Supplementary Information

Volatile Profile of Sparkling Wines Produced with the Addition of Mannoproteins or Lees before Second Fermentation Performed with Free and Immobilized Yeasts

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Table S1. Physicochemical parameters of base wines obtained from the *assemblage* of four grape cultivars (Chardonnay 30%, Pinot Noir 30%, Viognier 30% and Riesling 10%), after the addition of *liqueur de tirage* (suspension of yeasts and sugar) used to perform the second fermentation of traditional sparkling wines

Parameter	Result ± SD[a]
pH	3.22 ± 0.07
Free SO_2 / (mg L^{-1})	18.0 ± 2.2
Total SO_2 / mg L^{-1})	109 ± 4
Density / (g L^{-1})	1005 ± 10
Alcohol / %	11.0 ± 1
Total acidity / (mequiv L^{-1})	83.0 ± 9.0
Volatile acidity / (mequiv L^{-1})	6.0 ± 0.3
Sugar[b] / (g L^{-1})	33.2 ± 1.1

[a]SD: standard deviation; [b]residual sugar of base wine was 3.2 g L^{-1} (before correction through the addition of *liqueur de tirage*). The amount of sugar added to the base wine (30 g L^{-1}) followed the protocol traditionally used by the winery partner of this study. The sugar consumed by the yeast during the second fermentation in the bottle resulted in at least 7 atm of pressure. However, the pressure was reduced to around 5 atm after *dégorgement*. Brazilian legislation establishes that the pressure of the sparkling wines must be higher than 4 atm.[1]

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Table S2. Percentages of chromatographic areas and Fisher ratios of the compounds found in base wines and their corresponding sparkling wines (T1 to T9) produced according to treatments described in Table 1 and analyzed by gas chromatography coupled to mass spectrometric detection (GC-MS) using a polar column (DB-Wax). Chromatographic conditions and statistics procedures are described in sub-sections "Determination of volatile profile" and "Chemometric analysis", respectively

No.	Compound	FR	FR[a] / %	Chromatographic area ± standard deviation / %									
				Base	T1	T2	T3	T4	T5	T6	T7	T8	T9
13	2-nonanone	331.63	100	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.11 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
31	ethyl hexadecanoate	120.22	36	0.06 ± 0.00	0.14 ± 0.00	0.09 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.57 ± 0.05	0.51 ± 0.01	1.15 ± 0.01	0.96 ± 0.01	0.19 ± 0.03
14	β-damascenone	72.77	22	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.06 ± 0.00	0.00 ± 0.00
21	ethyl decanoate	64.33	19	16.89 ± 0.02	3.67 ± 0.18	6.43 ± 0.36	2.75 ± 0.13	3.32 ± 0.07	6.80 ± 0.14	5.13 ± 0.08	4.83 ± 0.08	4.68 ± 0.07	11.32 ± 0.22
30	methyl hexadecanoate	60.90	18	4.60 ± 0.29	8.78 ± 0.17	13.12 ± 0.83	13.36 ± 0.29	10.49 ± 0.18	6.43 ± 0.04	12.23 ± 0.31	10.26 ± 0.11	10.50 ± 0.29	8.59 ± 0.43
34	nerolidol	60.00	18	0.00 ± 0.00	0.17 ± 0.01	0.27 ± 0.01	0.21 ± 0.01	0.14 ± 0.00	0.14 ± 0.00	0.20 ± 0.01	0.13 ± 0.00	0.14 ± 0.01	0.13 ± 0.01
3	**decanoic acid**	57.75	17	4.53 ± 0.06	**5.09 ± 0.12**	**3.22 ± 0.11**	**3.10 ± 0.03**	**4.98 ± 0.07**	5.41 ± 0.01	4.42 ± 0.08	6.43 ± 0.04	4.93 ± 0.02	7.53 ± 0.06
4	**dodecanoic acid**	55.85	17	0.19 ± 0.01	**0.18 ± 0.00**	**0.00 ± 0.00**	**0.00 ± 0.00**	**0.00 ± 0.00**	0.27 ± 0.01	0.15 ± 0.00	0.16 ± 0.00	0.15 ± 0.01	0.19 ± 0.01
16	**ethyl hexanoate**	50.44	15	2.63 ± 0.25	**7.78 ± 0.17**	**10.91 ± 0.06**	**10.94 ± 0.06**	**5.11 ± 0.14**	5.43 ± 0.45	5.59 ± 0.12	5.60 ± 0.27	4.63 ± 0.03	3.54 ± 0.02
33	linalool	23.33	7	0.09 ± 0.01	0.00 ± 0.00	0.12 ± 0.01	0.00 ± 0.00	0.14 ± 0.01	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.16 ± 0.00	0.00 ± 0.00
8	2,3-butanediol	22.05	7	0.07 ± 0.00	0.15 ± 0.01	0.10 ± 0.01	0.22 ± 0.01	0.00 ± 0.00	0.18 ± 0.00	0.00 ± 0.00	0.19 ± 0.01	0.19 ± 0.01	0.19 ± 0.00
23	diethyl succinate	22.01	7	5.46 ± 0.08	13.51 ± 0.43	7.91 ± 0.32	15.33 ± 0.15	21.11 ± 0.37	15.63 ± 0.49	17.62 ± 0.42	19.44 ± 0.37	16.54 ± 0.24	11.17 ± 0.50
35	α-terpineol	19.57	6	0.00 ± 0.00	0.00 ± 0.00	0.10 ± 0.00	0.00 ± 0.00	0.07 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
1	**hexanoic acid**	17.27	5	0.08 ± 0.00	**0.18 ± 0.01**	**0.00 ± 0.00**	**0.00 ± 0.00**	**0.00 ± 0.00**	0.38 ± 0.02	0.29 ± 0.04	0.36 ± 0.01	0.00 ± 0.00	0.00 ± 0.00
7	2-nonanol	15.21	5	0.00 ± 0.00	0.00 ± 0.00	0.04 ± 0.01	0.00 ± 0.00	0.00 ± 0.00	0.12 ± 0.01	0.00 ± 0.00	0.00 ± 0.00	0.11 ± 0.01	0.13 ± 0.00
17	isoamyl butyrate	14.71	4	0.86 ± 0.05	0.76 ± 0.00	0.70 ± 0.02	0.50 ± 0.02	0.62 ± 0.01	1.27 ± 0.04	1.68 ± 0.04	1.27 ± 0.01	0.82 ± 0.07	0.30 ± 0.03
20	ethyl octanoate	14.45	4	53.49 ± 0.40	27.62 ± 0.14	46.11 ± 0.59	32.20 ± 0.53	45.27 ± 0.92	35.52 ± 0.13	36.60 ± 0.38	31.69 ± 0.23	43.54 ± 1.16	35.49 ± 0.35
28	ethyl dodecanoate	13.30	4	0.29 ± 0.02	0.27 ± 0.01	0.32 ± 0.01	0.31 ± 0.01	0.00 ± 0.00	0.33 ± 0.01	0.14 ± 0.02	0.27 ± 0.02	0.35 ± 0.02	0.88 ± 0.02
18	**hexyl acetate**	12.89	4	0.26 ± 0.01	**0.33 ± 0.01**	**0.36 ± 0.00**	**0.34 ± 0.01**	**0.33 ± 0.02**	0.20 ± 0.00	0.16 ± 0.00	0.11 ± 0.01	0.16 ± 0.00	0.17 ± 0.00
29	**methyl tetradecanoate**	12.12	4	0.10 ± 0.01	0.22 ± 0.00	**0.15 ± 0.00**	**0.00 ± 0.00**	**0.00 ± 0.00**	0.27 ± 0.00	0.22 ± 0.01	0.29 ± 0.00	0.27 ± 0.00	0.19 ± 0.01
26	2-phenethyl acetate	11.76	4	1.30 ± 0.04	0.73 ± 0.02	0.80 ± 0.02	0.87 ± 0.00	1.16 ± 0.02	0.77 ± 0.03	1.36 ± 0.02	1.28 ± 0.01	1.13 ± 0.03	1.02 ± 0.03
19	ethyl lactate	11.47	3	1.80 ± 0.34	10.79 ± 0.19	2.86 ± 0.08	7.07 ± 0.31	10.12 ± 0.08	6.18 ± 0.46	6.29 ± 0.08	7.05 ± 0.24	7.12 ± 0.18	7.38 ± 0.36

24	ethyl 9-decenoate	11.40	3	0.12 ± 0.00	0.12 ± 0.00	0.15 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.44 ± 0.01	0.22 ± 0.03	0.26 ± 0.01	0.32 ± 0.00	0.26 ± 0.01
6	**2-ethyl-1-hexanol**	10.92	3	0.08 ± 0.01	**0.13 ± 0.00**	**0.15 ± 0.00**	**0.24 ± 0.02**	**0.25 ± 0.02**	0.11 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.08 ± 0.00	0.08 ± 0.00
9	**1-octanol**	10.01	3	0.00 ± 0.00	**0.14 ± 0.01**	**0.11 ± 0.01**	**0.12 ± 0.01**	**0.07 ± 0.01**	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.00 ± 0.00
2	**octanoic acid**	9.26	3	0.00 ± 0.01	**0.00 ± 0.00**	**0.00 ± 0.01**	**0.00 ± 0.00**	**0.00 ± 0.00**	0.20 ± 0.01	0.00 ± 0.00	0.06 ± 0.00	0.11 ± 0.00	0.10 ± 0.00
10	2-phenylethanol	7.19	2	0.28 ± 0.03	0.65 ± 0.01	0.38 ± 0.00	0.24 ± 0.01	0.44 ± 0.02	1.43 ± 0.01	1.28 ± 0.04	1.42 ± 0.07	1.21 ± 0.04	0.50 ± 0.02
11	1-dodecanol	4.46	1	0.15 ± 0.00	0.29 ± 0.00	0.25 ± 0.01	0.17 ± 0.02	0.50 ± 0.03	0.97 ± 0.02	0.53 ± 0.03	0.51 ± 0.02	0.22 ± 0.01	0.37 ± 0.01
25	ethyl phenyl acetate	4.36	1	0.08 ± 0.02	0.13 ± 0.01	0.17 ± 0.01	0.26 ± 0.00	0.25 ± 0.01	0.15 ± 0.00	0.26 ± 0.00	0.26 ± 0.00	0.20 ± 0.00	0.18 ± 0.01
15	**isoamyl acetate**	2.91	1	1.51 ± 0.04	**5.42 ± 0.27**	**8.25 ± 0.55**	**4.18 ± 0.41**	**1.44 ± 0.20**	2.41 ± 0.14	1.18 ± 0.08	1.05 ± 0.16	1.41 ± 0.03	5.76 ± 0.58
22	**isoamyl octanoate**	2.48	1	0.25 ± 0.02	**0.00 ± 0.00**	**0.04 ± 0.03**	**0.26 ± 0.05**	**0.24 ± 0.02**	0.15 ± 0.01	0.00 ± 0.00	0.00 ± 0.00	0.12 ± 0.01	0.12 ± 0.00
5	**1-hexanol**	0.64	0	0.37 ± 0.03	**1.28 ± 0.17**	**0.15 ± 0.01**	**0.47 ± 0.06**	**0.99 ± 0.16**	1.46 ± 0.06	0.36 ± 0.02	0.71 ± 0.44	1.61 ± 0.07	1.55 ± 0.06

[a]Percentage of the Fisher ratio (FR) obtained in relation to the most discriminant compound (with higher FR value). The highest FR value is defined as 100% and the others correspond to x%. The number 0.00 does not mean that the contribution of this compound in terms of chromatographic area percentage is below the criteria of detection employed in this study. However, it may be present in lower amounts. In green and bold font are the names, numbers and chromatographic percentages of the compounds that positively contribute to the aroma of the headspace of the sparkling wines and are generally found in higher percentage in wines from T1 to T4. In red and bold font are the ones that negatively contribute to the odor of sparkling wines.

Table S3. Loadings obtained in the principal component analysis of 9 volatile compounds indicated by Fisher ratio as the most discriminating among the samples of base and sparkling wines (T1 to T9). Their vinification followed the treatment described in Table 1. The variables highlighted in gray were the ones with higher loading values, which contributed the most to explain that specific factor

No.	Principal component (PC)	PC1	PC2
	eigenvalue	23.85	4.7
	variance / %	81.58	16.06
	cumulative variance / %	81.58	97.64
13	2-nonanone	0.098	0.226
31	ethyl hexadecanoate	0.026	0.521
14	β-damascenone	0.070	0.282
21	ethyl decanoate	–0.972	–0.231
34	nerolidol	0.067	–0.385
30	methyl hexadecanoate	0.145	–0.633
4	dodecanoic acid	–0.479	0.384
3	decanoic acid	–0.857	0.237
16	ethyl hexanoate	0.752	–0.655

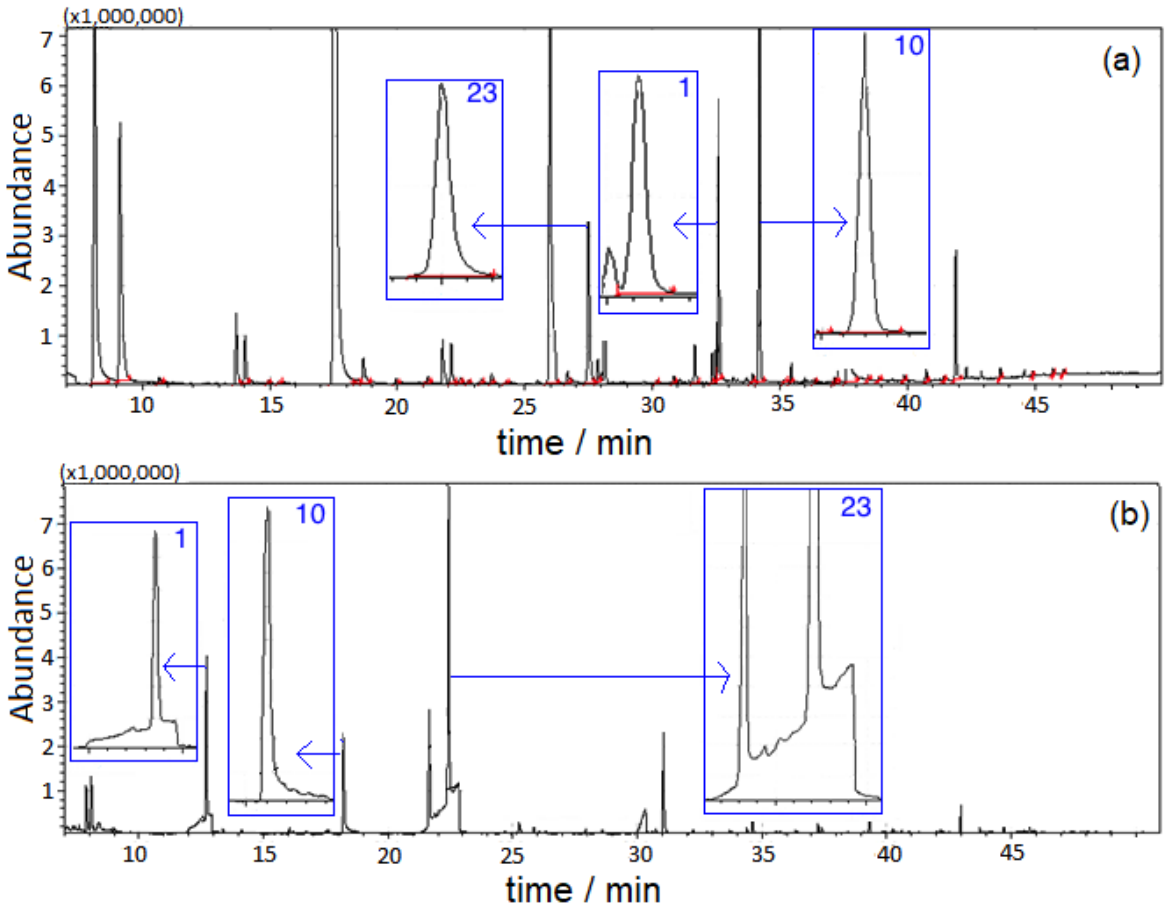

Figure S1. Chromatograms of a sparkling wine (T9, produced according to experimental conditions presented in Table 1) analyzed by gas chromatography coupled to mass spectrometric detection (GC-MS) using (a) a polar column (DB-Wax)) and (b) a nonpolar column (DB-5), with emphasis on the shape of the peaks corresponding to hexanoic acid (No. **1**), 2-phenylethanol (No. **10**) and diethyl succinate (No. **23**).

Reference

1. http://www.planalto.gov.br/ccivil_03/_ato2004-2006/2004/lei/l10.970.htm, accessed in March 2018.