

## Supporting Information for

# Maturation of Moristel in different vineyards. Amino acid and aroma composition of mistelles and wines with particular emphasis in Strecker aldehydes

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**Table S1.** Vineyard characterization. List of characteristics which define the selected vineyards.

	Vineyard		
	A	B	C
<b>Vineyard conditions</b>			
Soil type	Fine sandy loam	Loam	Fine sandy loam
Altitude (m)	463	398	514
Vineyard age (years)	38	24	22
Row orientation	W	SW	SW
Vine spacing (mxm)	3.1x1.2	3.3x1.2	3.1x1.2
Number of vines / ha	2366	2222	2366
<b>Yield and vegetative growth</b>			
Number of bunches in 10 vines	12.6	20.4	9.8
Average bunch weight (Kg)	0.178	0.198	0.166
Yield (Kg/Ha)	5306	8976	3848
Canopy width (m)	0.5	0.6	0.4
Canopy height (m)	0.8	1	0.8
Canopy solar exposure %	60	20	40
Exposed Leaf Area (m <sup>2</sup> / vine)	1.92	2.4	1.92
Exposed Leaf Area/yield (m <sup>2</sup> /Kg)	0.90	0.59	1.2
<b>Agricultural practices</b>			
Pruning	4x2	6x1	4x3
Shoot thinning	Yes	No	Yes
Shoot tipping	Yes	Yes	Yes
Desuckering	Yes	No	Yes
Irrigation	No	No	No
Trellising	Double guyot	Double guyot	Double guyot
Mulching	No	No	No
Leaf plucking	No	No	No
Tilling	Yes	Yes	Yes

**Table S2.** Conventional oenological parameters of 33 samples of must expressed as the average and standard deviation (s).

Vineyard	A								B								C							
Days Postvéraison	42		49		56		62		42		49		56		62		41		48		60			
	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s		
density (g/L)	1120	1.22	1121	2.04	1119	3.72	1125	0.85	1108	2.03	1111	1.25	1108	3.22	1117	2.06	1109	3.41	1110	4.42	1119	2.08		
TSS* (°Brix)	25.1	0.29	25.4	0.47	25.0	0.92	26.5	0.22	22.4	0.45	23.2	0.24	22.6	0.67	24.8	0.40	22.8	0.75	23.0	1.00	25.0	0.52		
pH	2.87	0.02	3.43	0.02	3.42	0.02	3.39	0.01	2.79	0.05	3.31	0.03	3.35	0.03	3.39	0.02	3.36	0.03	3.38	0.04	3.42	0.01		
total acidity (g tartaric acid/L)	4.16	0.27	3.99	0.07	4.18	0.18	4.11	0.06	6.10	0.52	6.12	0.34	5.68	0.37	5.50	0.16	6.15	0.20	6.41	0.25	5.47	0.09		
YAN** (mg/L)	328	21.4	144	15.2	148	10.2	186	9.1	408	24.2	250	21.9	233	21.1	304	12.6	199	19.3	234	9.1	237	7.5		

\*TSS: Total soluble solids content

\*\*YAN: yeast assimilable nitrogen

**Table S3.** Conventional oenological parameters, concentration values of volatiles and amino acids found in the set of the 10 *mistelles* (all expressed in micrograms per litre, except the oenological classical parameters).

Vineyard	A				B			C		
Days Postvéraison	42	49	56	62	42	49	56	62	48	60
Classical parameters										
pH	3.68	3.91	3.87	3.74	3.69	3.85	3.91	4.04	3.83	3.86
TPI	51	57.9	57.3	57.4	48.6	57.6	57.5	59.2	39.4	46.4
Carbonyl compounds										
Fermentative origin										
acetoine	1383	2687	3768	2490	289	702	471	548	556	1101
diacetyl	15.57	25.14	46.10	26.07	9.90	14.80	2.84	15.85	12.56	17.16
Oxidation-related										
acetaldehyde (total)	10113	10482	11042	10990	11591	9907	10609	9808	10974	10960
acetaldehyde (free)	1280	1309	1440	1227	978	1379	1353	1090	1071	836
Norisoprenoids										
$\beta$ -damascenone	8.43	5.34	7.78	8.74	11.84	11.14	9.82	11.04	7.48	7.68
$\alpha$ -ionone	0.26	0.20	0.18	0.19	0.30	0.20	0.20	0.20	0.08	0.12
$\beta$ -ionone	0.75	0.75	0.71	0.66	0.75	0.76	0.74	0.75	0.68	0.69
TDN	2.11	1.29	1.24	1.77	4.01	2.84	1.99	1.61	0.95	0.94
vitispirane A	0.073	0.022	0.033	0.052	0.075	0.060	0.035	0.026	0.006	0.006
vitispirane B	0.048	0.016	0.022	0.034	0.053	0.041	0.025	0.020	0.006	0.006
Riesling acetal	0.056	0.022	0.027	0.038	0.075	0.066	0.039	0.030	0.012	0.011
Strecker aldehydes										
isobutyraldehyde	5.78	11.16	14.15	19.60	10.82	22.06	10.38	25.09	15.03	18.75
isovaleraldehyde	7.41	14.45	16.98	18.96	15.93	27.28	5.78	32.11	19.55	28.16
2-methylbutanal	2.98	6.29	8.05	11.32	4.67	10.36	5.66	11.94	6.32	10.79
methional	6.18	5.57	8.55	12.24	10.46	10.54	5.43	16.71	8.83	10.69
phenylacetaldehyde	3.47	13.70	4.20	6.84	2.90	11.36	-	10.39	4.93	5.10
Others										
(Z)-3-hexenal	0.81	0.62	0.49	0.12	0.84	0.41	0.17	0.45	0.49	0.48

Vineyard	A				B				C	
Days <i>Postvéraison</i>	42	49	56	62	42	49	56	62	48	60
Esters										
Linear fatty acid derivatives										
ethyl propanoate	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
ethyl butyrate	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
ethyl hexanoate	38.1	82.7	55.2	44.6	49.7	72.4	63.7	49.1	34.4	42.7
ethyl octanoate	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
ethyl decanoate	<LD	23.3	<LD	<LD	<LD	15.9	<LD	<LD	<LD	<LD
Branched acid derivatives										
ethyl isobutyrate	1.98	1.69	2.18	1.94	2.20	1.85	2.08	1.88	1.77	2.20
ethyl 2-methylbutyrate	0.41	0.78	0.84	0.83	0.47	0.88	0.83	0.42	0.80	0.84
ethyl isovalerate	0.30	<LD	<LD	<LD	0.36	<LD	<LD	<LD	<LD	<LD
ethyl 4-methylpentanoate	<LD	<LD	<LD	<LD	<LD	<LD	<LD	0.012	0.009	<LD
ethyl cyclohexanoate	<LD	0.044	<LD	<LD	<LD	<LD	<LD	<LD	0.034	<LD
Varietal origin										
methyl vanillinate	4.17	7.12	7.12	6.11	4.65	6.35	7.61	8.16	5.08	6.90
ethyl vanillate	99	195	265	217	105	228	336	316	122	172
ethyl dihydrocinnamate	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
ethyl cinnamate	0.29	0.29	0.50	0.57	1.09	1.66	2.05	1.95	1.09	3.20
Fermentative origin										
ethyl lactate	167	117	125	103	161	178	161	122	119	97.4
diethyl succinate	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
ethyl acetate	9916	10429	10363	7524	6893	6737	5295	3278	2982	3466
isoamyl acetate	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
isobutyl acetate	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
phenylethyl acetate	3.29	2.56	3.03	3.51	4.90	5.10	4.18	4.64	2.68	2.71
Alcohols										
isobutanol	13.6	27.2	32.0	26.1	11.9	24.1	45.1	22.6	54.9	80.7
1-butanol	67.5	55.7	36.3	29.4	23.8	38.1	22.0	32.6	31.9	23.8
isoamyl alcohol	54.4	72.0	96.2	48.8	60.2	96.5	107.8	53.3	110.9	99.2
methionol	<LD	<LD	<LD	<LD	17.9	<LD	<LD	<LD	<LD	22.2
benzylic alcohol	67.2	117	105	84.0	107	154	169	157	213	164

Vineyard	A				B				C	
Days <i>Postvéraison</i>	42	49	56	62	42	49	56	62	48	60
Alcohols										
β-phenylethanol	103	118	110	100	138	178	140	171	122	114
1-penten-3-ol	29.1	19.8	24.6	20.0	21.7	29.2	24.7	22.8	27.9	22.5
C6 Alcohols										
1-hexanol	360	561	432	369	387	750	542	648	634	574
(Z)-3-hexenol	26.3	21.2	16.3	18.9	30.4	40.0	24.9	26.3	35.3	22.5
(E)-2-hexenol	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
(E)-3-hexenol	25.7	34.5	26.2	22.9	28.5	24.2	32.2	38.5	40.9	24.0
Unsaturated C8 Alcohols										
1-octen-3-ol	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
(E)-2-octen-1-ol	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
Acids										
Linear acids										
acetic acid	55454	99997	93663	45422	39513	51697	38641	37585	30336	37029
butyric acid	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
hexanoic acid	77.0	217	140	120	87.7	208	142	174	110	122
octanoic acid	60.8	10.5	16.3	16.4	32.8	32.1	14.3	17.3	19.2	23.1
decanoic acid	11.0	<LD	<LD	<LD	<LD	<LD	<LD	<LD	23.5	13.9
Branched acids										
isobutyric acid	0.063	0.093	0.111	0.086	0.034	0.070	0.082	0.065	0.097	0.102
isovalerianic acid	22.0	<LD	<LD	12.3	15.8	13.8	23.1	14.6	16.7	17.4
Terpenols										
linalool	3.59	3.71	3.52	3.75	4.84	5.19	5.20	5.97	4.26	3.52
α-terpineol	2.51	2.11	2.29	2.90	3.46	3.08	2.16	2.06	1.93	1.80
β-citronelol	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
geraniol	3.32	13.33	4.91	5.64	4.57	5.39	6.03	8.59	5.87	6.54
rose oxide	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
Lactones										
whiskylactone	0.32	0.32	0.30	0.16	0.32	0.31	0.24	0.18	0.28	0.32
γ-nonolactone	5.66	3.37	2.79	2.77	5.19	3.49	2.94	1.33	1.46	0.94
γ-butyrolactone	936	1130	1222	979	1151	1568	1098	1540	1475	1015

Vineyard	A				B				C	
Days <i>Postvéraison</i>	42	49	56	62	42	49	56	62	48	60
Volatile phenols										
guaiacol	8.53	13.24	11.95	8.55	6.70	8.27	11.94	9.08	3.93	4.06
<i>o</i> -cresol	0.62	0.73	0.70	0.62	1.07	1.16	1.15	1.19	0.87	0.74
4-ethylguaiacol	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
<i>m</i> -cresol	0.27	0.22	0.29	0.23	0.37	0.36	0.29	0.27	0.22	0.21
eugenol	2.10	2.21	1.97	1.49	2.78	3.14	3.01	3.13	1.76	1.12
4-ethylphenol	0.13	0.12	<LD	0.09	0.17	0.16	0.14	0.13	0.09	0.12
4-vinylguaiacol	85.6	57.9	75.3	81.1	194	217	220	204	54.7	56.2
( <i>E</i> )-isoeugenol	1.38	<LD	<LD	<LD	<LD	<LD	1.21	<LD	<LD	<LD
2,6-dimethoxyphenol	60.7	61.8	60.4	55.1	55.8	64.1	70.0	64.9	18.6	19.4
4-vinylphenol	83.7	66.0	71.3	50.9	124	178	138	98.9	64.9	54.7
4-propylguaiacol	<LD	0.0021	0.0040	<LD	<LD	<LD	<LD	<LD	<LD	0.042
4-allyl-2,6-dimethoxyphenol	<LD	<LD	<LD	0.76	1.37	<LD	<LD	<LD	<LD	0.53
vanillin	83.8	106	80.1	56.2	93.2	116	80.0	79.3	39.9	39.7
acetovanillone	10.8	<LD	10.59	<LD	18.2	<LD	<LD	<LD	<LD	<LD
Amino acids										
alanine (ALA)	75590	72970	76535	72149	107977	130142	123442	133650	132416	111788
asparagine (ASN)	3236	1748	1652	4147	12682	13814	7003	13086	7695	6139
aspartic acid (ASP)	25376	29396	28740	29429	39511	59153	59983	49544	31651	42118
arginine (ARG)	63913	116483	117995	144420	241301	503629	429757	553273	336037	266283
cysteine (CYS)	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD
$\gamma$ -aminobutyric acid (GABA)	163956	187839	187316	167990	139389	158668	154533	191248	184088	209267
glutamine (GLN)	<LD	<LD	<LD	6291	<LD	<LD	<LD	17692	<LD	<LD
glutamic acid (GLU)	34683	33045	36666	53914	57701	55987	63875	93523	96135	88015
glycine (GLY)	4185	4867	5371	3450	6833	8730	10253	7662	5249	5844
histidine (HIS)	31821	32702	36640	38037	38541	54743	45782	60217	42386	47722
isoleucine (ILE)	4757	6887	9337	10157	7389	13018	12796	15829	9786	14806
leucine (LEU)	9554	13219	16604	18940	17225	28283	27544	32773	21359	28442
lysine (LYS)	5688	7698	9107	7200	15309	17215	23542	16283	13316	13907
methionine (MET)	3028	3642	5509	4820	5153	8340	8661	8937	4318	5116
ornithine (ORN)	13379	9089	9724	8368	22918	21216	20520	11843	21154	17601

Vineyard		A				B			C	
Days Postvéraison	42	49	56	62	42	49	56	62	48	60
Amino acids										
phenylalanine (PHE)	11022	15610	17319	14952	14982	20568	27191	20451	18752	19320
proline (PRO)	538462	813274	812030	795274	562836	895815	881742	1172368	897536	1143722
serine (SER)	28274	34659	37489	37422	42998	62108	57891	66441	36750	39496
threonine-ammonium (THR)	237135	320468	278875	281212	444224	582466	447672	457008	440790	330583
tyrosine (TYR)	5815	8057	8816	7942	13230	18877	20880	17151	13872	13635
valine (VAL)	14013	17853	20363	21934	21191	32187	27846	34181	24175	29101



**Table S4.** Conventional oenological parameters and concentration values of compounds found in the set of the 30 wines (all expressed in micrograms per litre, except the oenological classical parameters). The data was expressed as the average (among replicated measurements) and standard deviation (s).

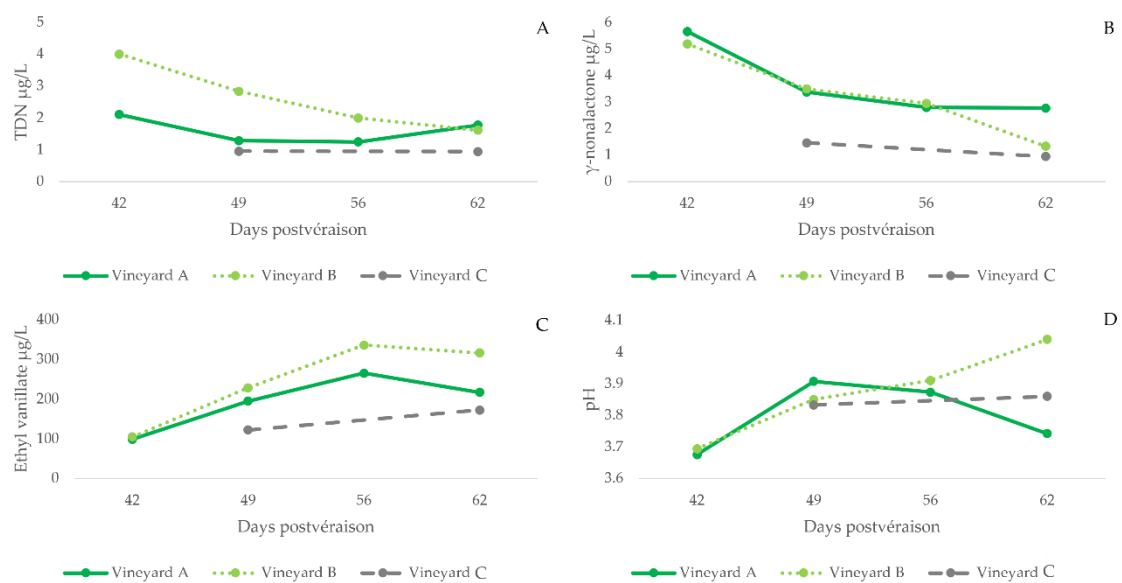
Vineyard	A										B										C										Odo- res thres- hold
Days Postvéraison	42		49		56		62		42		49		56		62		41		48		60										
	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s									
Classical parameters																															
pH	3.34	0.02	3.35	0.03	3.37	0.02	3.37	0.03	3.36	0.02	3.30	0.05	3.40	0.03	3.43	-	3.31	0.04	3.32	0.01	3.32	0.02	-								
volatile acidity (g/L)	0.637	0.040	0.570	0.070	0.515	0.049	0.727	0.193	0.527	0.021	0.490	0.000	0.550	0.020	1.085	-	0.590	0.050	0.353	0.040	0.450	0.026	-								
total acidity (g tartaric acid/L)	7.63	0.33	7.10	0.27	6.64	0.32	6.94	0.44	7.25	0.22	7.58	0.69	6.39	0.25	6.66	-	4.49	0.31	4.51	0.19	4.56	0.13	-								
reductive sugar (g/L)	0.383	0.230	0.063	0.110	0.460	0.297	0.220	0.195	0.940	0.106	0.290	0.020	0.413	0.081	1.022	-	0.923	0.259	0.667	0.501	0.993	0.202	-								
malic acid (g/L)	0.913	0.064	0.700	0.121	0.690	0.099	0.733	0.085	0.523	0.031	0.583	0.025	0.330	0.030	0.420	-	0.490	0.050	1.34	0.63	0.907	0.248	-								
lactic acid (g/L)	0.950	0.036	0.980	0.053	1.01	0.02	0.840	0.030	1.01	0.02	0.953	0.064	1.14	0.02	0.873	-	1.22	0.06	0.907	0.219	0.910	0.046	-								
ethanol (%)	15.7	0.1	15.4	0.16	15.69	0.86	16.78	0.35	12.6	0.2	12.65	0.27	13.13	0.46	13.97	-	12.66	0.67	13.08	0.46	14.32	0.55	-								
TPI	48.5	2.5	48.6	1.0	52.2	2.6	56.1	2.4	44.5	1.8	46.7	1.4	46.9	3.8	48.3	-	26.4	1.9	27.1	1.4	30.0	1.3	-								
CI	11.2	0.6	13.4	0.8	9.73	3.74	13.4	0.4	11.0	0.8	14.4	1.1	12.2	0.1	9.17	-	6.20	0.42	7.21	0.78	9.14	0.53	-								
Carbonyl compounds																															
Strecker aldehydes																															
isobutyraldehyde	23.3	5.5	26.1	4.2	26.2	6.9	24.1	9.2	29.0	3.6	32.8	8.0	20.6	1.5	26.8	-	38.6	4.1	36.5	4.1	34.1	3.1	6 <sup>1</sup>								
isovaleraldehyde	18.3	2.2	20.0	9.0	15.1	5.3	8.7	1.7	38.4	4.4	24.1	5.9	26.2	0.7	13.6	-	41.6	6.7	53.4	2.6	21.2	3.4	4.6 <sup>1</sup>								
2-methylbutanal	7.53	0.70	8.82	0.73	8.26	1.43	8.52	3.39	9.47	2.15	10.19	0.21	6.27	0.27	10.12	-	11.53	3.16	11.53	1.10	11.29	1.95	16 <sup>1</sup>								
methional	22.9	3.2	17.3	1.9	11.05	1.64	12.6	1.3	22.1	1.4	16.5	0.4	15.7	0.5	12.0	-	17.7	2.9	18.8	1.2	14.6	0.6	0.5 <sup>1</sup>								
phenylacetaldehyde	15.1	1.9	9.7	0.9	10.2	4.0	7.0	0.4	17.0	1.8	11.3	1.1	13.1	1.1	9.3	-	16.8	4.2	18.2	3.5	14.3	2.8	1 <sup>1</sup>								
Others aldehydes																															
(Z)-3-hexenal	19.8	0.6	15.7	0.6	17.2	0.7	23.6	2.3	16.9	0.2	14.9	2.2	15.8	0.9	23.7	-	17.4	0.9	17.4	0.7	19.5	0.3	0.12 <sup>2</sup>								
Esters																															
Branched acid derivatives																															
ethyl isobutyrate	132	25	147	15	109	6	92.2	19.7	94.4	21.4	103	7	70.2	12.5	59.7	-	101	6	103	10	85.7	4.7	15 <sup>3</sup>								
ethyl 2-methylbutyrate	17.2	0.6	16.2	2.0	10.6	0.4	11.7	1.7	11.0	1.0	12.3	2.3	8.44	0.74	9.43	-	19.0	1.0	17.0	0.2	15.9	0.5	18 <sup>3</sup>								
ethyl isovalerate	58.1	3.8	28.2	5.3	20.5	2.1	19.2	2.6	45.1	1.9	23.6	3.8	17.4	1.5	14.2	-	20.3	0.4	16.9	0.4	15.4	1.5	3 <sup>3</sup>								
Fermentative origin																															
isoamyl acetate	123	14	138	4	171	4	121	50	92.9	1.3	99.3	6.3	104	26	285	-	232	63	196	72	274	45	30 <sup>4</sup>								
isobutyl acetate	6.62	1.00	6.32	0.59	6.96	0.72	10.4	4.9	5.60	0.40	5.48	0.18	5.73	0.39	19.8	-	6.22	0.47	6.23	0.76	7.79	0.05	1600 <sup>5</sup>								
phenylethyl acetate	5.98	0.65	6.39	0.16	6.95	0.17	6.04	2.01	3.91	0.21	4.34	0.15	4.98	0.36	8.00	-	3.05	0.26	2.68	0.25	3.31	0.38	250 <sup>4</sup>								

Vineyard	A										B										C										Odor thres- hold <sup>a</sup>
Days Postvéraison	42		49		56		62		42		49		56		62		41		48		60										
	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s									
	Alcohols																														
isobutanol	29844	1160	33245	747	38116	1480	31066	2176	29151	1371	28198	960	29192	933	33961	-	31924	1195	36641	4274	31887	1459	40000 <sup>4</sup>								
isoamyl alcohol	255953	10166	262100	3515	281089	12159	229127	9072	255297	19329	245167	3437	270537	9289	253260	-	255954	6558	272488	12835	262139	5568	30000 <sup>4</sup>								
methionol	1754	137	2538	1190	1967	43	1036	93	2066	241	1859	130	2316	139	437	-	215	4	218	17	184	13	1000 <sup>3</sup>								
β-phenylethanol	35143	582	38796	730	42320	1270	33784	2781	27928	1531	27190	1628	35139	7627	17377	-	3440	19	3521	119	3188	222	14000 <sup>3</sup>								
Acids																															
Branched acids																															
isobutyric acid	2699	216	2713	256	2200	5	2208	300	1867	63	2021	207	1808	55	2914	-	2692	21	2491	145	2585	95	50 <sup>6</sup>								
isovaleric acid	3491	135	3465	231	2681	99	2297	159	2396	39	2446	115	2137	53	2214	-	108	5	72.3	10.5	69.9	10.2	33 <sup>3</sup>								
Amino acids																															
alanine (ALA)	22390	162	18171	3491	15110	7591	21995	2226	35761	3068	29575	1284	34879	391	41632	-	23682	2406	25380	3037	19859	1528	-								
asparagine (ASN)	5776	355	4730	661	4566	1042	2258	1915	14454	1517	12283	1019	9905	904	14579	-	5175	3028	5520	1572	5164	1909	-								
arginine (ARG)	11127	1860	9502	940	9175	3665	11785	2034	6049	1401	16909	4586	7742	1764	12351	-	15243	4468	27819	1905	24263	2175	-								
aspartic acid (ASP)	7774	2269	7453	2786	7947	5039	16562	4457	17209	1483	12850	473	15370	2858	31872	-	16590	3716	21116	8506	14453	2563	-								
cysteine (CYS)	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	-	<LD	<LD	<LD	<LD	<LD	<LD	-								
γ-aminobutyric acid (GABA)	17311	1406	13553	2427	10201	4745	10146	476	46886	4508	38177	8240	37743	793	28486	-	27848	2644	29412	2017	17352	1776	-								
glutamine (GLN)	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	<LD	-	<LD	<LD	<LD	<LD	<LD	<LD	-								
glutamic acid (GLU)	12272	297	9510	1879	9298	5072	14473	397	25544	1990	18472	1617	21228	1455	30735	-	18451	2155	21625	3271	15398	2662	-								
glycine (GLY)	6975	362	6838	2360	6508	3570	10015	1158	14558	1105	13857	796	15333	1004	21427	-	8898	1002	9856	872	8519	827	-								
histidine (HIS)	4811	378	4080	1429	4021	2328	7200	503	13471	2336	13034	2108	13664	554	757	-	8647	1889	9350	1363	8515	2020	-								
isoleucine (ILE)	610	47	338	301	224	364	1788	412	4099	895	3773	815	3722	484	8367	-	5502	1894	5328	1462	3672	940	-								
leucine (LEU)	5222	740	3584	1095	2585	834	6990	652	15703	681	11240	1206	12813	1872	16119	-	14018	3533	14992	3273	10156	2848	-								
lysine (LYS)	9063	1420	6925	1804	5660	2500	11782	1322	24273	820	20418	2339	21816	2554	21200	-	21869	4183	23835	4010	19916	5180	-								
methionine (MET)	2358	587	2147	192	1908	109	3201	276	6052	1437	5015	401	3979	453	3867	-	2563	746	2981	1711	2772	1607	-								
ornithine (ORN)	4125	320	2961	2394	2425	1812	4486	655	10698	9113	3096	1356	3979	1318	24638	-	14268	8788	8408	886	8535	1655	-								
phenylalanine (PHE)	3972	1904	4088	767	4732	1772	7858	636	16384	868	12552	2027	14713	1715	14895	-	12740	2514	14072	2356	11544	3317	-								
proline (PRO)	276837	55278	435702	17694	659188	399625	1015638	101649	821160	174531	782749	333453	975427	127727	2017104	-	486432	53509	581326	106862	981786	176606	-								
serine (SER)	6141	1874	5850	4054	4705	3228	6307	264	11082	643	8010	273	10348	2006	13669	-	9290	3312	7901	2837	8281	710	-								
threonine- ammonium (THR)	25630	3967	20493	4120	16744	6945	35667	6837	69435	4560	58819	4709	59493	4560	88683	-	48916	4462	29894	5019	23221	5478	-								

Vineyard	A										B								C						Odor thres- hold <sup>a</sup>
Days Postvéraison	42		49		56		62		42		49		56		62		41		48		60				
	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s	Mean	s			
Amino acids																									
tyrosine (TYR)	3494	170	2874	786	2730	1388	6214	544	12448	688	9836	1872	11579	1661	12477	-	9652	2377	10974	1714	9158	2279	-		
valine (VAL)	3333	315	2659	981	2264	1250	5146	817	9251	378	6624	592	8489	1000	12435	-	7017	1327	7350	1585	5036	1109	-		

<sup>a</sup> Reference in which the odour threshold value has been calculated is given in brackets. [1-6]

**Figure S1.** Evolution of some varietal aroma compounds and pH during maturation in mistelle samples aged 8 months. **A**, TDN; **B**,  $\gamma$ -nonalactone; **C**, ethyl vanillate; **D**, pH.



**Table S5.** Correlations between amino acid consumed proportions and the quotients ALA/GABA, 1/GABA and GLU/GABA in must.

	ALA/GABA			1/GABA			GLU/GABA		
	R <sup>2</sup>	R	<i>p</i>	R <sup>2</sup>	R	<i>p</i>	R <sup>2</sup>	R	<i>p</i>
ASN	0.290	0.539	0.104	0.030	0.173	0.631	0.603	0.776	0.007
GABA	0.783	-0.885	0.000	0.619	-0.787	0.006	0.243	-0.493	0.143
GLU	0.175	-0.418	0.226	0.716	-0.846	0.002	0.002	0.045	0.901
GLY	0.013	-0.114	0.752	0.016	-0.126	0.727	0.180	-0.424	0.218
HIS	0.639	-0.799	0.004	0.621	-0.788	0.006	0.308	-0.555	0.092
ILE	0.612	-0.782	0.006	0.073	-0.270	0.448	0.812	-0.901	0.000
LEU	0.365	-0.604	0.060	0.354	-0.595	0.066	0.333	-0.577	0.077
LYS	0.038	-0.194	0.589	0.028	-0.167	0.644	0.252	-0.502	0.135
MET	0.034	-0.185	0.607	0.392	-0.626	0.049	0.008	-0.091	0.801
PHE	0.600	-0.775	0.007	0.033	-0.182	0.614	0.919	-0.959	0.000
THR	0.222	-0.472	0.165	0.201	-0.448	0.190	0.189	-0.434	0.206
TYR	0.197	-0.444	0.194	0.128	-0.357	0.307	0.505	-0.711	0.019
VAL	0.468	-0.684	0.026	0.324	-0.569	0.082	0.465	-0.682	0.027
ALA	0.025	-0.157	0.664	0.401	-0.633	0.046	0.000	-0.012	0.973
ASP	0.019	-0.138	0.703	0.031	0.177	0.624	0.414	-0.644	0.041
SER	0.061	-0.248	0.488	0.053	-0.230	0.521	0.227	-0.477	0.159
ARG	0.471	0.686	0.026	0.087	0.295	0.406	0.270	0.519	0.120
ORN	0.094	0.306	0.386	0.025	0.158	0.662	0.069	-0.263	0.460
PRO	0.191	-0.437	0.202	0.026	0.162	0.654	0.130	-0.360	0.303

## References

1. Culleré, L., Cacho, J., & Ferreira, V. An assessment of the role played by some oxidation-related aldehydes in wine aroma. *J. Agric. Food Chem.* **2007**, *55*(3), 876-881. doi: 10.1021/jf062432k
2. Sellami, I., Mall, V., & Schieberle, P. Changes in the Key Odorants and Aroma Profiles of Hamlin and Valencia Orange Juices Not from Concentrate (NFC) during Chilled Storage. *J. Agric. Food Chem.* **2018**, *66*(28), 7428-7440. doi: 10.1021/acs.jafc.8b02257
3. Ferreira, V., López, R., & Cacho, J. F. Quantitative determination of the odorants of young red wines from different grape varieties. *J. Sci. Food Agric.* **2000**, *80*(11), 1659-1667. doi: 10.1002/1097-0010(20000901)80:11<1659::aid-jsfa693>3.0.co;2-6
4. Guth, H. Quantitation and Sensory Studies of Character Impact Odorants of Different White Wine Varieties. *J. Agric. Food Chem.* **1997**, *45*(8), 3027-3032. doi: 10.1021/jf970280a
5. Ferreira, V., Ortín, N., Escudero, A., López, R., & Cacho, J. Chemical characterization of the aroma of Grenache rose wines: Aroma extract dilution analysis, quantitative determination, and sensory reconstitution studies. *J. Agric. Food Chem.* **2002**, *50*(14), 4048-4054. doi: 10.1021/jf0115645
6. Gemert, L. J. N., A. H. (2003). Compilation of odour threshold values in air and water; National Institute for Water Supply: Zeist. Zeist, The Netherlands.