DOI: https://doi.org/10.20870/oeno-one.2024.58.4.8080

OPEN ACCESS

ORIGINAL RESEARCH ARTICLE

Impact of *Botrytis cinerea* on γ-Nonalactone concentration: analysis of New Zealand white wines using SIDA-SPE-GC-MS

Gillean C. Miller[1], David Barker[1,2], Lisa I. Pilkington[1,3], Rebecca C. Deed[1,4*]

[1] School of Chemical Sciences, University of Auckland, Auckland, 1010, New Zealand
[2] The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, 6012, New Zealand
[3] Te Pūnaha Matatini, Auckland, 1142, New Zealand
[4] School of Biological Sciences, University of Auckland, Auckland, 1010, New Zealand

*correspondence:
rebecca.deed@auckland.ac.nz

Associate editor:
Maurizio Ugliano

Received:
10 April 2024

Accepted:
27 September 2024

Published:
18 October 2024

This article is published under the **Creative Commons licence** (CC BY 4.0).

Use of all or part of the content of this article must mention the authors, the year of publication, the title, the name of the journal, the volume, the pages and the DOI in compliance with the information given above.

ABSTRACT

Noble rot, caused by infection of grapes with the fungus *Botrytis cinerea*, is commonly used in the production of dessert-style white wines, imparting desirable aroma descriptors, including dried fruit, honey, and stone fruit. γ-Nonalactone is an aroma compound that is ubiquitous in wine yet has been overlooked in literature for some time. Previously, this compound has been found in higher concentrations in noble rot wines. New Zealand (NZ) is world-renowned for its high-quality white wines, particularly Sauvignon blanc; however, limited research has been carried out on the aroma features of wines produced in lower volumes, such as botrytised dessert styles, and those produced from aromatic grape varieties such as Riesling. Therefore, this work quantified γ-Nonalactone concentrations in 38 NZ commercial white wines, representing botrytised (18) and non-botrytised (20) styles, using SIDA-SPE-GC-MS. These wines were selected to represent a cross-section of NZ white wines, made from Sauvignon blanc, Riesling, and Sauvignon-Sémillon blends, and derived across a range of vintages (2014–2021), and NZ wine regions (Central Otago, Gisborne, Hawke's Bay, Marlborough, Waiheke Island, Waipara Valley, and Wairarapa). Multivariate data analyses were carried out using vitivinicultural data from wine producers, wine, and measured technical parameters and γ-Nonalactone concentrations. Analyses revealed that γ-Nonalactone concentration was significantly higher in botrytised wines (p-value = 3×10^{-8}), with a maximum of 43.5 µg L^{-1}, compared to a maximum of 8.7 µg L^{-1} in the non-botrytised samples. No significant associations were found between γ-Nonalactone concentration and region or grape variety, suggesting that the precursors to γ-Nonalactone are produced by *B. cinerea* itself, or through alterations in grape metabolism induced by *B. cinerea*. Additional research is needed to elucidate the mechanism(s) by which noble rot leads to higher γ-Nonalactone concentrations in wines.

KEYWORDS: *Botrytis cinerea*, GC-MS, New Zealand, noble rot, γ-Nonalactone, Riesling, Sauvignon blanc

INTRODUCTION

Noble rot, produced by the infection of grape species such as *Vitis vinifera*, by the Ascomycete fungus *Botrytis cinerea*, is a widespread viticultural technique used to produce high-quality dessert wine styles. Microclimatic conditions determine whether *B. cinerea* infection of grape berries will result in noble rot, or detrimental grey rot (Fournier *et al*., 2013). When vineyard conditions are appropriate, with moist nights, morning fog, and dry, sunny days, grape berries undergo shrivelling, resulting in substantial changes in the concentrations of aroma compounds and their precursors, with some increasing significantly, and others decreasing (Negri *et al*., 2017). Descriptors attributed to the resulting wines often include honey, dried fruits, stone fruits (peach and apricot), and caramel (Magyar and Soós, 2016; Vannini and Chilosi, 2013).

Botrytised wines can be made with a range of suitable grape varieties. A large proportion of research on botrytised wines has focused on the renowned Sauternes wines, made primarily with Sauvignon blanc and Sémillon (Magyar and Soós, 2016), and Hungarian Tokaji Aszú, which can be made using six different grape varieties, including Furmint (Vyviurska and Špánik, 2020). Riesling is also commonly used to produce high-quality botrytised wines, with famed examples hailing from Germany (Magyar and Soós, 2016). Previous works have highlighted the extensive sensory and chemical differences between botrytised and non-botrytised wines. Compounds produced by the fungus or the grapes themselves, due to *B. cinerea* induced changes in berry metabolism, may be responsible for these changes. Studies have looked at the composition of both the grape must and the resulting wine, either through artificial induction of *B. cinerea* infection (Negri *et al*., 2017; Wang *et al*., 2017); by harvesting grapes at two-time points, standard and late harvest times, with *B. cinerea* infection (Genovese *et al*., 2007); or by comparing botrytised and non-botrytised wines made using visually-selected grapes from the same vineyard (Tosi *et al*., 2012).

By comparing Garganega wines made from grapes withered with and without the influence of *B. cinerea*, Negri *et al*. (2017) found that a range of compounds were present in higher concentrations in wines made from botrytised grapes, including benzaldehyde, 1-octen-3-ol, lactones (sherry lactone and γ-Nonalactone), and esters (such as ethyl phenylacetate), to name a few. These differences were attributed to the influence of *B. cinerea* and were primarily associated with "spicy", "floral" and "mushroom" descriptors in these wines, compared to the "fresh fruit" attributes associated with the non-botrytised wine. Similar findings were reported by comparing wines produced from non-botrytised and artificially botrytised Chardonnay grapes. Compared to the non-botrytised wine, the botrytised wine exhibited higher concentrations of a range of aroma compounds including esters, lactones (including γ-Nonalactone), and thiols. A "dry apricot" aroma descriptor was attributed to the botrytised wine and found to be associated with several aroma compounds, including γ-Nonalactone (Wang *et al*., 2017).

Highlighted above, one potentially key aroma compound in dessert wine styles shown to be significantly impacted by noble rot infection is γ-Nonalactone. This compound, containing a five-membered lactone ring, is commonly found in a wide range of wines and is associated with coconut and stone fruit descriptors, with a relatively low odour detection threshold in wine (ODT, 30 μg L^{-1}) (Miller *et al*., 2022; Nakamura *et al*., 1988). A large survey of Australian red and white wines showed that significantly higher concentrations of γ-Nonalactone were present in noble rot wines, with a maximum of 59 μg L^{-1} (Cooke *et al*., 2009).

One possible precursor to γ-Nonalactone in botrytised wines is linoleic acid. Analysis of the extracellular matrix of *B. cinerea* germlings found that linoleic acid constituted approximately 3.6 % of the acyl glycerides present (Cooper *et al*., 2000). Incubation experiments have shown that γ-Nonalactone is produced from linoleic acid during fermentation by *Sporobolomyces odorus* and *Saccharomyces cerevisiae* yeasts, *via* lipoxygenation, yielding its 9- and 13-hydroperoxide derivatives, which are subsequently further broken down to produce γ-Nonalactone (Garbe *et al*., 2001). It, therefore, follows that during fermentation, *S. cerevisiae* could be producing high levels of γ-Nonalactone in botrytised wines from the increased linoleic acid in botrytised grapes compared to non-botrytised.

The process of fatty acid biosynthesis in plants is similar to that in fungi, with the extension of fatty acid chains through the use of acetyl-CoA (Zhang *et al*., 2022), and fatty acids are also present in grapes, being essential to plant metabolism. Of the fatty acids found in grapes, linoleic acid tends to be the most abundant, with the highest concentrations detected in the grape skins (≥ 10 % total weight), as shown by a recent study of New Zealand (NZ) Sauvignon blanc and Pinot noir grapes (Sherman *et al*., 2023). Concentrations of linoleic acid in Pinot noir grapes were higher than in Sauvignon blanc grapes (Sherman *et al*., 2023), which may explain the higher γ-Nonalactone levels generally found in dry red wines compared to dry white wines (Cooke *et al*., 2009). Fatty acids in general can have a significant impact on wine aroma when used to supplement grape must (Pinu *et al*., 2019), however, many of the processes involved in this relationship are unclear. This may be due to the misconception that the hydrophobic nature of fatty acids limits their extraction during winemaking, but this has been proven false (Sherman *et al*., 2023). Further investigation is required to understand the complex relationship between fatty acids and grape aroma, and what vitivinicultural factors may impact this relationship.

Another compound speculated to be a γ-Nonalactone precursor is 4-oxononanoic acid, supplementation with which was shown by deuterium-labelling to result in the production of γ-Nonalactone in Merlot and Cabernet-Sauvignon (de Ferron *et al*., 2020). (2*E*,4*E*)-2,4-Nonadien-1-ol was also suggested as a downstream product of the 9-hydroperoxide derivative of linoleic acid (Garbe *et al*., 2001). Neither of

these compounds nor the lipoxygenation products of linoleic acid have yet been linked to the influence of *B. cinerea*.

The impact of grape stress events on wine aroma and quality is well-documented. When grapes are stressed due to a variety of factors, including infection, water stress, extreme heat, and extreme cold, metabolic processes within the grapes are altered (Blanco-Ulate *et al*., 2015; Ma *et al*., 2021; Pons *et al*., 2017; Venios *et al*., 2020). A study of alterations in the metabolism of Sémillon grapes infected with *B. cinerea* via transcriptomic and metabolomic methods demonstrated an increase in fatty acid biosynthesis, suggested to lead to alterations in the resulting wine aroma (Blanco-Ulate *et al*., 2015). However, neither lactones nor linoleic acid were investigated specifically in this work, thus, further research is required in this area.

NZ is known worldwide for its famed Sauvignon blanc wines, with their characteristic tropical passionfruit aroma (Parr *et al*., 2007). In addition to dry table styles of Sauvignon blanc, NZ also produces high-quality noble rot white wines from this variety, often as a single variety but sometimes blended with Sémillon, as used in Sauternes (New Zealand Winegrowers Inc., 2023a). Although a significant amount of work has investigated the aroma profiles of dry styles of NZ Sauvignon blanc wines, little research has been conducted on sweeter wine styles.

Previous work by this group involved the design and synthesis of an isotopically labelled γ-Nonalactone analogue ($^2H_2{}^{13}C_2$-γ-Nonalactone, Figure 1), and its use for the quantification of γ-Nonalactone using a stable isotope dilution assay (SIDA) in a range of 12 NZ Pinot noir samples, *via* solid phase extraction-gas chromatography-mass spectrometry [SPE-GC-MS] (Miller *et al*., 2023). This robust SIDA γ-Nonalactone quantification method allows for very different wine styles, with a range of matrices (varying sugar and ethanol levels) to be analysed using a single method.

This current work aims to quantify γ-Nonalactone in a range of NZ botrytised and non-botrytised white wines, and to determine whether γ-Nonalactone concentrations are higher in noble rot wines compared to their non-botrytised counterparts. It is hypothesised that γ-Nonalactone concentration will not be significantly impacted by grape variety, region, nor vintage and that *Botrytis* influence will be the most important factor in determining γ-Nonalactone concentration.

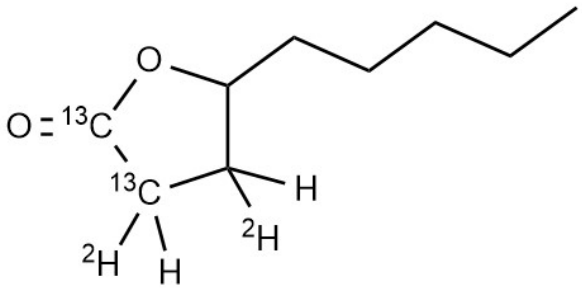


FIGURE 1. Structure of $^2H_2{}^{13}C_2$-γ-Nonalactone, used as an isotopically labelled internal standard in this work (Miller *et al.*, 2023).

MATERIALS AND METHODS

1. Chemicals and reference compounds

$^2H_2{}^{13}C_2$-γ-Nonalactone was synthesised previously according to the literature procedure (Miller *et al*., 2023). γ-Nonalactone (> 97 %) was purchased from Sigma-Aldrich (MO, USA). Sodium sulfate and all organic solvents were purchased from ECP Ltd (Auckland, NZ). Sartorius (Göttingen, Germany) Arium Pro ultrapure water system was used for Type 1 water production.

2. Analytical procedure

γ-Nonalactone was extracted and quantified in wine samples following the stable isotope dilution assay-solid phase extraction-gas chromatography-mass spectrometry (SIDA-SPE-GC-MS) method used previously, with $^2H_2{}^{13}C_2$-γ-Nonalactone as an isotopically labelled internal standard (Miller *et al*., 2023). This method was based on an additional method used for the quantification of four saturated linear aliphatic lactones in Australian wines (Cooke *et al*., 2009). Wine samples (50 mL) were spiked with internal standard (IS, 100 µL of 10,000 µg L^{-1} ethanolic solution), in triplicate. Samples were then passed through Bond Elut ENV SPE cartridges (200 mg, 3 mL), previously conditioned with methanol (2 mL) and water (4 mL). Cartridges were then washed with water (5 mL), then an aqueous solution (20 mL) of methanol (40 % v/v) and sodium bicarbonate (1 % w/v). Cartridges were allowed to dry by passing air through them for 30 min, then extracts were eluted with CH_2Cl_2 (2.5 mL). This eluate was collected and then concentrated under a gentle stream of nitrogen to a final volume of approximately 100 µL.

For analysis of samples, an Agilent 6890N Network GC coupled to an Agilent 5973 GCMS Single Quad inert mass selective detector was used. Samples (1 µL) were injected directly onto the column (Agilent HP-INNOWax, 60 m length, 0.25 internal diameter, 0.25 µm film thickness) using an Agilent 77683B Series Injector, in splitless mode. The carrier gas was He, at a flow rate of 1 mL min^{-1}. The temperature programme of the GC oven was as follows: from a starting temperature of 50 °C, the temperature was increased to 60 °C at a rate of 1 °C min^{-1}, then to 250 °C at a rate of 10 °C min^{-1}. Finally, the temperature was held at 25 °C for 25 minutes, giving a total run time of 54 minutes.

Ion monitoring was conducted in SCAN mode. For quantification of γ-Nonalactone 1, the base peaks of γ-Nonalactone and $^2H_2{}^{13}C_2$-γ-Nonalactone (*m/z* 85 and 89, respectively) were used. The relative responses of γ-Nonalactone and $^2H_2{}^{13}C_2$-γ-Nonalactone were compared to the calibration curve, with concentrations of γ-Nonalactone up to 100 µg L^{-1}. Qualifier ions used for the identification of compounds were *m/z* 99 and 114 for γ-Nonalactone and *m/z* 103 and 118 for $^2H_2{}^{13}C_2$-γ-Nonalactone.

Alcohol levels (% v/v) in commercial wine samples were analysed using an Alcolyzer Wine M from Anton Paar (Graz, Austria). pH and titratable acidity (TA) of commercial wine samples were determined using a Hanna Instruments (RI,

TABLE 1. Technical and vitivinicultural data associated with wine samples analysed in this work. (part. 1/2)

Code	Vintage	Age (years)	Grape variety	*Botrytis*	Lees ageing	Oak	Harvest	NZ region
BR1	2016	7	Riesling	Yes	No	No	Hand	Waipara Valley
BR2	2018	5	Riesling	Yes	Yes	Yes	Hand	Marlborough
BR3	2018	5	Riesling	Yes	No	No	Hand	Waipara Valley
BR4	2019	4	Riesling	Yes	No	No	Hand	Waipara Valley
BR5	2018	5	Riesling	Yes	No	No	Hand	Marlborough
BR6	2019	4	Riesling	Yes	No	Yes	Hand	Martinborough
BR7	2019	4	Riesling	Yes	No	No	Hand	Marlborough
BR8	2018	5	Riesling	Yes	No	No	Hand	Marlborough
BR9	2014	9	Riesling	Yes	No	No	Hand	Marlborough
BR10	2018	5	Riesling	Yes	No	No	Hand	Marlborough
BS1	2019	4	Sémillon	Yes	No	No	Hand	Hawke's Bay
BSB1	2015	8	Sauvignon blanc	Yes	No	No	Hand	Marlborough
BSB2	2017	6	Sauvignon blanc	Yes	No	No	Hand	Martinborough
BSB5	2018	5	Sauvignon blanc	Yes	No	No	Hand	Wairarapa
BSB6	2017	6	Sauvignon blanc	Yes	No	Yes	Hand	Marlborough
BSB7	2018	5	Sauvignon blanc	Yes	No	No	Hand	Marlborough
BSB8	2016	7	Sauvignon blanc	Yes	No	No	Hand	Hawke's Bay
BSS1	2019	4	Sauvignon blanc/ Sémillon	Yes	Yes	Yes	Hand	Waipara Valley
NR1	2019	4	Riesling	No	No	No	NS*	Marlborough
NR2	2017	6	Riesling	No	No	No	Hand	Marlborough
NSB1	2021	2	Sauvignon blanc	No	No	No	Machine	Marlborough
NSB2	2021	2	Sauvignon blanc	No	Yes	No	Hand	Marlborough
NSB3	2021	2	Sauvignon blanc	No	No	No	Machine	Gisborne
NSB4	2021	2	Sauvignon blanc	No	No	No	Machine	Marlborough
NSB5	2020	3	Sauvignon blanc	No	No	No	Machine	Marlborough
NSB6	2020	3	Sauvignon blanc	No	No	No	Machine	Marlborough
NSB7	2021	2	Sauvignon blanc	No	No	No	Machine	Marlborough
NSB8	2020	3	Sauvignon blanc/ Sémillon	No	Yes	No	Hand	Hawke's Bay
NSB9	2018	5	Sauvignon blanc	No	Yes	No	Hand	Central Otago
NSB10	2018	5	Sauvignon blanc	No	Yes	Yes	Hand	Martinborough
NSB11	2020	3	Sauvignon blanc	No	No	No	Machine	Marlborough
NSB13	2021	2	Sauvignon blanc	No	Yes	Yes	Hand	Central Otago
NSB14	2021	2	Sauvignon blanc	No	No	No	Machine	Marlborough
NSB15	2021	2	Sauvignon blanc	No	No	No	Machine	Wairarapa
NSB16	2021	2	Sauvignon blanc	No	No	No	Machine	Marlborough

TABLE 1. Technical and vitivinicultural data associated with wine samples analysed in this work. (part. 2/2)

NSB17	2020	3	Sauvignon blanc	No	No	No	Machine	Central Otago
NSS1	2018	5	Sauvignon blanc/ Sémillon	No	Yes	Yes	Hand	Waipara Valley
NSS2	2018	5	Sauvignon blanc/ Sémillon	No	Yes	Yes	Hand	Waiheke Island

*NS = not specified.

USA) Wine Titrator, equipped with a Hanna Instruments pH meter. Residual sugar (RS), free (FSO_2), and total (TSO_2) sulfite levels were determined in commercial wine samples using the Megazyme (Bray, Ireland) D-Fructose/D-Glucose Assay Kit and Total and Megazyme Free Sulfite Assay Kit, respectively.

3. Wine Samples

Thirty-eight white wines were purchased from retailers within Auckland, NZ. Wine samples represented a wide range of NZ wine-producing regions (Central Otago, Gisborne, Hawke's Bay, Marlborough, Waiheke Island, Waipara Valley, Wairarapa), vintages (2014, 2015, 2016, 2017, 2018, 2019, 2020, and 2021) and grape varieties (Riesling, Sauvignon blanc, Sémillon, and Sauvignon blanc-Sémillon blend) [Table 1]. Of the wine samples analysed, 18 were botrytised and 20 were non-botrytised, according to the information provided by the producers. All vitivinicultural data provided by winemakers, including vintage, grape variety, region, presence of *Botrytis*, lees ageing, oak use, and harvest method are shown in Table 1. All technical parameters measured in this work including RS, pH, TA, alcohol percentage, FSO_2, and TSO_2 are shown in Table 1.

4. Quantification of γ-Nonalactone in NZ white wine samples

As previously performed (Miller *et al*., 2023), calibration was conducted in model wine (12 % v/v ethanol in Type 1water, 5 g L^{-1} tartaric acid, adjusted to pH 3.2 with NaOH). Model wine samples (50 mL) were spiked with $^2H_2{}^{13}C_2$-γ-Nonalactone (100 µL, 10,000 µg L^{-1}) and a range of concentrations of γ-Nonalactone (eight concentrations, 0–100 µg L^{-1}), in triplicate. Relative peak areas of analyte and internal standard were plotted against γ-Nonalactone concentration to produce a calibration curve (R^2 = 0.9985) with a limit of detection (LOD) of 0.4 µg L^{-1}.

In triplicate for each wine, white wine samples (50 mL) were spiked with $^2H_2{}^{13}C_2$-γ-Nonalactone (100 µL, 10,000 µg L^{-1}), prior to extraction and analysis by SIDA-SPE-GC-MS. γ-Nonalactone concentrations in these samples were determined by comparing the relative peak area of γ-Nonalactone and the internal standard with the aforementioned calibration curve (Miller *et al*., 2023).

5. Statistical analysis of γ-Nonalactone concentrations alongside technical data and winemaking parameters

R: A language and environment for statistical computing [version 4.3.1] (R Core Team, 2022), and accompanying RStudio [version 2023.09.1] (RStudio Team, 2020) were used for data processing and analysis. For data visualisation, the R packages ggplot2 (version3.5.0) and factoextra (version 1.0.7) were used. To carry out statistical analyses, the base stats package (R Core Team, 2022) randomForest (version 4.7-1.1) and mdatools (version 0.14.1) were used (Kassambara and Mundt, 2020; Kucheryavskiy, 2020; Wickham, 2016). Microsoft Excel (version 2402) was used for additional data processing.

The heatmap dendrogram was produced using an agglomeration method for hierarchical cluster analysis, whereby each object was assigned to its own cluster and then proceeded iteratively, joining the two most similar clusters and continuing until there was just one cluster. Distances between clusters were calculated using the Lance-Williams dissimilarity update formula.

The final PLS-R model (number of components = 1) was chosen to minimise the cross-validation RMSE. A series of random forest models were fit to the data, using an out-of-bag cross-validation approach. In the model fitting process, 500 trees were fit for each forest model and three variables were randomly sampled at each split.

RESULTS AND DISCUSSION

A previously verified analytical method was selected for the quantification of γ-Nonalactone in NZ white wines. Considering this diversity in sample matrices, stable isotope dilution analysis was used for the quantification of γ-Nonalactone. The stability of the internal standard, $^2H_2{}^{13}C_2$-γ-Nonalactone, in wine, and the repeatability and reproducibility of this analytical method were verified, as described previously (Miller *et al*., 2023). Average γ-Nonalactone concentrations and associated standard deviation values in commercial wine samples are shown in Table 2.

Of the 36 wines analysed, 29 had γ-Nonalactone concentrations above the LOQ, and only one sample had no detectable γ-Nonalactone. All samples with γ-Nonalactone concentrations below the LOQ or LOD were non-botrytised. Therefore, the most notable factor related to the concentrations of γ-Nonalactone was associated with *Botrytis* influence; botrytised wines showed significantly higher concentrations of γ-Nonalactone, compared to non-botrytised wines (two-sample t-test, p-value = 3×10^{-8}) [Figure 2]. This result was in agreement with previous research which included seven botrytised wines in a large survey of 178 Australian wines (Cooke *et al*., 2009). The concentration of γ-Nonalactone in

TABLE 2. Average γ-Nonalactone concentrations and associated standard deviations were measured in commercial white wine samples in this work. Measured technical parameters of samples (RS, pH, TA, alcohol (Alc), TSO_2, and FSO_2) were also provided. (part. 1/2)

	γ-Nonalactone							
Code	Concentration (μg L^{-1})	Standard deviation (±) (μg L^{-1})	RS (g L^{-1})	pH	TA (g L^{-1})	Alc % (v/v)	TSO_2 (ppm)	FSO_2 (ppm)
BR1	13.02	0.27	223.10	2.98	9.15	11.3	273.93	6.91
BR2	11.89	0.18	181.12	3.41	8.69	9.3	268.55	27.81
BR3	9.07	0.14	60.37	3.26	8.82	11.7	302.57	44.67
BR4	7.80	0.13	7.19	3.12	6.18	14.0	219.51	6.08
BR5	23.37	0.30	210.85	3.62	6.92	8.8	152.98	12.30
BR6	29.30	0.56	116.87	3.46	5.87	11.2	157.26	12.74
BR7	4.04	0.13	34.85	3.23	8.35	8.9	123.64	6.95
BR8	31.28	1.69	251.98	3.65	12.20	9.0	152.79	33.31
BR9	19.00	0.31	39.86	2.95	9.05	11.4	165.61	9.89
BR10	19.67	0.50	99.53	3.23	11.10	9.1	176.78	14.79
BS1	13.60	0.76	88.75	3.30	7.16	11.8	179.96	28.38
BSB1	37.83	1.13	262.45	3.92	9.79	9.5	231.75	21.86
BSB2	32.83	1.60	148.95	3.54	9.14	10.5	400.42	50.49
BSB5	5.23	0.05	118.69	3.34	7.64	10.2	284.21	6.39
BSB6	17.79	0.44	195.63	3.71	10.70	12.3	263.04	54.63
BSB7	8.58	0.50	137.76	3.75	6.45	7.8	265.75	11.18
BSB8	43.51	0.59	127.09	3.66	8.38	11.1	189.96	32.73
BSS1	11.86	0.13	199.77	3.37	7.75	12.8	298.05	26.12
NR1	ND	-	4.71	2.82	10.10	11.4	47.19	4.63
NR2	< LOQ	-	6.08	2.74	8.29	11.2	109.30	13.45
NSB1	1.78	0.14	3.49	2.85	8.53	12.2	90.06	8.25
NSB2	< LOQ	-	1.93	3.15	8.15	11.6	93.01	5.50
NSB3	4.79	0.22	3.99	3.21	8.64	10.7	148.03	10.24

TABLE 2. Average γ-Nonalactone concentrations and associated standard deviations were measured in commercial white wine samples in this work. Measured technical parameters of samples (RS, pH, TA, alcohol (Alc), TSO_2, and FSO_2) were also provided. (part. 2/2)

NSB4	1.52	0.06	12.65	3.18	7.72	11.2	94.98	3.41
NSB5	< LOQ	-	5.18	3.14	7.28	11.1	97.67	3.06
NSB6	1.43	0.17	3.64	3.21	7.77	11.7	91.56	6.04
NSB7	< LOQ	-	3.61	3.17	7.60	12.3	126.94	4.78
NSB8	1.47	0.22	0.46	3.00	5.84	12.9	108.24	9.89
NSB9	< LOQ	-	3.30	2.77	7.06	8.7	66.68	3.47
NSB10	3.02	0.13	0.55	3.20	7.44	12.0	126.46	4.63
NSB11	1.18	0.06	3.81	3.05	5.94	11.6	88.49	15.26
NSB13	< LOQ	-	4.11	2.59	8.06	12.6	83.16	12.99
NSB14	1.85	0.13	1.05	3.32	8.45	13.6	129.12	32.73
NSB15	< LOQ	-	2.60	2.79	7.73	11.8	100.20	7.44
NSB16	< LOQ	-	4.64	2.97	7.25	11.3	114.70	3.18
NSB17	1.11	0.13	2.43	3.18	6.65	10.9	104.54	15.93
NSS1	8.67	0.31	1.85	3.21	6.79	14.0	171.86	12.16
NSS2	7.39	0.12	1.12	3.23	7.56	10.5	185.61	25.21

ND = below the limit of detection < LOQ = detected, but below the limit of quantitation (1.1 μg L^{-1}).

botrytised wines ranged from 4.1 μg L^{-1} to 43.5 μg L^{-1}, four of which were above the ODT of this compound (30 μg L^{-1}). Meanwhile, the highest concentration of γ-Nonalactone in non-botrytised wines was 8.7 μg L^{-1}, which was well below the ODT of 30 μg L^{-1} [Figure 2] (Nakamura *et al*., 1988). Again, these results are similar to those observed previously; Cooke *et al*. (2009), reported γ-Nonalactone concentrations ranging from 8.9–59.3 μg L^{-1} in botrytised samples, while in the dry white wines analysed, the highest concentration of γ-Nonalactone was 4.7 μg L^{-1} in a sample of Viognier.

The other winemaking-associated variables investigated in this study were region, vintage, grape variety, oak usage, and harvest method (hand or machine). Notably, all samples possessed the same bottle closure (screwcap), so bottle closure was not considered as a variable in this work. Oak usage and harvest method did not appear to be associated with γ-Nonalactone concentration (two-sample t-test, *p*-values > 0.05). The grape variety was generally not associated with γ-Nonalactone concentration, except for the non-botrytised Sauvignon blanc-Sémillon samples NSS1 and NSS2, which had concentrations of 8.67 and 7.39 μg L^{-1}, respectively. The γ-Nonalactone concentration in non-botrytised Sauvignon blanc-Sémillon blends was higher than the concentration in non-botrytised samples of non-Sémillon containing wines (*p*-value < 0.05, Figure 5); however, concentrations were still below the ODT of γ-Nonalactone (30 μg L^{-1}). This result suggests that there is either a varietal factor contributing to γ-Nonalactone concentration, with Sémillon grapes perhaps containing higher levels of precursors to γ-Nonalactone, or that the grapes used to make these wines had some noble rot or grey rot, which would therefore contribute to the higher concentration of γ-Nonalactone. The latter is more likely, given that Sémillon grapes tend to be reasonably susceptible to *B. cinerea* infection due to their thin cuticles, and it is not common for botrytis influence to be mentioned for dry white wines (Köycü *et al*., 2018; Paňitrur-De La Fuente *et al*., 2018). However, the number of samples of Sémillon analysed in this study was very

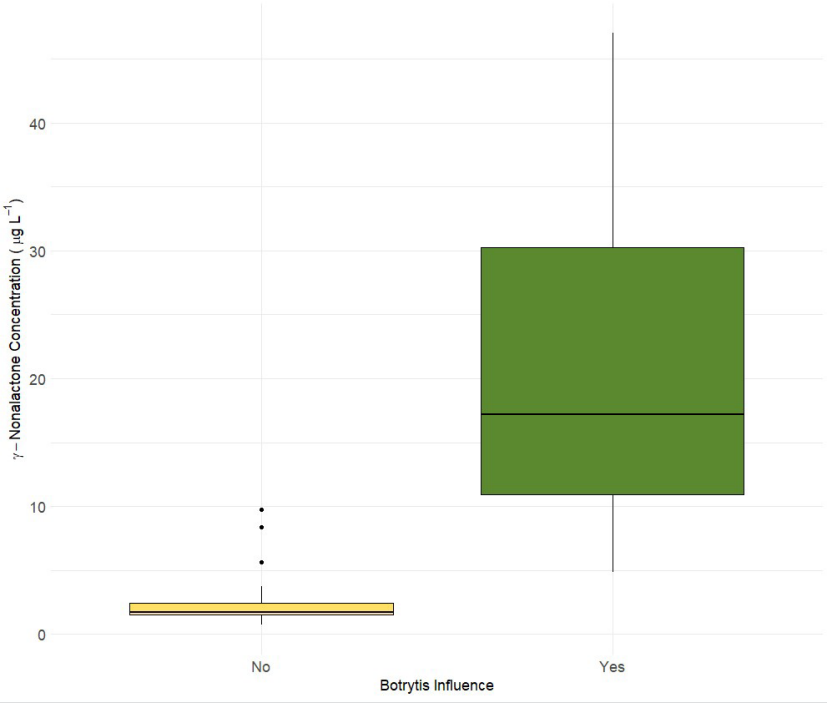


FIGURE 2. γ-Nonalactone concentration in white wine samples analysed in this work, grouped based on whether the wines were made with botrytised grapes or not. The horizontal line in the middle of each box indicates the median γ-Nonalactone concentration in the corresponding group, while the boxes themselves represent the interquartile range of the γ-Nonalactone concentration of each group.

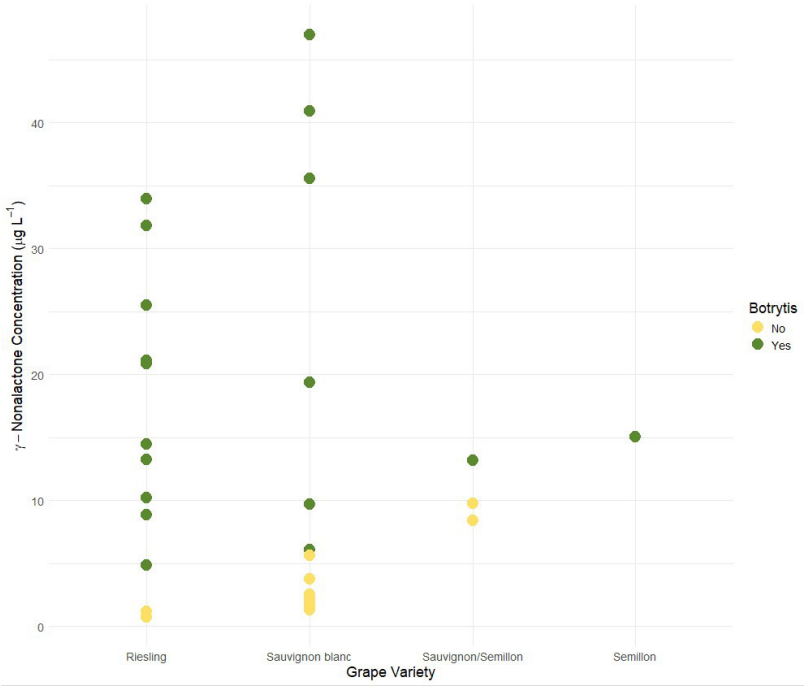


FIGURE 3. γ-Nonalactone concentration in white wine samples analysed in this work, arranged by grape variety.

limited, reflecting the low abundance of this grape variety in NZ winemaking (< 0.1 % of grapes in 2022, by mass) (New Zealand Winegrowers Inc., 2023b). Notably, γ-Nonalactone concentration was relatively low in the non-botrytised Sauvignon blanc samples analysed, suggesting that this aroma compound is unlikely to contribute to the acclaimed aroma of NZ Sauvignon blanc (Parr *et al.*, 2007).

Residual sugar in the botrytised wines ranged from off-dry (7.2 g L^{-1}) in an unusual style of botrytised Riesling (BR4) to sweet (262.5 g L^{-1}), and alcohol percentage ranged from 7.8 to 14.0 % (v/v). The non-botrytised wines were dry or off-dry (0.6 to 12.7 g L^{-1} RS) with alcohol levels ranging from 8.7 to 14.0 % (v/v). pH was, on average, higher in the botrytised wines compared to the non-botrytised wines

(two-sample t-test, p-value = 3.6×10^{-5}). There was some evidence that TA was higher in botrytised samples (two-sample t-test, p-value = 0.068). These relationships were demonstrated via principal component analysis (PCA), hierarchical clustering analysis (HCA), partial-least-squares regression (PLS-R), and random forest methods. For a more comprehensive analysis of the data collected, to determine relationships between different factors, PCA was carried out (Figure 4). Principal components 1 and 2 accounted for 53.6 % and 13.9 % of variability in the data, respectively, indicating a notable portion of the variability in the wine profile could be captured when analysing these principal components. PCA showed that, as expected, RS and TA were positively correlated with γ-Nonalactone concentration. This association can be explained by the strong links between these parameters and *Botrytis* influence. Botrytised wines commonly have higher RS levels (fructose and glucose) due to the concentration of sugars during grape berry infection and resulting shrivelling (Magyar and Soós, 2016). TA tends to be higher in dessert-style wines, to balance the high sugar levels. Unexpectedly, in the PCA the pH and TA appeared to be weakly correlated, according to Figure 4. This relationship was further investigated with correlation tests (Pearson and Spearman tests), which showed that contrary to what is suggested by the PCA, pH, and TA were not significantly correlated (p-values = 0.2 and 0.3, respectively). It is also worth mentioning that PCA can indicate weak correlations between variables that are not necessarily present when all the data is considered, with principal components only accounting for a set amount of variation in the data. Lower alcohol levels were generally present in wines with higher γ-Nonalactone concentration, which is consistent with the expectation that higher-sugar botrytised wines do not tend to be fermented to dryness, and fermentation is often stopped early via the addition of sulfur dioxide (Magyar, 2011). However, the statistical significance of the relationship between alcohol % and γ-Nonalactone concentration was none-to-weak (Spearman correlation test, p-value = 0.09). γ-Nonalactone concentration was found to be significantly positively correlated to FSO_2 and TSO_2 in the wines analysed (Spearman correlation test, p-values = 5×10^{-5} and 3×10^{-7}, respectively). This is not unexpected, as sweet wines are permitted to have higher levels of SO_2 in NZ (Giacosa *et al*., 2019).

Interestingly, year of vintage was shown to be negatively correlated with γ-Nonalactone concentration, with older samples having higher γ-Nonalactone concentrations. This result may be due to the limitations of commercially available wines at the time this study was carried out. Non-botrytised samples were mainly available from more recent vintages (mainly 2020–2021), compared to the older botrytised samples from 2014–2019. Therefore, it is hypothesised that this relationship is related to confounding of vintage and *Botrytis* influence, rather than reflecting an actual vintage-related trend. The possibility of wine ageing having an impact on the concentration of γ-Nonalactone has previously been evaluated in the scientific literature. Analyses of Malvasia and Moscato white wines before and after bottle storage for 18 months showed that the concentration of γ-Nonalactone decreased significantly in both wines (Del Caro *et al*., 2014). Further work to investigate the negative correlation between γ-Nonalactone concentration and vintage could include a longitudinal study, looking at dry and botrytised Sauvignon blanc wines over successive years and determining if there is a significant trend between vintages.

Two-way analysis of variance (ANOVA) was carried out to explore the relationships between γ-Nonalactone concentration and the variables *Botrytis*, vintage, oak, and harvest method. Two-way effects between these variables were also assessed. None of the two-way effects on γ-Nonalactone concentration

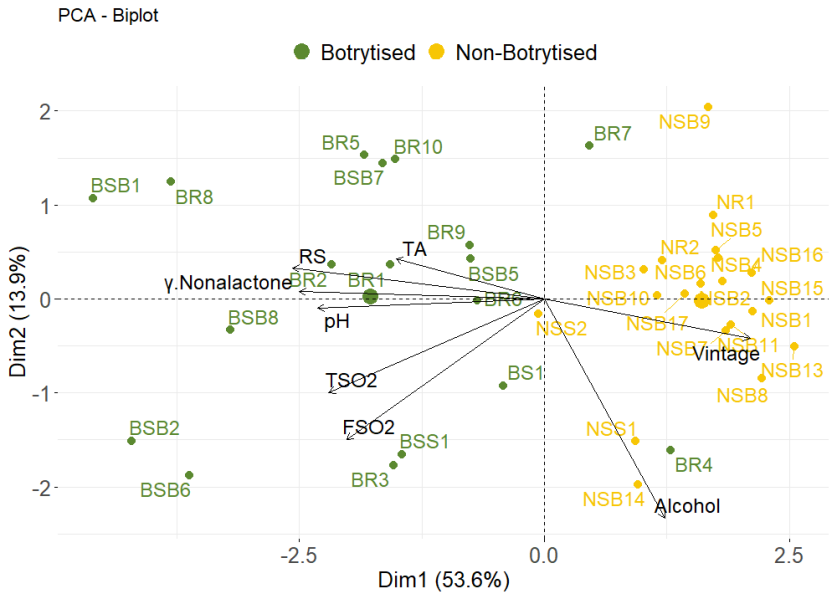


FIGURE 4. PCA visualising relationships between studied winemaking variables (alcohol level, free and total SO_2, pH, TA, RS, vintage) and γ-Nonalactone concentration. Samples are coloured according to whether they are botrytised (green) or non-botrytised (yellow).

were statistically significant, (p-values > 0.05), and nor were the main effects of oak or harvest method (p-value > 0.05). The only significant effects were observed for vintage and *Botrytis* (p-values = 3×10^{-6} and 0.002, respectively), which was in line with observations from the PCA in Figure 4.

To explore how the winemaking variables and γ-Nonalactone concentration were related to other wine parameters, the PCA scores plots showing the samples were coloured according to *Botrytis* influence or lack thereof, grape variety used, oak usage, and harvest method (Figure 5A-D). Ellipses to represent 95 % confidence levels associated with these groups are shown. Figure 5A shows the non-botrytised samples are much more tightly clustered compared to the botrytised samples. While there is an overlap of the 95 % ellipses for the groups, the botrytised wines were almost exclusively to the left of the PCA scores plot and the non-botrytised to the right. Based on the loadings for the PCA, it can be said that the botrytised wines were from later vintages, as discussed above, and had higher γ-Nonalactone concentration, pH, TA, and RS.

The other variables visualised, grape variety (Figure 5B), oak usage (Figure 5C) and harvest method (Figure 5D) do not show distinct separate clusters. In literature, grape variety has been demonstrated to have a significant impact on lactone concentrations, particularly in red wines, evidenced in studies directly comparing volatile profiles of different red grape wines (de Ferron *et al*., 2020; Fan *et al*., 2010; Martínez-Pinilla *et al*., 2013). Varietal differences are likely due to differences in concentrations of precursors in the grapes (de Ferron *et al*., 2020). However, as dry white wines generally tend to have low concentrations of γ-Nonalactone, this relationship appears to be less prevalent in white wines, as evidenced in work by Cooke *et al*. in the analysis of Australian white wines (Cooke *et al*., 2009). Alternatively, or perhaps in addition to this factor, different treatments of grapes during winemaking, such as extended maceration commonly used in red wine production, may enable increased extraction of γ-Nonalactone precursors, resulting in higher concentrations of this compound in the finished wine.

The use of oak during winemaking is a widespread practice within the wine industry and is known to impart aroma compounds to the wine, including oak lactone, which is similar in chemical structure to γ-Nonalactone (Piggott *et al*., 1995). Perhaps due to this structural similarity, γ-Nonalactone has been suggested to be extracted from oak during wine ageing (Jarauta *et al*., 2005). Based on this theory, it might be expected that the wines in this study which have had oak exposure during winemaking, either through fermentation in barrel and/or maturation, would have higher concentrations of γ-Nonalactone. During winemaking, there are also many different options for oak usage, such as using new oak or old oak, duration of oak exposure, the portion of wine exposed to oak, the oak source (American and French), oak species, or the level of toast the oak has (Garde-Cerdán and Ancín-Azpilicueta, 2006). Unfortunately, the information on oak use in the production of the wines analysed in this study was very limited, and the data was consequently reduced to a simple "yes" or "no" concerning the use of oak. The current results suggest that oak is unlikely to influence γ-Nonalactone concentration in wine, but further study using controlled types and amounts of oak during winemaking would enable a better assessment of whether this is truly the case.

The harvest method was classified in this work as either hand harvesting or machine harvesting. Generally, botrytised grapes are hand-harvested and visually selected depending on the extent of *B. cinerea* infection, and the desired wine style (Magyar, 2011). On the other hand, non-botrytised grapes are commonly machine-harvested in NZ, particularly for varieties such as Sauvignon blanc. This technique is chosen because it is faster than hand harvesting, allows grapes to be processed more quickly, and retains positive fruity attributes that are characteristic of the variety (Parr *et al*., 2013). The machine-harvested samples in this study are more tightly clustered and situated more to the right of the scores plot (Figure 5D), compared to the hand-harvested samples. This is likely indicative of the typicity of non-botrytised machine-harvested New Zealand Sauvignon blanc.

An additional method, hierarchical cluster analysis (HCA), was employed to explore the measured wine properties and the white wines analysed in this research. HCA allowed the construction of a heatmap from the known numerical data and the grouping of samples based on the similarity of their observed properties (Figure 6). In the HCA, as shown in Figure 7, four distinct clusters were formed. Except for samples BR7, NSS1, and NSS2, it can be seen that all of the botrytised samples were clustered separately from non-botrytised clusters. Closer examination of these samples reveals that BR7 had the lowest concentration of γ-Nonalactone of all the botrytised samples (4.04 μg L^{-1}) which may be contributing to its clustering with non-botrytised samples with similarly low γ-Nonalactone concentrations. BR7 also has a relatively low RS concentration (35 g L^{-1}) compared to the mean (139 g L^{-1}) and median (132 g L^{-1}) RS concentrations in the botrytised samples. Generally, in agreement with previous analyses, the red, purple, and orange groupings (primarily botrytised samples, shown in Figure 6) exhibited higher concentrations of γ-Nonalactone, while the latter two groups exhibited higher concentrations of FSO_2, TSO_2, and RS, based on the heat map. The orange and purple groups appear to be separated based on their RS, γ-Nonalactone concentration, and TA to some extent. The results of these analyses further demonstrate the main grouping within the samples is due to the presence or absence of *B. cinerea* during winemaking.

PCA and HCA are unsupervised statistical techniques that do not take into account any response (*i.e*., γ-Nonalactone). As an additional statistical approach, the supervised modelling techniques, partial least-squares regression (PLS-R), and random forest analyses were also carried out. These models were created to understand variables that were most closely linked to γ-Nonalactone concentration, by having γ-Nonalactone as the response and the range of explanatory variables being alcohol %, FSO_2, pH, RS, TA, TSO_2, and vintage. The PLS-R model appeared to fit the data well, with excellent agreement between the actual and predicted values (Figure S2D). In the developed PLS-R model, RS

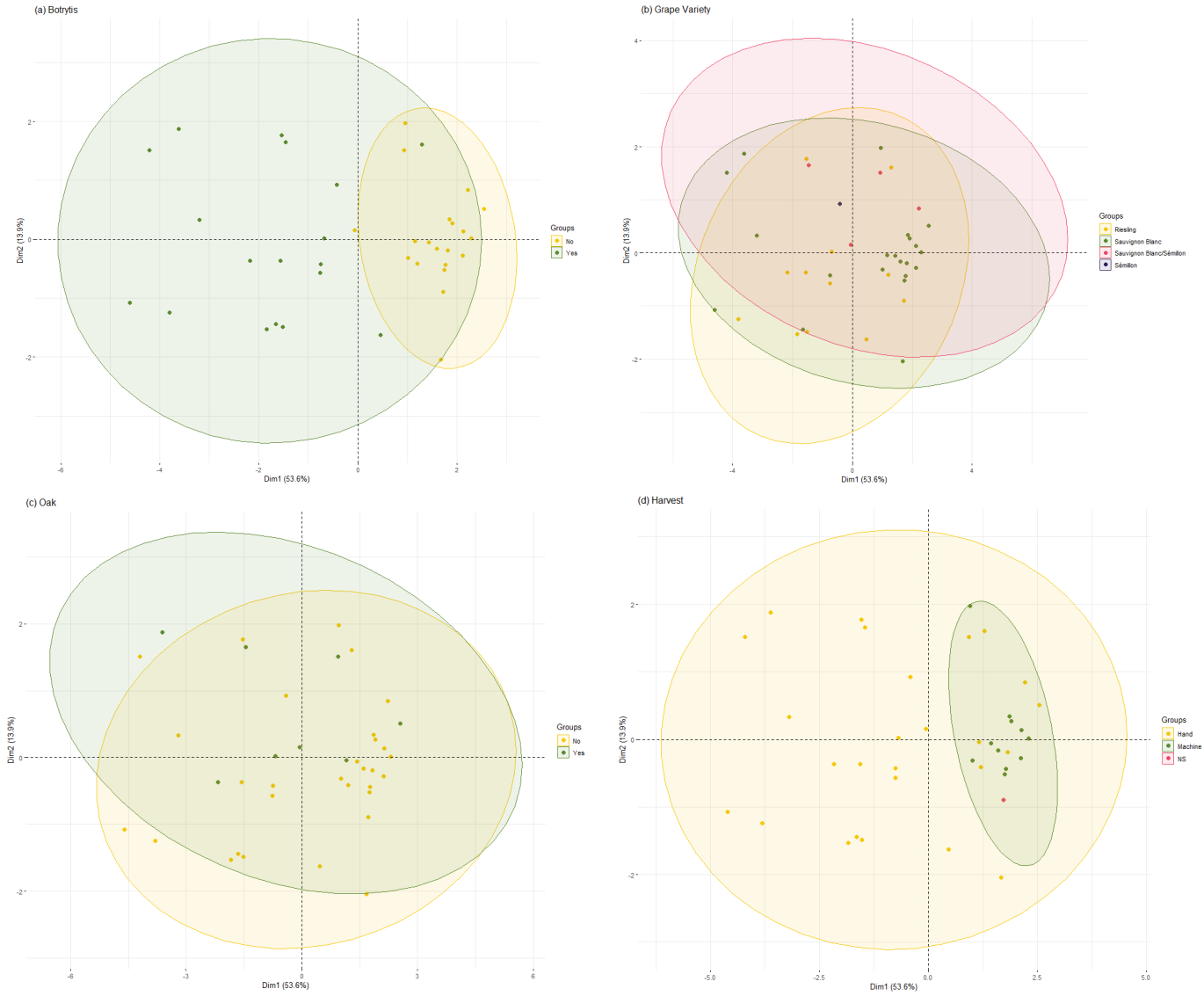


FIGURE 5A-D. PCA scores plots with white wine samples coloured according to wine-related properties and the PCA shown in Figure 4. The 95 % ellipsoids represent clusters based on key variables (A) *Botrytis cinerea* presence, (B) grape variety, (C) oak use, and (D) harvest method. Colours corresponding to categories are provided in the figure legends. In (D) "NS" refers to "not specified" where the data was not available from the wine's technical data.

and pH were the strongest numerical explanatory variables for the response variable (γ-Nonalactone concentration), whilst vintage and both free and total SO_2 were correlated with higher γ-Nonalactone concentration based on their variable importance (VIP) and selectivity ratios (Figure S2E and S2F). Random Forest models were also developed with γ-Nonalactone concentration as the response. Several random forest models were fit, with these generally corroborating the importance of the parameters highlighted in the PLS-R model, with pH and RS again being the strongest predictors (Figure S3).

CONCLUSION

This work provides the foundation for further research into γ-Nonalactone origins in wines and has corroborated the trend of higher concentrations of γ-Nonalactone being present in botrytised white wines compared to non-botrytised white wines, while the region of wine production, grape variety, oak usage, and harvest method do not appear to have a significant impact. This research also showed that NZ botrytised and non-botrytised white wines show similar trends in γ-Nonalactone concentration, compared to those produced in other countries, such as Australia (Cooke *et al*., 2009).

The mechanisms behind the possible relationship between γ-Nonalactone concentration and noble rot have yet to be fully investigated. The higher concentrations of γ-Nonalactone in dry red wines compared to dry white wines found in other works suggest the presence of some precursors in grapes which are more highly concentrated in red grapes (Cooke *et al*., 2009; Miller *et al*., 2023) or are extracted to a greater extent during the production of red wines. The presence of *B. cinerea* may alter the concentrations of precursors

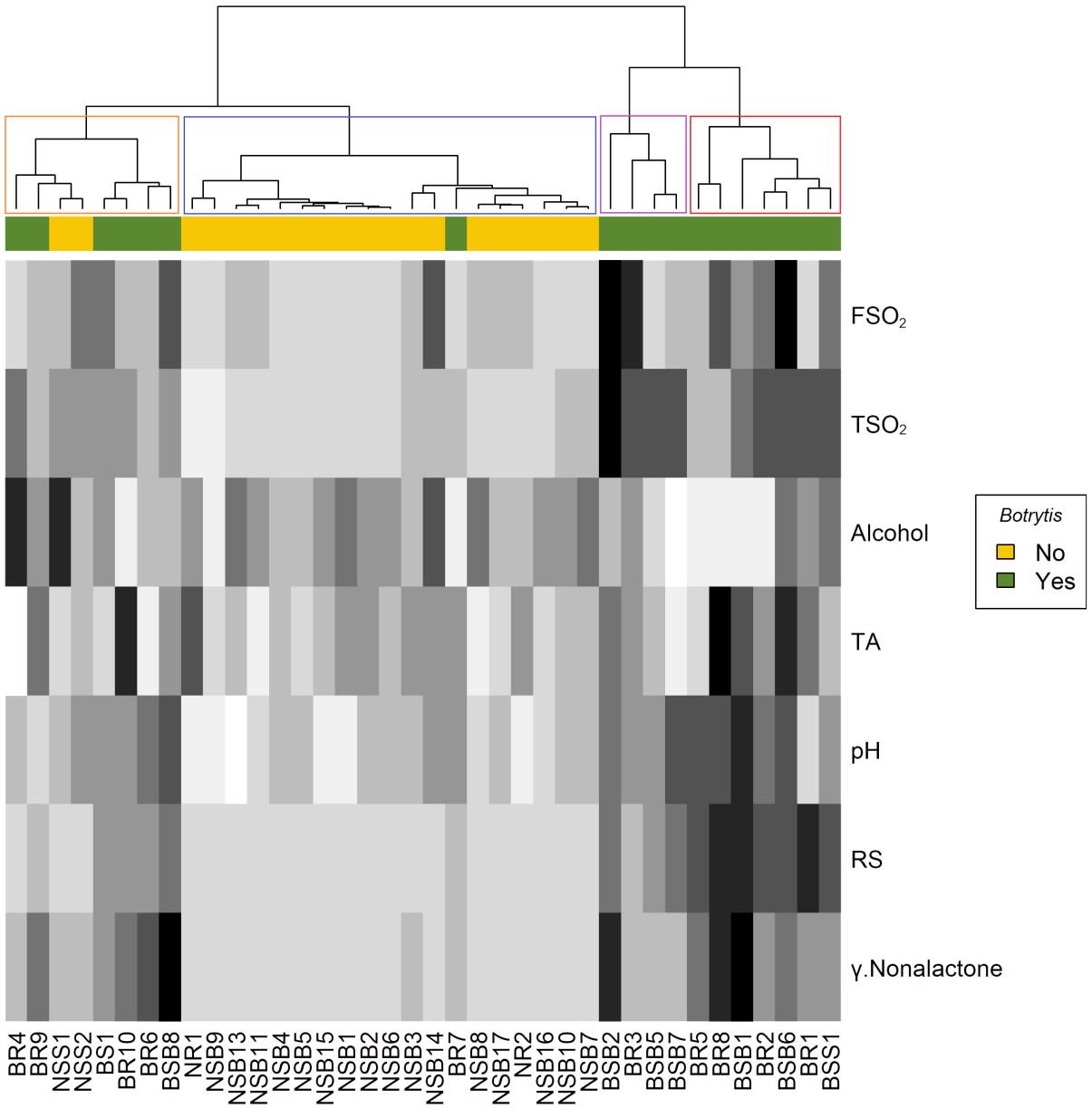


FIGURE 6. Heatmap visualising the interaction of different winemaking and chemical variables (γ-Nonalactone concentration, region, vintage, grape variety, oak usage, and harvest method). Clusters are indicated by the coloured boxes in the dendrogram.

present in white grapes, either through the production of precursors, such as linoleic acid, by the fungus itself, and/or effected alterations in grape metabolism, leading to increased concentrations of precursors (also possibly including linoleic acid) or γ-Nonalactone itself. Additionally, physical changes induced by *B. cinerea* infection of grapes may induce greater extraction of γ-Nonalactone precursors whilst grapes are still on the vine.

It is worth considering whether there is any relationship between γ-Nonalactone and grape stress in future studies. In this case, the identification of γ-Nonalactone precursors in grapes could be useful markers of grape stress for winemakers. Particularly with the prospect of climate change impacting wine aroma by creating more stressful events for grapevines, it will be important to have a thorough understanding of the mechanisms by which this may occur.

ACKNOWLEDGMENTS

This research was undertaken with the assistance of the University of Auckland Doctoral Scholarship, and the Frederick Douglas Brown Postgraduate Science Research Scholarship (G.C.M). The Faculty Research Development Fund (FRDF) was also received for this work (R.C.D.). Thanks also to Jennifer Muhl for assistance with collecting technical data for the commercial white wines analysed in this work.

AUTHOR CONTRIBUTION

G.C.M.: Conceptualisation, methodology, formal analysis, investigation, writing-original draft, writing-review & editing, visualisation. D.B.: resources, writing-review & editing, supervision. L.I.P.: Methodology, resources, writing-review & editing, visualisation, supervision. R.C.D.: Conceptualisation, resources, writing-review & editing, project administration, writing-review & editing, supervision, funding acquisition.

REFERENCES

Blanco-Ulate, B., Amrine, K. C. H., Collins, T. S., Rivero, R. M., Vicente, A. R., Morales-Cruz, A., Doyle, C. L., Ye, Z., Allen, G., Heymann, H., Ebeler, S. E., & Cantu, D. (2015). Developmental and Metabolic Plasticity of White-Skinned Grape Berries in Response to *Botrytis cinerea* during Noble Rot. *Plant Physiology*, *169*(4), 2422–2443. https://doi.org/10.1104/pp.15.00852

Cooke, R. C., Capone, D. L., van Leeuwen, K. A., Elsey, G. M., & Sefton, M. A. (2009). Quantification of Several 4-Alkyl Substituted γ-Lactones in Australian Wines. *Journal of Agricultural and Food Chemistry*, *57*(2), Article 2. https://doi.org/10.1021/jf8026974

Cooper, L. L. D., Oliver, J. E., De Vilbiss, E. D., & Doss, R. P. (2000). Lipid composition of the extracellular matrix of *Botrytis cinerea* germlings. *Phytochemistry*, *53*(2), Article 2. https://doi.org/10.1016/S0031-9422(99)00495-1

de Ferron, P., Thibon, C., Shinkaruk, S., Darriet, P., Allamy, L., & Pons, A. (2020). Aromatic Potential of Bordeaux Grape Cultivars: Identification and Assays on 4-Oxononanoic Acid, a γ-Nonalactone Precursor. *Journal of Agricultural and Food Chemistry*, *68*(47), 13344–13352. https://doi.org/10.1021/acs.jafc.0c04171

Del Caro, A., Piombino, P., Genovese, A., Moio, C., & Piga, A. (2014). Effect of Bottle Storage on Colour, Phenolics and Volatile Composition of Malvasia and Moscato White Wines. *South African Journal of Enology and Viticulture*, *35*(1), 128-138. https://doi.org/10.21548/35-1-992

Fan, W., Xu, Y., Jiang, W., & Li, J. (2010). Identification and Quantification of Impact Aroma Compounds in 4 Nonfloral *Vitis vinifera* Varieties Grapes. *Journal of Food Science*, *75*(1), S81–S88. https://doi.org/10.1111/j.1750-3841.2009.01436.x

Fournier, E., Gladieux, P., & Giraud, T. (2013). The 'Dr Jekyll and Mr Hyde fungus': Noble rot versus gray mold symptoms of *Botrytis cinerea* on grapes. *Evolutionary Applications*, *6*(6), 960–969. https://doi.org/10.1111/eva.12079

Garbe, L.-A., Lange, H., & Tressl, R. (2001). Biosynthesis of γ-Nonalactone in Yeast. In *Aroma Active Compounds in Foods*. American Chemical Society, 794, 176–182. https://doi.org/10.1021/bk-2001-0794.ch014

Garde-Cerdán, T., & Ancín-Azpilicueta, C. (2006). Review of quality factors on wine ageing in oak barrels. *Trends in Food Science & Technology*, *17*(8), 438–447. https://doi.org/10.1016/j.tifs.2006.01.008

Genovese, A., Gambuti, A., Piombino, P., & Moio, L. (2007). Sensory properties and aroma compounds of sweet Fiano wine. *Food Chemistry*, *103*(4), Article 4. https://doi.org/10.1016/j.foodchem.2006.10.027

Giacosa, S., Río Segade, S., Cagnasso, E., Caudana, A., Rolle, L., & Gerbi, V. (2019). SO_2 in Wines. In A. Morata (Ed.), *Red Wine Technology*. Academic Press. 309–321. https://doi.org/10.1016/B978-0-12-814399-5.00021-9

Jarauta, I., Cacho, J., & Ferreira, V. (2005). Concurrent Phenomena Contributing to the Formation of the Aroma of Wine during Aging in Oak Wood: An Analytical Study. *Journal of Agricultural and Food Chemistry*, *53*(10), 4166–4177. https://doi.org/10.1021/jf0481960

Kassambara, A., & Mundt, F. (2020). *factoextra: Extract and Visualize the Results of Multivariate Data Analyses* (1.0.7) [Computer software]. https://CRAN.R-project.org/package=factoextra

Köycü, N., Özer, C., Solak, E., Delen, N., & Tarihi, G. (2018). Infection of *Botrytis cinerea* in Different Fungicide Application Programs in Semillon Grape. *Journal of Tekirdag Agricultural Faculty*, *15*, 15.

Kucheryavskiy, S. (2020). Mdatools – R package for chemometrics. *Chemometrics and Intelligent Laboratory Systems*, *198*, 103937. https://doi.org/10.1016/j.chemolab.2020.103937

Ma, Y., Xu, Y., & Tang, K. (2021). Aroma of Icewine: A Review on How Environmental, Viticultural, and Oenological Factors Affect the Aroma of Icewine. *Journal of Agricultural and Food Chemistry*, *69*(25), 6943–6957. https://doi.org/10.1021/acs.jafc.1c01958

Magyar, I. (2011). Chapter 6—Botrytized Wines. In R. S. Jackson (Ed.), *Advances in Food and Nutrition Research* (). Academic Press. 63, 147–206. https://doi.org/10.1016/B978-0-12-384927-4.00006-3

Magyar, I., & Soós, J. (2016). Botrytized wines – current perspectives. *International Journal of Wine Research*, *8*, 29–39. https://doi.org/10.2147/IJWR.S100653

Martínez-Pinilla, O., Guadalupe, Z., Ayestarán, B., Pérez-Magariño, S., & Ortega-Heras, M. (2013). Characterization of volatile compounds and olfactory profile of red minority varietal wines from La Rioja. *Journal of the Science of Food and Agriculture*, *93*(15), 3720–3729. https://doi.org/10.1002/jsfa.6211

Miller, G. C., Barker, D., Pilkington, L. I., & Deed, R. C. (2023). Synthesis of a novel isotopically labelled standard for quantification of γ-Nonalactone in New Zealand Pinot noir via SIDA-SPE-GC–MS. *Analytical and Bioanalytical Chemistry*, *415*(20), 5035–5047. https://doi.org/10.1007/s00216-023-04789-2

Miller, G. C., Pilkington, L. I., Barker, D., & Deed, R. C. (2022). Saturated Linear Aliphatic γ- and δ-Lactones in Wine: A Review. *Journal of Agricultural and Food Chemistry*, *70*(49), 15325–15346. https://doi.org/10.1021/acs.jafc.2c04527

Nakamura, S., Crowell, E. A., Ough, C. S., & Totsuka, A. (1988). Quantitative Analysis of γ-Nonalactone in Wines and Its Threshold Determination. *Journal of Food Science*, *53*(4), Article 4. https://doi.org/10.1111/j.1365-2621.1988.tb13578.x

Negri, S., Lovato, A., Boscaini, F., Salvetti, E., Torriani, S., Commisso, M., Danzi, R., Ugliano, M., Polverari, A., Tornielli, G. battista, & Guzzo, F. (2017). The Induction of Noble Rot (*Botrytis cinerea*) Infection during Postharvest Withering Changes the Metabolome of Grapevine Berries (*Vitis vinifera* L., cv. Garganega). *Frontiers in Plant Science*, *8*. https://doi.org/10.3389/fpls.2017.01002

New Zealand Winegrowers Inc. (2023a). *New Zealand Wine: A comprehensive guide to the regions and varieties*. https://www.nzwine.com/en/trade/learning/textbook/

New Zealand Winegrowers Inc. (2023b). *NZ Winegrowers Annual Report 2022*. https://www.nzwine.com/en/media/statistics/annual-report/

Paňitrur-De La Fuente, C., Valdés-Gómez, H., Roudet, J., Acevedo-Opazo, C., Verdugo-Vásquez, N., Araya-Alman, M., Lolas, M., Moreno, Y., & Fermaud, M. (2018). Classification of winegrape cultivars in Chile and France according to their susceptibility to *Botrytis cinerea* related to fruit maturity. *Australian Journal of Grape and Wine Research*, *24*(2), 145–157. https://doi.org/10.1111/ajgw.12315

Parr, W. V., Green, J. A., White, K. G., & Sherlock, R. R. (2007). The distinctive flavour of New Zealand Sauvignon blanc: Sensory characterisation by wine professionals. *Food Quality and Preference*, *18*(6), 849–861. https://doi.org/10.1016/j.foodqual.2007.02.001

Parr, W. V., Schlich, P., Theobald, J. C., & Harsch, M. J. (2013). Association of selected viniviticultural factors with sensory and chemical characteristics of New Zealand Sauvignon blanc wines. *Food Research International*, *53*(1), 464–475. https://doi.org/10.1016/j.foodres.2013.05.028

Piggott, J. R., Conner, J. M., & Melvin, J. L. (1995). The contribution of oak lactone to the aroma of wood-aged wine. In G. Charalambous (Ed.), *Developments in Food Science*. Elsevier. *37*, 1695–1702. https://doi.org/10.1016/S0167-4501(06)80258-X

Pinu, F. R., Villas-Boas, S. G., & Martin, D. (2019). Pre-fermentative supplementation of fatty acids alters the metabolic activity of wine yeasts. *Food Research International*, *121*, 835–844. https://doi.org/10.1016/j.foodres.2019.01.005

Pons, A., Allamy, L., Schüttler, A., Rauhut, D., Thibon, C., & Darriet, P. (2017). What is the expected impact of climate change on wine aroma compounds and their precursors in grape? *OENO One*, *51*(2), Article 2. https://doi.org/10.20870/oeno-one.2017.51.2.1868

R Core Team. (2022). *R: A language and environment for statistical computing*. [Computer software]. R Foundation for Statistical Computing. https://www.R-project.org/

RStudio Team. (2020). *RStudio: Integrated Development for R* [Computer software]. http://www.rstudio.com/

Sherman, E., Yvon, M., Grab, F., Zarate, E., Green, S., Bang, K. W., & Pinu, F. R. (2023). Total Lipids and Fatty Acids in Major New Zealand Grape Varieties during Ripening, Prolonged Pomace Contacts and Ethanolic Extractions Mimicking Fermentation. *Fermentation*, *9*(4), Article 4. https://doi.org/10.3390/fermentation9040357

Tosi, E., Fedrizzi, B., Azzolini, M., Finato, F., Simonato, B., & Zapparoli, G. (2012). Effects of noble rot on must composition and aroma profile of Amarone wine produced by the traditional grape withering protocol. *Food Chemistry*, *130*(2), Article 2. https://doi.org/10.1016/j.foodchem.2011.07.053

Vannini, A., & Chilosi, G. (2013). Botrytis Infection: Grey Mould and Noble Rot. In *Sweet, Reinforced and Fortified Wines*. John Wiley & Sons, Ltd. 159-169. https://doi.org/10.1002/9781118569184.ch11

Venios, X., Korkas, E., Nisiotou, A., & Banilas, G. (2020). Grapevine Responses to Heat Stress and Global Warming. *Plants*, *9*(12), Article 12. https://doi.org/10.3390/plants9121754

Vyviurska, O., & Špánik, I. (2020). Assessment of Tokaj varietal wines with comprehensive two-dimensional gas chromatography coupled to high resolution mass spectrometry. *Microchemical Journal*, *152*, 104385. https://doi.org/10.1016/j.microc.2019.104385

Wang, X., Tao, Y., Wu, Y., An, R., & Yue, Z. (2017). Aroma compounds and characteristics of noble-rot wines of Chardonnay grapes artificially botrytized in the vineyard. *Food Chemistry*, *226*, 41–50. https://doi.org/10.1016/j.foodchem.2017.01.007

Wickham, H. (2016). *ggplot2: Elegant Graphics for Data Analysis*. Springer-Verlag New York. https://ggplot2.tidyverse.org

Zhang, X.-Y., Li, B., Huang, B.-C., Wang, F.-B., Zhang, Y.-Q., Zhao, S.-G., Li, M., Wang, H.-Y., Yu, X.-J., Liu, X.-Y., Jiang, J., & Wang, Z.-P. (2022). Production, Biosynthesis, and Commercial Applications of Fatty Acids From Oleaginous Fungi. *Frontiers in Nutrition*, *9*. https://doi.org/10.3389/fnut.2022.873657