

Research on the improvement of the aromatic profile of white wines through maturation: study case on Chardonnay and Sauvignon Blanc cultivars

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Abstract

This research aims to improve the aromatic profile of white wines, with a special emphasis on the Chardonnay and Sauvignon Blanc cultivars, by refining maturation processes for making more complex wines that are stable and reflect varietal typicity. The main objective was to identify methods for preserving varietal aromas—fruity, floral, or vegetal notes—while enriching them with secondary and tertiary notes derived from oak barrels, fine lees, and controlled oxidation. The research findings prove that oak (by its type, toasting intensity, and tannic potential) had a significant impact on the final aroma profile. Chardonnay is more tolerant to oak aging, developing harmonious notes of vanilla, caramel, and toasted bread, whereas Sauvignon Blanc is much more sensitive: extended maturation can significantly reduce the concentration of volatile thiols, which are responsible for its distinctive tropical and vegetal aromas. Lees aging (*sur lie*) and *bâtonnage* significantly improve the flavour profile, providing flavours of brioche and butter while improving oxidative stability. Furthermore, maturation length must be carefully considered: shorter periods preserve freshness, whilst extended aging increases complexity but has the risk of reducing primary aromas. Finally, these investigations show that increasing the aromatic profile of white wines requires a balanced management of maturation processes that are adapted to the unique characteristics of each variety.

Keywords: Chardonnay, Sauvignon blanc, barrels, lees, aroma profile

Introduction

White wines play a significant position in the worldwide viticultural industry due to their freshness, balanced acidity, and aromatic richness [15]. Unlike red wines, which are frequently associated with extended maturity, white wines are usually associated with immediate consumption after bottling in order to preserve their essential grape-derived aromas [10]. However, current research and advances in enological technologies have revealed that controlled maturation can provide major benefits to white wines [20; 11].

Maturation improves the aromatic profile, stabilize volatile components, and boost mouthfeel. This process occurs in stainless steel tanks, oak barrels, or with alternate materials such chips and staves [30]. Lees aging (*sur lie*) combined with periodic stirring (*bâtonnage*) are commonly used for increasing volume, creaminess, and protecting the wine from oxidation [14]. Regarding aromatic composition, aging promotes the synthesis of esters, lactones, and phenolic compounds, which contribute to notes of vanilla, almonds, honey, toasted bread, or licorice [4]. Depending on the grape variety, secondary and tertiary aromas might perfectly balance the initial fruity or fragrant notes [8]. The maturation must be adjusted to the desired style, grape variety, and target market [29]. Several variables influence the duration and efficiency of wine maturation, including storage temperature and humidity, vessel type, acceptable oxidation level, SO₂ concentration, and the biological properties of the wine (cultivar, alcohol strength, pH, and tannin content) [23]. Depending on the desired style, maturation can last from a few months (for young wines) to several years (for premium wines with aging potential) [6;27].

The objective of the study, was to create white wines that are not only expressive and well-balanced, but also distinctive, with a particular aromatic identity and the potential to evolve successfully in the bottle. The

inclusion of aging as a strategic stage in current white wine production represents a scientific and creative approach to enology that emphasizes quality and expression of flavours.

Material and Method

The study focused on the aromatic profiles of Chardonnay and Sauvignon Blanc grape cultivars, and their development during maturation concerning the diversity of aromatic components influenced by climate, barrel oak type, oak chip toasting levels, and the yeasts involved during fermentation, specifically indigenous or selected yeasts.

The experimental trial was carried out during the 2024 growing season in the experimental plots of the USV “Mihai I” vineyard from Timișoara, Romania, on two white grape cultivars: ‘Chardonnay’ and ‘Sauvignon Blanc’. Grapes were harvested at technological maturity, determined on sugar content, total acidity, and berry tasting, ensuring representativeness for each cultivar. Harvesting was performed manually in the morning to minimize temperature-related degradation of volatile compounds. Immediately after harvest, grapes were transported under refrigerated conditions to the oenology laboratory for vinification and analysis.

The vinification protocol followed classical white winemaking techniques, including destemming, crushing, gentle pressing, cold settling of must at 10 °C for 24 h, and alcoholic fermentation at a controlled temperature of 16–18 °C using a selected *Saccharomyces cerevisiae* commercial strain. Wines were stabilized post-fermentation and stored in two-liter glass vessels under inert gas at 4 °C until analysis.

To characterize the aromatic profiles, volatile compounds were extracted by headspace solid-phase microextraction (HS-SPME) using a DVB/CAR/PDMS fibre, which provides efficient extraction of esters, higher alcohols, terpenes, norisoprenoids, and volatile sulphur compounds. Analyses were performed with gas chromatography coupled with mass spectrometry (GC–MS; Agilent 7890B GC system coupled to a 5977A MSD, Agilent Technologies, USA) equipped with a DB-Wax column (30 m × 0.25 mm × 0.25 μm). The oven program ranged from 40 °C (held 5 min) to 240 °C at 4 °C/min, with helium as carrier gas at 1.0 mL/min. MS conditions were electron impact ionization at 70 eV, with scanning from 30–350 m/z. Identification of compounds was achieved through comparison with the NIST 14 Mass Spectral Library and retention indices calculated with n-alkane standards. Quantification was carried out using calibration curves with authentic standards, with results expressed in μg/L of wine.

In addition, a sensory evaluation was conducted by a trained panel of 12 assessors, using descriptive analysis under ISO 8589 standardized conditions. Wines were evaluated for fruity, floral, vegetal, and woody aromatic descriptors, alongside overall aroma intensity and balance.

All chemical determinations were performed in triplicate, and statistical analysis of variance (ANOVA) followed by Tukey’s HSD test (p < 0.05) was conducted using Microsoft Excel 2021.

Results and Discussion

Chardonnay is one of the world’s most widely cultivated grape cultivars, distinguished by its versatility and capacity to adapt to diverse terroirs and winemaking practices [24]. Its aromatic expression can vary considerably depending on growing climate and post-harvest processing. In cool climates, Chardonnay wines often exhibit green and citrus notes such as green apple, lemon, and grapefruit, along with high acidity and occasionally minerality [7]. Under moderate temperate climate, the flavor profile tends to become rounder and more nuanced, with aromas of white peach, nectarine, and subtle floral hints [25]. In warm climates, Chardonnay may develop ripe tropical fruit characters—pineapple, mango or banana—coupled with reduced acidity and richer mouthfeel [6].

The material of the vessel for maturation also significantly influences Chardonnay’s aroma. Oak aging (in barrels or with chips) ‘borrow’ compounds like vanillin, lactones, and toasted notes, which give the wine additional complexity, such as vanilla, butter, caramel, and nutty or toasty flavors [13]. Fermentation and maturation in stainless steel preserve freshness and emphasize primary varietal fruit aromas, resulting in wines that are lighter, crisper, and more vivid in acidity [18].

Table 1. Aromatic profile of Chardonnay vs. Sauvignon Blanc

Characteristic	Chardonnay	Sauvignon Blanc
Primary aromas	Apple, peach, pineapple; vanilla notes (in oak-aged)	Green bell pepper, fresh-cut grass, grapefruit, passion fruit
Vegetal aromas	Minimal to absent	Pronounced and intense
Acidity	Medium to high	Generally high
Texture / Body	Ranges from light to full-bodied, often creamy with oak influence	Light to medium-bodied, typically crisp and refreshing

Characteristic	Chardonnay	Sauvignon Blanc
Expression of terroir	Highly adaptable; aromatic expression varies significantly with region and vinification	Strongly terroir-expressive (e.g., mineral notes in Sancerre; vegetal tones in New World regions)

Sauvignon Blanc is renowned for its distinct, powerful, and easily identifiable fragrances. This cultivar has an intense flavour, and the resulting wines are typically crisp, refreshing, and high in acidity. Sauvignon Blanc can be identified by the presence of green plant flavours, such as green bell pepper, asparagus, newly cut grass, and blackcurrant bud, which are predominantly derived from methoxypyrazines such as 3-isobutyl-2-methoxypyrazine (IBMP) [3;1]. Citrus aromas—particularly lemon, lime, and grapefruit—are also prominent. In warmer climates, Sauvignon Blanc may develop tropical fruit flavours like passion fruit and melon [16]. Regarding oak chip maturation, the aromatic complex is influenced by both the oak species and the degree of toasting of the chips. For example, aging with American oak (*Quercus alba*) tends to confer higher levels of cis-whiskey lactone and vanillin (which are associated with coconut and vanilla flavours) [9]. French oak (*Quercus robur* and *Q. petraea*) has more ellagitannins, resulting in a more balanced tannic structure while preserving primary fruit flavours. French oak also produces more delicate and complex characteristics, such as caramel, roasted almond, coffee, and spice (e.g., cinnamon and clove) [26; 19]. The toasting (or toast) level of oak chips directly transforms wood compounds, producing new fragrances. During toasting, cellulose, hemicellulose, and lignin are decomposed, generating volatile compounds such as furfural, methylfurfural, volatile phenols, and lactones [31]. As the toast level increases, studies show elevated concentrations of furfural and 5-methylfurfural (which give toasted, almond, caramel, and spicy notes), whereas lighter, less intense toasts preserve more vanillin and oak lactones (cis- and trans-whiskey lactone) [28]. The evolution of aromatic compounds depending on the degree of roasting is presented in Table 2.

Table 2. Aromatic compounds in oak chips depending on the roasting level

Toasting level	Predominant flavours	Associated chemical compounds
Light	Vanilla, caramel, fresh wood	Cis-lactone, vanillin
Medium	Vanilla, caramel, coffee, chocolate, roasted almond	Vanillin, furfural, furans
Heavy	Smoky, coffee, dark chocolate, cinnamon	Guaiacol, eugenol, furfural

Another major influence on a wine’s aromatic profile is the yeast population involved in alcoholic fermentation. Indigenous yeasts, also known as wild yeasts, are microorganisms that naturally occur on grape skins and in the winery environment. They can contribute to superior aromatic complexity because they comprise a wide range of yeast strains—including non-*Saccharomyces* species—which coexist and contribute diverse aromas such as earthy, spicy, and subtler notes. This supports the concept of *terroir*, reflecting the specific origin of the grapes [12]. However, spontaneous fermentation is less predictable and carries greater risks, such as sluggish or delayed fermentation, the development of off-aromas (e.g. acetic or volatile phenols), and reduced control over the process [22]. Wild fermentations can offer greater aromatic complexity and expression of terroir, as Franco et al. (2021) [12] studies show for seven grape cultivars in the Maule Region of Chile and found that fresh grape juice harbored a large diversity of non-*Saccharomyces* yeasts, which significantly influenced the early volatile aroma profile after 7 days of spontaneous fermentation. They noted genera such as *Hanseniaspora*, *Metschnikowia*, and *Rhodotorula* were abundant, contributing desirable aroma compounds.

Table 3. Advantages and disadvantages of indigenous vs. selected yeasts in winemaking

Characteristic	Indigenous yeasts	Selected yeasts
Control	Low; fermentation process is less predictable	High; fermentation process is controlled and consistent
Complexity	Contributes to complex, subtle aromas that express terroir	Produces clean, varietal-driven aromas with lower influence from terroir
Aromas	Earthy, spicy, and terroir-specific notes	Fruity, floral, and varietal aromas
Risks	Higher risk of slow, stuck fermentations or development of faults	Low risk; generally, ensures rapid and complete fermentation
Typical use	Natural, biodynamic, and artisanal wines	Most commercial wines

Another objective of the study was to assess the effect of oak chip type (French and American) on the evolution of key flavor components in Chardonnay wine during three-month maturation. Vanillin, furfural, and guaiacol were among the chemicals studied, all of which play important roles in defining the fragrance profile of oak-aged wines. The results suggest that vanillin levels were more evident in American oak chips. Furfural increased gradually in both options with a small dominance in French oak. Guaiacol concentrations were roughly comparable although slightly higher in French oak.

The concentration of vanillin in wines aged with American oak chips increased substantially, rising from 2.0 mg/L to 4.2 mg/L over three months; French oak chips contributed more moderately, ranging from 1.2 to 2.8 mg/L. According to Garde-Cerdán et al. (2002) [5], vanillin adds vanilla, toasted almond, and caramel flavors to full-bodied Chardonnay. This trend aligns with prior research indicating that *Quercus alba* (American oak) contains more cis- and trans-oak lactones and vanillin than *Quercus robur* or *Quercus petraea* (French oak), resulting in sweeter and more strong aromatic expressions [2].

Furfural showed a balanced progression across both treatments, with slightly higher concentrations in wines aged with French oak chips. This compound contributes notes of caramel, toasted bread, and almond, which enhance the wine's delicacy and roundness.

Similar patterns were observed by Jordão et al. (2006) [17], who reported that French oak tends to favor furfural extraction due to its denser grain structure, which promotes slower but more complex aromatic release. Guaiacol developed modestly in both treatments, with no discernible difference between American and French oak. It is associated with smoky, spicy, and charred wood notes, which provide complexity without emphasizing the varietal flavor. These findings are comparable with those of Garde-Cerdán et al. (2002) [5], who discovered that guaiacol levels are less dependent on oak species and more impacted by the level of toasting, with medium-to-heavy toasts favoring its release. Overall, the findings support the accepted idea that American wood increases sweetness and vanilla-driven notes, while French oak provides more subtle, spicy, and structural complexity, aligning well with literature on oak–wine interactions [21].

Table 4. Comparative influence of French and American oak on the aromatic profile of Chardonnay wine

Compound	French oak (<i>Q. robur</i> , <i>Q. petraea</i>)	American oak (<i>Quercus alba</i>)	Recommended style
Vanillin	Subtle, balanced expression	Intense, dominant character	Full-bodied Chardonnay
Furfural	Contributes balance and finesse	Slightly lower concentration	Classic, elegant style
Guaiacol	Delicate smoky notes	Similar, but more attenuated	Enhances aromatic complexity

The results show that oak wood—through its species type, toast level, and tannin potential—significantly influences the aromatic composition of wines. Chardonnay appears more receptive to the integration of woody notes, while Sauvignon Blanc is more sensitive to the loss of its characteristic volatile compounds. Aging on lees (“sur lies”) and ‘bâtonnage’ contributes to increased body, additional brioche and butter notes, and improved antioxidant protection in the wine.

Conclusions

Studies on enhancing the aromatic profile of white wines during maturation demonstrate that improvements depend largely on a balanced management of maturation techniques. For Chardonnay, by carefully combining oak, stainless steel, and yeast management, winemakers can obtain elegant wines that preserve varietal identity while gaining refinement and aging potential. In contrast, Sauvignon Blanc requires more precise handling to maintain its expressive character while also developing aromatic complexity. Fermentation methods play a decisive role. The choice between indigenous or selected yeasts, stainless steel tanks versus oak barrels, and maturation sur lie (in contact with lees) significantly affects the development of tertiary aromas such as vanillin, oak lactones, and esters. Temperature control and fermentation are essential variables in shaping the aromatic profile: stable temperatures between 10–15 °C favor a slow and balanced aromatic evolution.

Oak maturation contributes additional layers of complexity, while stainless steel preserves varietal freshness and typicity. The final wine style thus results from the careful assemblage of these technical decisions. For Sauvignon Blanc, achieving high concentrations of volatile thiols (3MH, 3MHA, 4MMP) requires cool climates, controlled solar exposure, harvesting during cooler hours, and, interestingly, mechanical harvesting, which has been shown to increase thiol potential.

Cold fermentation (10–15 °C) preserves the balance between green and fruity notes. While the overall density of aromas may not necessarily increase, the resulting profile tends to be more harmoniously balanced. Managing reductive conditions (H₂S control, protection from oxygen, and early SO₂ additions) is critical for stabilizing volatile thiols.

In conclusion, balanced management of maturation time and technique—integrating stainless steel with oak aging and lees contact—enables the production of expressive, complex, and stable white wines that maintain varietal typicity.

References

- [1] Baiano, A., Terracone, C., Longobardi, F., Ventrella, A., Agostiano, A., & Del Nobile, M. A. (2012), Effects of different vinification technologies on physical and chemical characteristics of Sauvignon blanc wines. *Food Chemistry*, 135(4), 2694-2701.
- [2] Canas, S., Anjos, O., Caldeira, I., & Belchior, A. P. (2019), Are the furanic aldehydes ratio and phenolic aldehydes ratios reliable to assess the addition of vanillin and caramel to the aged wine spirit? *Food Control*, 95, 77-84.
- [3] Capone, D. L., Francis, I. L., Clingeleffer, P. R., Maffei, S. M., & Boss, P. K. (2022), Evidence that methoxypyrazine accumulation is elevated in Shiraz rachis grown on Ramsey rootstock, increasing 'green'flavour in wine. *Australian Journal of Grape and Wine Research*, 28(2), 304-315.
- [4] Carpena, M., Pereira, A. G., Prieto, M. A., & Simal-Gandara, J. (2020), Wine aging technology: Fundamental role of wood barrels. *Foods*, 9(9), 1160.
- [5] Cerdán, T. G., Mozaz, S. R., & Azpilicueta, C. A. (2002), Volatile composition of aged wine in used barrels of French oak and of American oak. *Food research international*, 35(7), 603-610.
- [6] Chen, K., & Li, J. (2022), A glance into the aroma of white wine. In *White Wine Technology* (pp. 313-326). Academic Press.
- [7] Cordente, A.G., Espinase Nandorfy, D., Solomon, M., Schulkin, A., Kolouchova, R., Francis, I. L., & Schmidt, S.A. (2021), Aromatic higher alcohols in wine: Implication on aroma and palate attributes during chardonnay aging. *Molecules*, 26(16), 4979.
- [8] Dobrei, A.G., Nistor, E., Cirt, S., Mălaescu, M., Drăgulescu, A., & Dobrei, A.I. (2021), *Research concerning organic white wines production in a winery from Timis County*. JOURNAL of Horticulture, Forestry and Biotechnology. Volume 25(2), 69 – 73.
- [9] Dumitriu, G. D., Teodosiu, C., Gabur, I., Cotea, V. V., Peinado, R. A., & López de Lerma, N. (2019), *Evaluation of aroma compounds in the process of wine ageing with oak chips*. *Foods*, 8(12), 662.
- [10] Er, Y., & Atasoy, A. (2016), *The classification of white wine and red wine according to their physicochemical qualities*. *International Journal of Intelligent Systems and Applications in Engineering*, 4(Special Issue-1), 23-26.
- [11] Ferrero-del-Teso, S., Arias, I., Escudero, A., Ferreira, V., Fernández-Zurbano, P., & Sáenz-Navajas, M. P. (2020), *Effect of grape maturity on wine sensory and chemical features: The case of Moristel wines*. *Lwt*, 118, 108848.
- [12] Franco, W., Benavides, S., Valencia, P., Ramirez, C., & Urtubia, A. (2021), *Native yeasts and lactic acid bacteria isolated from spontaneous fermentation of seven grape cultivars from the maule region (Chile)*. *Foods*, 10(8), 1737.
- [13] Gambetta, J. M., Bastian, S. E., Cozzolino, D., & Jeffery, D. W. (2014), *Factors influencing the aroma composition of Chardonnay wines*. *Journal of Agricultural and Food Chemistry*, 62(28), 6512-6534.
- [14] Garcia, L., Poulain, B., Douliez, A., Naud, E., Valls-Fonayet, J., & Nioi, C. (2025), *White wine lees as a source of antioxidants: Insights into their chemical profile*. *Food Chemistry*, 146118.
- [15] Gawel, R., Smith, P. A., Cicerale, S., & Keast, R. (2018), *The mouthfeel of white wine*. *Critical reviews in food science and nutrition*, 58(17), 2939-2956.
- [16] Iobbi, A., Tomasino, E., & Di, Y. (2025), *Tropical Fruit Aroma in White Wines: Exploring the Role of Esters and Thiols in Chardonnay and Sauvignon Blanc Wines*. *Journal of Food Science*, 90(9), e70567.
- [17] Jordão, A. M., Ricardo-da-Silva, J. M., Laureano, O., Adams, A., Demyttenaere, J., Verhé, R., & De Kimpe, N. (2006), *Volatile composition analysis by solid-phase microextraction applied to oak wood used in cooperage (Quercus pyrenaica and Quercus petraea): effect of botanical species and toasting process*. *Journal of Wood Science*, 52(6), 514-521.
- [18] Liberatore, M. T., Pati, S., Del Nobile, M. A., & La Notte, E. (2010), *Aroma quality improvement of Chardonnay white wine by fermentation and ageing in barrique on lees*. *Food Research International*, 43(4), 996-1002.
- [19] Luchian, C. E., Focea, E. C., Scutarașu, E. C., Motrescu, I., Vlase, A. M., Vlase, L. & Cotea, V. (2023), *Oak aging and ultrasound treatment for improving the sensory profile of Sauvignon Blanc wines*.

In International Conference on Global Research and Education (pp. 104-121). Cham: Springer Nature Switzerland.

- [20] Lukić, I., Jedrejčić, N., Ganić, K. K., Staver, M., & Peršurić, Đ. (2015), *Phenolic and aroma composition of white wines produced by prolonged maceration and maturation in wooden barrels*. Food technology and biotechnology, 53(4), 407.
- [21] Martínez-Gil, A.M., del Alamo-Sanza, M., del Barrio-Galán, R., & Nevares, I. (2022), *Alternative woods in oenology: volatile compounds characterisation of woods with respect to traditional oak and effect on aroma in wine, a review*. Applied Sciences, 12(4), 2101.
- [22] Nisiotou, A., Sgouros, G., Mallouchos, A., Nisiotis, C. S., Michaelidis, C., Tassou, C., & Banilas, G. (2018), *The use of indigenous Saccharomyces cerevisiae and Starmerella bacillaris strains as a tool to create chemical complexity in local wines*. Food Research International, 111, 498-508.
- [23] Nistor, E., Dobrei, A. G., Mattii, G. B., & Dobrei, A. (2022), *Calcium and potassium accumulation during the growing season in Cabernet Sauvignon and Merlot grape varieties*. Plants, 11(12), 1536.
- [24] Seinform, B., Caillé, S., Nikolantonaki, M., & Saucier, C. (2025), *Evidence for Discriminant Specific Tastes in Chardonnay Wines Among Other White Wines*. Foods, 14(16), 2870.
- [25] Sereni, A., Phan, Q., Osborne, J., & Tomasino, E. (2020), *Impact of the timing and temperature of malolactic fermentation on the aroma composition and mouthfeel properties of Chardonnay wine*. Foods, 9(6), 802.
- [26] Spillman, P.J., Sefton, M.A., & Gawel, R. (2004), *The contribution of volatile compounds derived during oak barrel maturation to the aroma of a Chardonnay and Cabernet Sauvignon wine*. Australian Journal of Grape and Wine Research, 10(3), 227-235.
- [27] Swiegers, J. H., Kievit, R. L., Siebert, T., Lattey, K. A., Bramley, B. R., Francis, I. L. & Pretorius, I. S. (2009), *The influence of yeast on the aroma of Sauvignon Blanc wine*. Food microbiology, 26(2), 204-211.
- [28] Tsai, P.C., Araujo, L.D., & Tian, B. (2022), *Varietal aromas of Sauvignon Blanc: impact of oxidation and antioxidants used in winemaking*. Fermentation, 8(12), 686.
- [29] Vilela, A., Ferreira, R., Nunes, F., & Correia, E. (2020), *Creation and acceptability of a fragrance with a characteristic Tawny Port wine-like aroma*. Foods, 9(9), 1244.
- [30] White, W., & Catarino, S. (2023), *How does maturation vessel influence wine quality? A critical literature review*. Ciência e Técnica Vitivinícola, 38(2), 128-151.
- [31] Zhang, T., Liao, Z., Li, Z., Liu, Y., Bi, J., Liu, Y., & Qin, Y. (2025), *Revealing the flavor differences of Sauvignon Blanc wines fermented in different oak barrels and stainless-steel tanks through GC-MS, GC-IMS, Electronic, and Artificial Sensory Analyses*. Food Chemistry: X, 25, 102188.