



Identification criteria and quantification

Aroma compounds were subjected to an identification process that involved three stages. Firstly, a tentative identification of metabolites was considered when the similarity values were equal or greater than 75% between the mass spectrum obtained for each chromatographic peak in samples and the mass spectral libraries (NIST-08 and Willey-7). Secondly, a difference lower than 15 units was considered between the linear retention index obtained for each compound through Van Den Dool & Kraft method (LRIc) and those reported (LRIr) in the NIST webbook of Chemistry. Finally, those compounds that did not meet these two requirements, were subjected to a definitive confirmation with the mass spectrum of their relative pure standards.

The quantification process was carried out through the internal standard quantification method, using calibration curves obtained with standard solutions subjected to the same analytical conditions as wine samples. The selection of target and qualifiers ions used for this purpose were performed with the Chemstation software (Agilent Technologies, Palo Alto, CA). The calibration curves from compounds with the most similar chemical structures and/or similar number of C atoms was used to estimate the concentration of those volatiles without pure compounds commercially available.

Table S1. Major and minor volatile aroma compounds identified in the wines.

Compound	Prv [‡]	CAS ^c	LRI ^a	LRI ^b	Slope	Interception	R ²	LOD ^d (µg/L)	LOQ ^e (µg/L)
Isoamyl acetate	F	123-92-2	875	876	4.80E-02	1.12E-02	0.984	22	75
Ethyl acetate*	S	141-78-6	906	885	4.96E-03	-3.0E-04	0.998	2.1e+03	7,00E+03
2-phenylethyl acetate	S	103-45-7	1256	1256	6.22E-02	4.10E-03	0.995	3	9
Hexyl acetate	S	142-92-7	1014	1015	1.34E-01	1.65E-02	0.991	5	18
Isoamyl alcoholst*	M	123-51-3	1243	1230	8.7E+03	9.0E-03	0.999	4.2E+03	1,40E+04
2-phenylethanol*	S	60-12-8	2011	1892	1,10E-02	2,00E-03	0.999	3.6E+03	1,20E+04
Hexanol	F	111-27-3	867	867	1.00E-03	0.00E+00	0.944	3	11
2-ethyl-1-hexanol	S	104-76-7	1028	1027	1.04E-03	8.30E-06	0.955	11	36
Dodecanol	S	112-53-8	1461	1469	2.60E-03	8.65E-02	0.982	5	17
Guaiacol	S	90-05-1	1091	1088	3.30E-03	1.50E-03	0.933	2	6
4-vinylphenol ¹		2628-17-3	1225	1229					
2-methoxy-4-vinylphenol	S	2785-89-9	1313	1314	2.62E-01	-8.63E-02	0.969	2	8
Heptanal	S	111-71-7	903	901	7.90E-03	2.56E-03	0.961	0.4	1.3
Octanal	S	124-13-0	1004	1004	9.10E-03	1.80E-02	0.961	0.2	0.6
Nonanal	S	124-19-6	1104	1103	9.90E-03	1.79E-02	0.979	1.5	4.9
Decanal	S	112-31-2	1206	1206	8.90E-03	1.78E-02	0.959	0.3	1.1
Benzaldehyde	S	100-52-7	958.9	959	5.10E-03	7.00E-03	0.988	3	10
6-methyl-5-hepten-2-one ²		110-93-0	982	987					
Ethyl propanoate	S	105-37-3	708	705	2.20E-03	9.60E-03	0.967	12	39
Ethyl butanoate	S	105-54-4	802	802	7.80E-03	1.03E-03	0.989	23	76
Ethyl 3-methylbutanoate	S	108-64-5	851	847	7.78E-03	1.03E-02	0.989	5	15
Ethyl 4-hydroxybutanoate ³		999-10-0	1826	1819					
Ethyl hexanoate	F	123-66-0	1000	1001	7.02E-02	4.32E-02	0.917	10	34

Ethyl heptanoate ⁴		106-30-9	1102	1095					
Ethyl octanoate	F	106-32-1	1198	1196	1.78E-01	-4.70E-03	0.988	7	25
Ethyl decanoate	F	110-38-3	1395	1397	1.69E-01	6.90E-03	0.976	0.5	1.7
Ethyl dodecanoate	F	106-33-2	1594	1593	1.79E-01	7.10E-03	0.986	0.3	0.9
Ethyl hexadecanoate	F	628-97-7	1992	1996	1.83E-01	-2.60E-03	0.971	0.6	2.1
γ-Crotonolactone	S	497-23-4	913	916	1.00E-04	5.70E-03	0.972	9	29
γ-Butyrolactone	F	96-48-0	918	922	2.00E-04	4.70E-04	0.974	14	47
γ-Nonalactone	M	104-61-0	1363	1362	4.90E-03	-1.00E-04	0.943	1	4
Valerolactone ⁵		108-29-2	970	965					
β-Damascenone	S	23726-93-4	1385	1388	1.13E-02	5.85E-03	0.976	65	215
β-Ionone	S	8013-90-9	1420	1427	1.64E-02	2.89E-03	0.986	0.3	1.1
Vitispirane ⁶		65416-59-3	1279	1271					
Linalool	F	78-70-6	1090	1098	3.29E-02	2.50E-03	0.977	7	25
Limonene	S	138-86-3	1022	1030	3.30E-02	2.70E-03	0.976	1	4
β-Farnesene ⁷		18794-84-8	1478	1469					
E-Nerolidol	S	40716-66-3	1564	1562	1.78E-01	-8.09E-02	0.977	3	9
Z-Dihydrofarnesol ⁸		58001-87-9	1579	1587					
Farnesol 3	S	4602-84-0	1728	1740	6.65E-003	2.97E-01	0.992	5	16
Geranyl acetone	S	689-67-8	1442	1450	5.64E-03	6.32E-03	0.976	2	8
E-Methyl dihydrojasmonate	S	24851-98-7	1661	1649	4.62E-03	4.95E-02	0.968	1.4	4.7

LRI: Linear retention index using definition of Van den Dool and Kratz (1963) in a HP-5MS capillary column (30 m/0.25 mm/0.25 µm, He) and *CPWAX57-CB capillary column (60 m/0.25 mm/0.40 µm, He). . ^aCalculated values ^bData collected from the NIST Webbook of Chemistry. <http://webbook.nist.gov/chemistry>. ^cCAS: Chemical Abstracts Service number. ^dLOD: Limit of Detection. ^eLOQ: Limit of Quantification. + Isoamyl alcohols = 2-methylbutanol + 3-methylbutanol. ¹Quantified as 2-methoxy-4-vinylphenol. ²Quantified as octanal. ³Quantified as ethyl butanoate. ⁴Quantified as ethyl hexanoate. ⁵Quantified as butyrolactone. ⁶Quantified based on internal standard. ^{7,8}Quantified as farnesol. [†]Prv: Standard providers. F: Fluka; M: Merck; S: Sigma-Aldrich.

Table S2. Fermentation kinetic rates of the *Saccharomyces cerevisiae* strains during the fermentation process.

	220 g/L of initial sugars			250 g/L of initial sugars			250 g/L of initial sugars and 70 mg/L of SO ₂		
	Sc1	Sc5	Lc	Sc1	Sc5	Lc	Sc1	Sc5	Lc
Maximum dCO ₂ /dt values (g CO ₂ loss/day)	3.36	4.19	3.06	3.17	3.80	3.28	2.32	1.91	2.04
Time required for the maximum dCO ₂ /dt (days)	2.00	2.00	1.83	2.00	2.00	1.83	14.88	16.00	4.83
Fermentation duration (days)	21.88	21.88	14.92	26.8	24.88	18.92	32.88	33.92	21.83

Table S3. Odor perception thresholds and aromatic series assigned to the volatile compounds.

	Perception threshold ($\mu\text{g/L}$)		Perception threshold ($\mu\text{g/L}$)
Chemistry		Citrus	
Ethyl acetate	7500	2-Ethyl-1-hexanol	8000
Guaiacol	75	Limonene	10
Isoamyl alcohols	30000	Linalol	6
Limonene	10	Octanal	2,5
4-vinylphenol	180	Nonanal	2,5
Creamy		Decanal	1,25
γ -Butyrolactone	35000	6-Methyl-5-hepten-2-one	50
γ -Crotonolactone	35000	Green	
γ -Nonalactone	30	β -Farnesene	20
Floral		Heptanal	3
β -Damascenone	7	Hexanol	8000
Z-Dihydrofarnesol	20	6-Methyl-5-hepten-2-one	50
Farnesol 3	20	E-Nerolidol	700
Geranyl acetone	60	Green fruit	
β -Ionone	0,09	Ethyl 3-methyl butanoate	3
Linalol	6	Ethyl hexanoate	14
E-Nerolidol	700	Ethyl heptanoate	2,2
2-Phenylethyl acetate	250	Hexyl acetate	670
2-Phenylethanol	10000	Herbal	
E-Methyl dihydrojasmonate	70	β -Damascenone	7
Vitispirane	800	β -Farnesene	20
Fruity		β -Ionone	0,09
Benzaldehyde	350	Smoky	
Ethyl propanoate	10	Ethyl 4-OH-butanoate	1000
Ethyl butanoate	20	2-Methoxy-4-vinylphenol	125,8
Ethyl 3-methyl butanoate	3	Guaiacol	75
Ethyl hexanoate	14	Spice	
Ethyl heptanoate	2,2	Valerolactone	10
Ethyl octanoate	5	Waxy	
Ethyl decanoate	200	Decanal	1,25
Hexyl acetate	670	Dodecanol	1000
Isoamyl acetate	30	Ethyl octanoate	5
γ -Nonalactone	30	Ethyl decanoate	200
Honey		Ethyl dodecanoate	500
2-Phenylethyl acetate	250	Ethyl hexadecanoate	2000

Table S4. Weight of the aromatic series for the component selected in the principal component analysis.

	PC1	PC2	PC3
Fruity	0,4059	-0,0633	-0,1496
Green fruit	0,4102	0,0247	0,0098
Green	0,2698	-0,1748	-0,3432
Creamy	0,3050	0,1481	0,3469
Citrus	0,3887	0,1034	-0,0391
Chemistry	0,3025	-0,3383	-0,1252
Honey	0,1691	-0,2221	0,5420
Waxy	0,3663	0,0222	-0,3816
Spice	0,2876	0,0896	0,4941
Herbal	-0,0413	-0,5169	0,0558
Floral	-0,0211	-0,5032	0,1704
Smoky	-0,1049	-0,4894	-0,0812

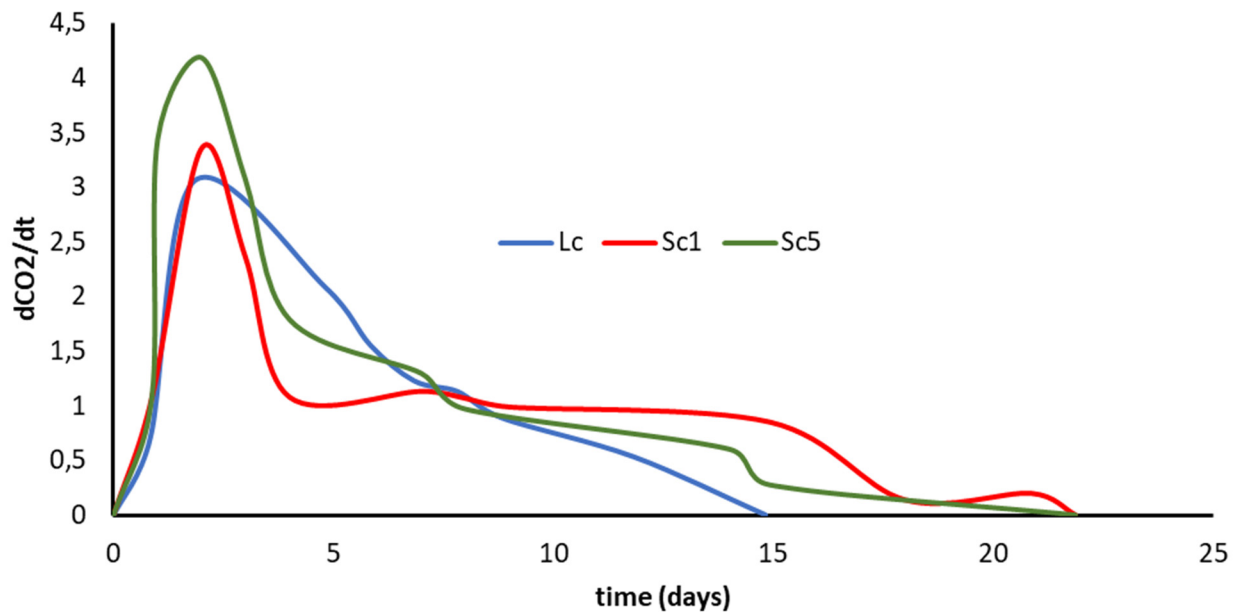


Figure S1a. Fermentation kinetic of the wild yeasts *Saccharomyces cerevisiae* 1 (Sc1) and *Saccharomyces cerevisiae* 5 (Sc5) and of the commercial strain (Lc) obtained when the initial sugar content of the must was 220 g/L.

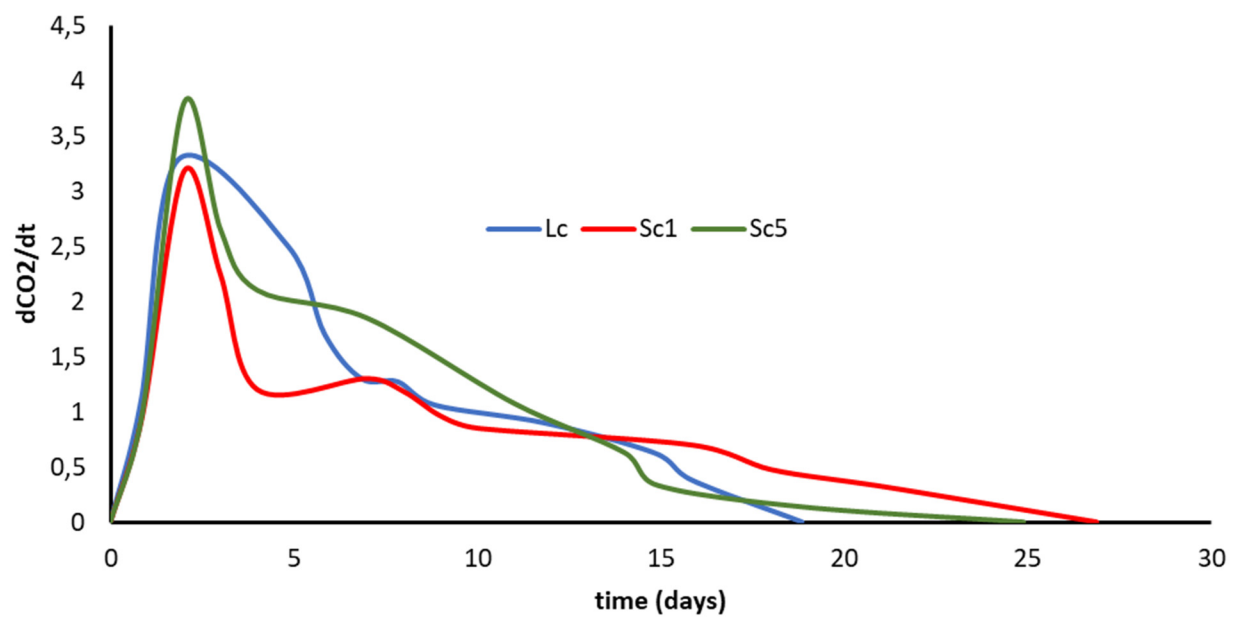


Figure S1b. Fermentation kinetic of the wild yeasts *Saccharomyces cerevisiae* 1 (Sc1) and *Saccharomyces cerevisiae* 5 (Sc5) and of the commercial strain (Lc) obtained when the initial sugar content of the must was 250 g/L.

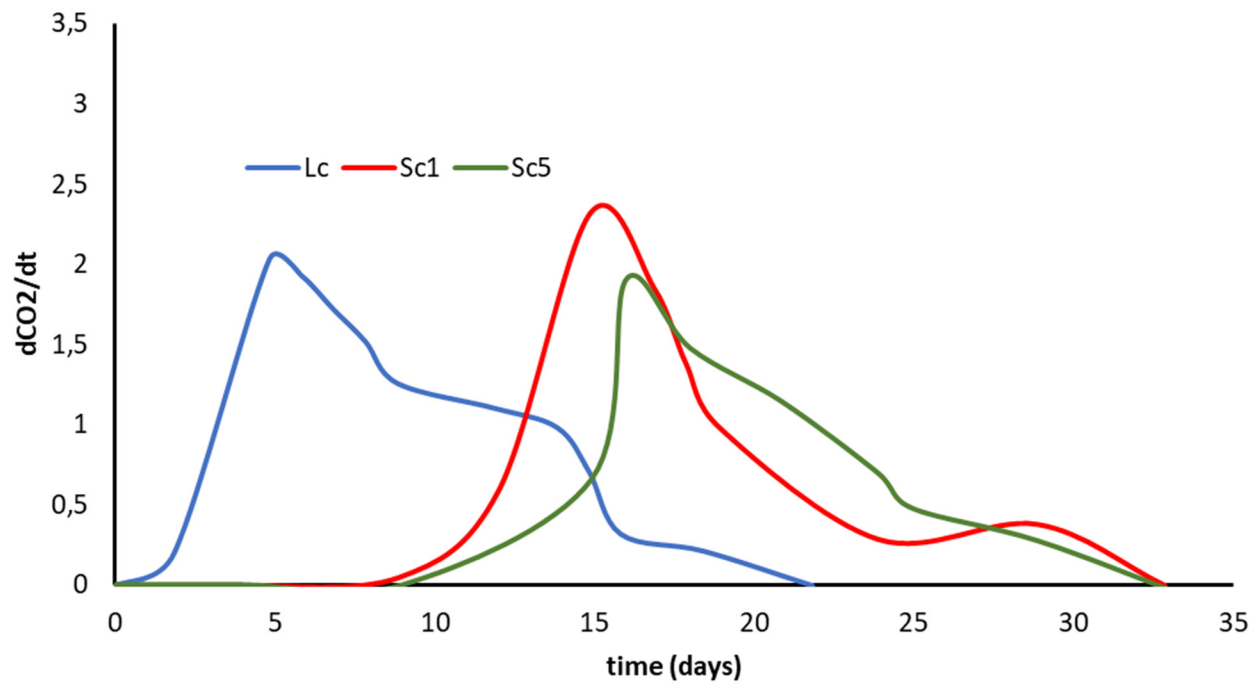


Figure S1c. Fermentation kinetic of the wild yeasts *Saccharomyces cerevisiae* 1 (Sc1) and *Saccharomyces cerevisiae* 5 (Sc5) and of the commercial strain (Lc) obtained when the initial sugar content of the must was 250 g/L and 75mg/L of sulphur dioxide was added prior to inoculation.