC 1 explained 95% of the variation observed (Figure 2a), and resulted in a strong separation of *cuvée* from *taille*. The spectral loadings for PC 1 showed features at 260 nm and 330 nm suggesting influence of hydroxycinnamates, with *cuvée* having higher levels. Absorbance at 280 nm is often used to estimate total phenolics; the spectral loadings for PC 1 show very little influence by 280 nm in separating *cuvée* from *taille*. One outlier was observed, i.e., an individual juice sample that did not cluster with other juice samples of the same treatment, namely a *taille* sample, that instead was represented in the lower left quadrant, but was still separated from *cuvée* on PC 1. The clustering pattern of press fractions likely relates to appreciable differences in the concentration of caffeic and ferulic acids, or their esters, between *cuvée* and *taille* samples.

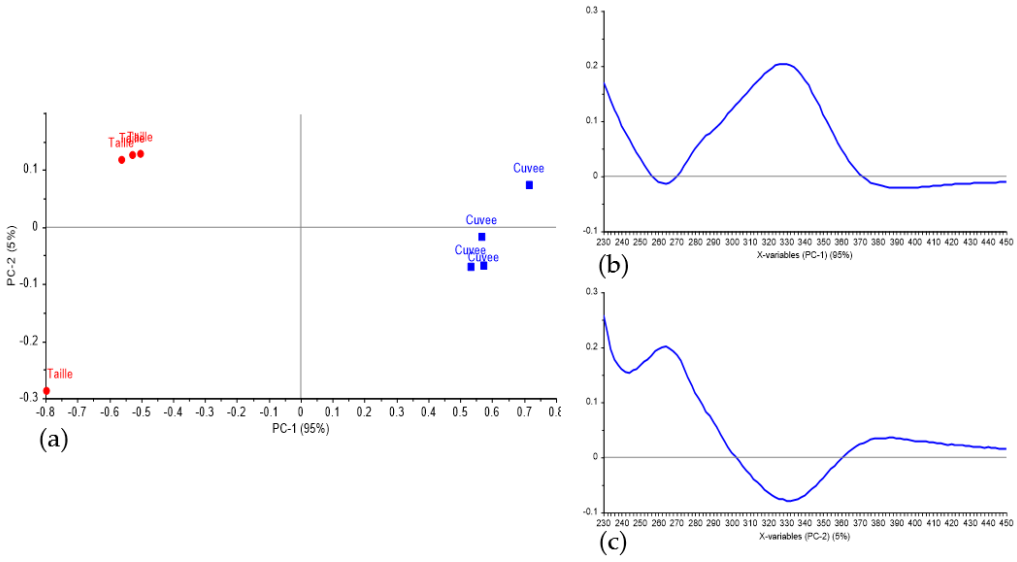

Figure 2. PCA scores and loadings plots of 2011 Chardonnay juice samples from the laboratory scale trial discriminating *cuvée* from *taille*. Scores plots (**a**); PC 1 (**b**) and PC 2 (**c**) loadings.

For Pinot noir samples, PC 1 accounts for 84% of the data variability (Figure 3a), and similar to Chardonnay, resulted in a clear separation of *cuvée* and *taille* samples. The greatest separation between the *cuvée* and *taille* clusters was observed along the horizontal (PC 1) axis. As with Chardonnay PC

1 was influenced by 260 nm and 330 nm features, with *cuvée* samples having higher absorbance at these wavelengths.

For both varieties, PC 2 provided some separation within each press fraction and it appeared to also be driven by 260 and 330 nm wavelengths, but differences were smaller than between the press fractions (Figures 2c and 3c).

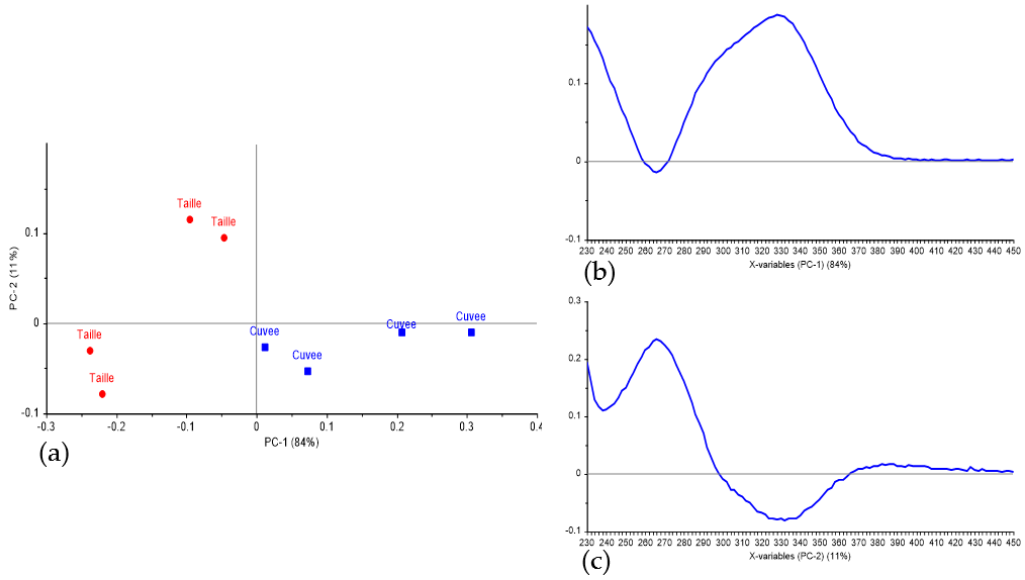

Figure 3. PCA scores and loadings plots of 2011 Pinot noir juice samples from the laboratory scale trial discriminating *cuvée* from *taille*. Scores plots (**a**); PC 1 (**b**) and PC 2 (**c**) loadings.

3.2. Classification of Press Fractions in the Commercial Scale Trial

PCA scores and loadings plots of commercial Chardonnay and Pinot noir grape juice press fractions, are reported in Figures 4 and 5 respectively. In the commercial scale trial, Chardonnay juice samples were strongly separated along PC 1 with 98% of the data variation explained (Figure 4a). Winemaker subjective assessment of juice quality as *cuvée* and *taille* corresponded with the UV-Vis SPF separation along PC 1. The loadings for PC 1 indicated that the *taille* fractions had higher phenolics, but unlike the laboratory press, the separation was not specifically influenced by the 330 nm peak indicative of hydroxycinnamates. This may be related to the operational nature of the press type [31] and oxidation conditions during the pomace break-up [32]. The laboratory press was a flat-bed press with only a thin layer of bunches that were pressed relatively quickly and with smaller fraction volumes, whereas the commercial press had greater skin contact time and the press load was rotated and pressed multiple times, allowing more extraction and oxidation. This again suggests that hydroxycinnamates are more readily extracted than other phenolics such as flavanols and tannin, possibly due to their different distribution within the berry of these varieties, or to skin contact conditions [9,33]. However, changes in phenolic composition with pressing could also be related to oxidation reactions occurring within the must when inside the press [8].

PCA of the 31 Pinot noir juice samples, gave similar associations as observed in the Chardonnay samples. PC 1 explained >99.9% of the data variability (Figure 5) and, the spectral loadings for PC 1 were indicative of higher phenolics in *taille* fractions without specificity for hydroxycinnamates. The press fractions were collected in chronological order during processing of a batch of grapes, so overlap of SPF would be expected at samples near the boundary of *cuvée* and *taille*. In the case of Figure 4a, PC 1 is the main component that separates fractions, but where samples overlap on PC 1, they are separated by PC 2, with *cuvée* having higher hydroxycinnamates on PC 2, agreeing with the

laboratory scale press. In the case of Figure 5a the close samples near the zero point of PC 1 represent the boundary of the *cuvée* and *taille* fractions.

For both Chardonnay and Pinot noir, the relatively minor PC 2 indicated that separation within the fractions was influenced by absorbance at 330 nm, a hydroxycinnamate peak (Figures 4c and 5c), particularly for Chardonnay.

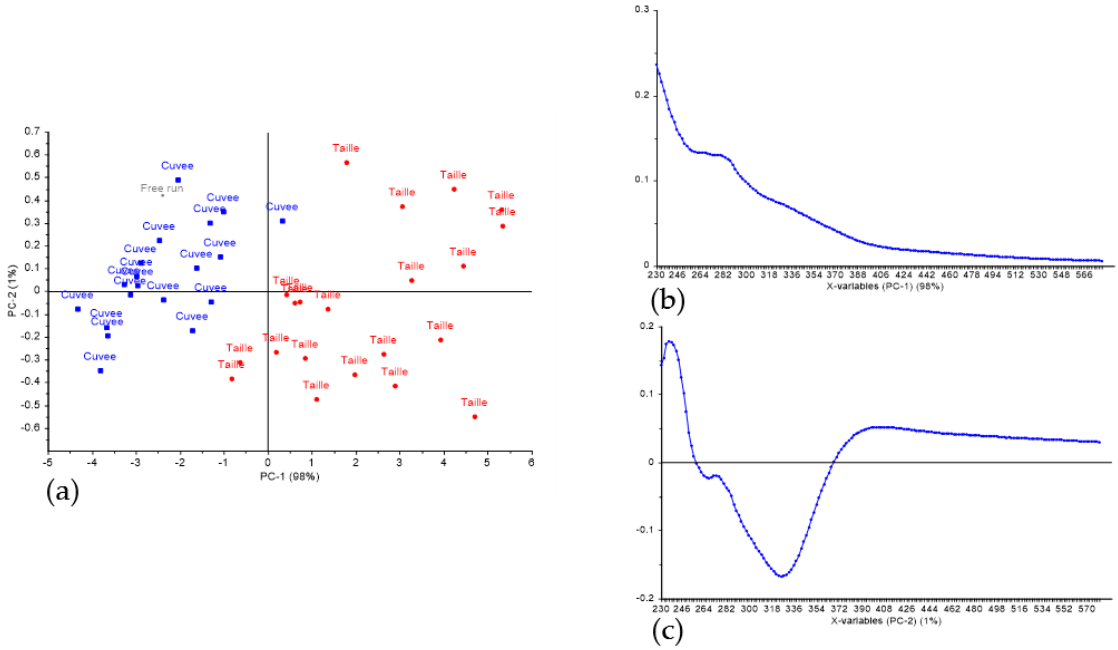

Figure 4. PCA scores and loadings plots of 2012 Chardonnay juice samples from the commercial scale trial discriminating *cuvée* from *taille*. Scores plots (**a**); PC 1 (**b**) and PC 2 (**c**) loadings.

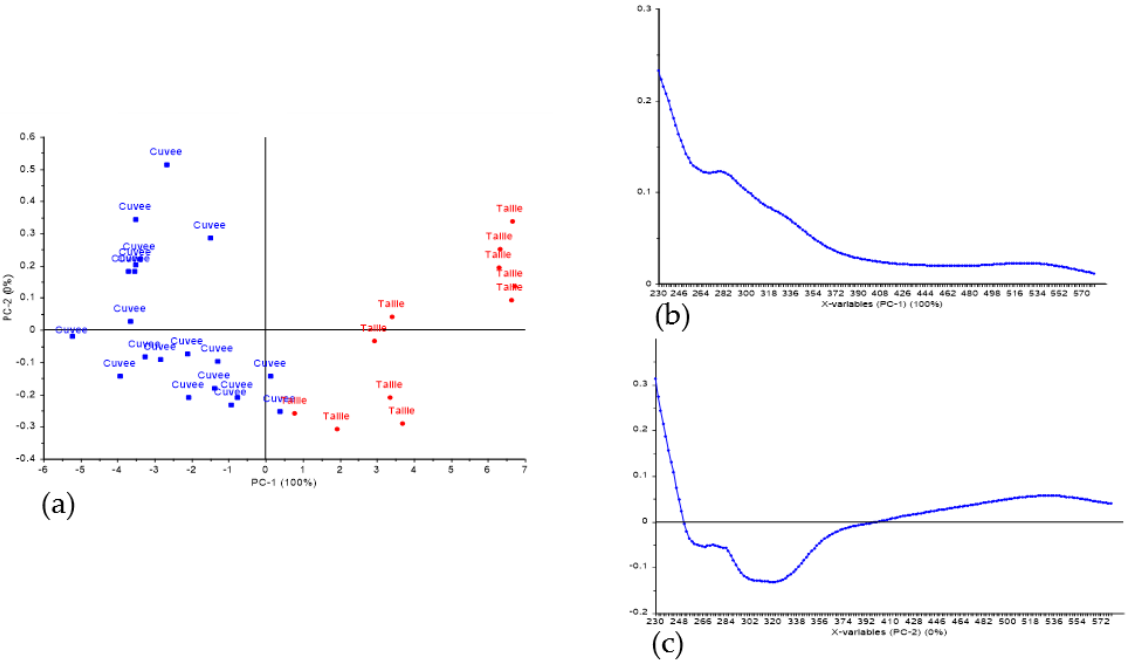

Figure 5. PCA scores and loadings plots of 2012 Pinot noir juice samples from the commercial scale trial discriminating *cuvée* from *taille*. Scores plots (**a**); PC 1 (**b**) and PC 2 (**c**) loadings.

4. Conclusions

Ultraviolet-Visible (UV-Vis) spectral phenolic fingerprinting (SPF) proved to be an effective tool when combined with PCA to qualitatively discriminate between *cuvée* (i.e., first grape juice press fraction) and *taille* (i.e., subsequent grape juice press fraction) of Chardonnay and Pinot noir grape varieties. As conventional methods for 'phenolic pick-up' (i.e., detection of drying, rough in-mouth perceptions) during grape juice press fractioning are often dependent on winemakers' subjective assessment, UV-Vis SPF could be used as a rapid, reliable, and cost-efficient objective measure for precise grape juice press fractioning. The differences observed between the experimental flat-bed press and the commercial airbag press indicates that juice phenolic composition can be strongly influenced by the pressing method. Further investigation at different ripeness levels and using a broader range of grape varieties is warranted. Finally, using information from spectral data a quantitative quality index may be developed.

Author Contributions: F.K. and R.D. conceived and designed the experiments; F.K and R.D. performed the experiments; F.K., R.D. and R.L. analyzed the data. All authors contributed to the preparation of the manuscript.

Funding: We thank the Australian Government's Industry Cooperative Innovation Program (**ANZSIC 9621**), the Tasmanian-based consortium, industry partners, Australian Wine Research Institute, Flextank, Croplands and Josef Chromy Wines.

Acknowledgments: We gratefully acknowledge Richard Smart and Angela Sparrow, formerly of the University of Tasmania, for their technical support and Karina Dambergs, formerly of Clover Hill Wines, for industry perspectives. We also thanks Matt Lowe, of Solutions in Stainless, for press co-design and construction.

Conflicts of Interest: The authors declare no conflicts of interest.

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