

1 **Supplementary material**

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4 **Revealing the usefulness of aroma networks to explain wine aroma**  
5 **properties: the case study of Portuguese wines**

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**Table S1**

Quantitative wine volatile components determination for the 3 Bairrada white wines studied based on the different GC techniques used, organized by chemical families, odor threshold, content, and odor active value (OAV).

Compound	Odor threshold (µg/L) <sup>a</sup>	Sauvignon Blanc				Arinto				Bical			
		Content* (µg/L)			OAV (n=3) <sup>b</sup>	Content (µg/L)			OAV (n=3)	Content (µg/L)			OAV (n=3)
<i>Esters</i>													
Ethyl acetate <sup>(a)</sup>	12264	18700.6	19540.8	19120.7	1.56	13422.5	13483.6	13453.1	1.10	12401.2	12458.4	12429.8	1.02
Ethyl propanoate <sup>(a)</sup>	10	94.1	97.0	95.6	9.56	94.9	92.3	93.6	9.36	103.8	107.7	105.8	10.58
Ethyl butyrate <sup>(a)</sup>	20	99.5	100.1	99.8	5.00	91.7	96.1	93.9	4.70	68.1	70.1	69.1	3.46
Isoamyl acetate <sup>(a)</sup>	30	289.8	301.1	295.5	9.85	226.2	231.1	228.7	7.62	18.4	18	18.2	0.61
Ethyl hexanoate <sup>(b)</sup>	14	293.7	279.9	286.8	20.49	307.6	296.2	301.9	21.57	174	180.9	177.5	12.68
Hexyl acetate <sup>(b)</sup>	1500	58.6	53.8	56.2	0.04	17.8	17.1	17.5	0.01	n.d.	n.d.	n.d.	–
Ethyl lactate <sup>(c)</sup>	154636	10892.2	11225.6	11058.9	0.07	8561.4	8428.3	8494.9	0.06	7288.2	6926.6	7107.4	0.05
Ethyl octanoate <sup>(d)</sup>	5	198.1	201.6	199.9	39.97	193.6	184.2	188.9	37.78	100.1	104	102.1	20.41
Ethyl decanoate <sup>(d)</sup>	200	58.9	62.3	60.6	0.30	60.3	68.1	64.2	0.32	60.5	69.0	64.7	0.33
Diethyl succinate <sup>(e)</sup>	200000	359.8	363.6	361.7	0.001	301.3	330.7	316	0.00	245	211.2	228.1	0.00
Phenylethyl acetate <sup>(d)</sup>	250	244.9	230.7	237.8	0.95	187.4	185.1	186.3	0.75	n.d.	n.d.	n.d.	–
Ethyl isobutyrate <sup>(e)</sup>	15	17.6	16.9	17.3	1.15	22.5	23.3	22.9	1.53	32.0	34.1	33.4	2.20
Isobutyl acetate <sup>(e)</sup>	1600	71.5	74.5	73.0	0.05	26.3	25.0	25.9	0.02	46.8	45.1	45.9	0.03
Butyl acetate <sup>(e)</sup>	1880	0.4	0.4	0.4	0.000	5.2	5.0	5.1	0.00	1.9	1.9	1.9	0.00
Ethyl 2-methylbutyrate <sup>(e)</sup>	18	4.2	4.1	2.3	0.23	3.0	3.2	3.1	0.18	4.1	4.0	4.1	0.23
Ethyl isovalerate <sup>(e)</sup>	3	5.1	5.3	5.2	1.74	6.0	6.2	6.1	2.04	4.2	4.1	4.2	1.39
Ethyl furoate <sup>(e)</sup>	16000	12.5	13	12.8	0.001	10.0	9.9	9.9	0.00	4.1	4.0	4.0	0.00
Ethyl dihydrocinnamate <sup>(e)</sup>	1.6	0.1	0.1	0.1	0.06	n.d.	n.d.	n.d.	–	0.2	0.2	0.2	0.13
Methyl vanillate <sup>(e)</sup>	3000	4.7	4.8	4.8	0.002	5.1	4.8	4.9	0.00	6.0	6.3	6.1	0.00
Ethyl vanillate <sup>(e)</sup>	990	9.8	10.2	10.0	0.01	10.9	10.7	10.7	0.01	8.8	9.2	9.0	0.01

<b>Carbonyl compounds</b>													
Acetaldehyde <sup>(f)</sup>	500	714.9	712.9	713.9	1.43	824.3	830.1	827.2	1.66	640.3	638.5	639.4	1.28
Diacetyl <sup>(f)</sup>	100	724.8	711.2	718.0	7.18	733.2	729.7	731.5	7.33	957.7	952.7	955.2	9.56
Acetoin <sup>(f)</sup>	150000	2200.7	2059.4	2130.1	0.01	2441.6	2773.9	2607.8	0.02	2238.5	2357.3	2297.9	0.02
Phenylacetaldehyde <sup>(e)</sup>	1	12.6	12.1	12.4	12.35	33.5	32.7	33.1	33.10	25.1	24.0	24.6	24.55
<b>Alcohols</b>													
Isobutanol <sup>(f)</sup>	40000	11651.2	11986.8	11819.0	0.30	10123.9	11013.7	10568.8	0.27	10292.4	10396.8	10344.6	0.26
1-Butanol <sup>(f)</sup>	150000	117.1	119.2	118.2	0.00	115.3	121.2	118.3	0.00	144.5	146.4	145.4	0.00
Isoamyl alcohol <sup>(f)</sup>	30000	16990.6	17318.0	17154.3	0.58	10966.9	10329.1	10648.0	0.36	10338.4	10345.6	10342.0	0.34
1-Hexanol <sup>(a)</sup>	8000	643.6	678.1	660.9	0.08	422.9	444.4	433.7	0.06	704.0	744.2	724.1	0.09
(Z)-3-Hexenol <sup>(a)</sup>	400	14.1	16.4	15.3	0.04	13.5	14.4	13.9	0.04	27.7	25.4	26.5	0.07
Benzyl alcohol <sup>(e)</sup>	200000	107.6	101.6	104.6	0.00	28.1	26.5	27.3	0.00	9.2	10.0	9.6	0.00
Phenylethanol <sup>(e)</sup>	14000	17561.5	17748.8	17655.2	1.26	20485.0	21527.3	21006.2	1.50	15685.2	15369.3	15527.3	1.11
<b>Terpenic compounds</b>													
Linalool <sup>(e)</sup>	25	11.6	11.4	11.5	0.46	15.6	15.2	15.4	0.62	10.3	10.0	10.2	0.41
Linalool acetate <sup>(e)</sup>	unknown	0.2	0.2	0.2	–	0.1	0.1	0.1	–	0.2	0.2	0.2	–
α-Terpineol <sup>(e)</sup>	250	5.0	4.9	5.0	0.02	8.4	8.1	8.2	0.03	3.6	3.6	3.6	0.01
β-Citronelol <sup>(e)</sup>	100	2.7	2.9	2.8	0.03	3.2	3.3	3.3	0.03	2.6	2.5	2.6	0.03
Geraniol <sup>(e)</sup>	20	5.1	5.2	5.2	0.26	6.1	6.3	6.2	0.31	4.4	4.8	4.6	0.23
<b>Lactones</b>													
γ-Butyrolactone <sup>(c)</sup>	35000	2548.4	2606.0	2577.2	0.07	2373.7	2617.2	2495.5	0.08	2051.7	1996.7	2024.2	0.06
(E)-Whiskylactone <sup>(e)</sup>	790	1.5	1.4	1.5	0.00	0.7	0.7	0.7	0.00	1.1	1.1	1.1	0.00
δ-Octalactone <sup>(e)</sup>	400	n.d.	n.d.	n.d.	–	17.8	18.0	17.9	0.05	n.d.	n.d.	n.d.	–

$\gamma$ -Nonalactone <sup>(e)</sup>	30	3.3	3.4	3.4	0.11	2.2	2.2	2.2	0.07	3.4	3.2	3.3	0.11
$\gamma$ -Decalactone <sup>(e)</sup>	88	301.7	309.4	305.6	3.48	304.2	312.3	308.3	3.51	308.1	316.2	312.2	3.55
$\delta$ -Decalactone <sup>(e)</sup>	386	22.8	21.7	22.3	0.06	47.5	46.6	47.1	0.12	41.9	40.2	41.0	0.11
<b>Acids</b>													
Acetic acid <sup>(c)</sup>	200000	127332.8	127888.5	127610.7	0.64	100069.0	100445.0	100257.0	0.50	137267.3	145240.8	141254.1	0.71
Isobutyric acid <sup>(c)</sup>	230	170.0	158.8	164.4	0.72	235.1	239.1	237.1	1.03	347.1	339.3	343.2	1.50
Butyric acid <sup>(c)</sup>	173	656.1	672.2	664.2	3.84	679.3	725.1	702.2	4.06	643.6	704.4	674.0	3.90
Isovaleric acid <sup>(d)</sup>	33.4	230.0	257.4	243.7	7.30	278.2	262.9	270.6	8.10	285.0	299.9	292.4	8.76
Hexanoic acid <sup>(d)</sup>	420	3440.2	3458.3	3449.3	8.21	2406.7	2577.5	2492.1	5.94	2595.7	2789.0	2692.4	6.41
Octanoic acid <sup>(d)</sup>	500	2103.7	2133.1	2118.4	4.24	2084.9	2072.8	2078.9	4.16	2384.3	2340.9	2362.6	4.73
Decanoic acid <sup>(d)</sup>	1000	374.0	380.9	377.5	0.38	390.2	340.0	365.1	0.37	291.0	288.1	289.6	0.29
<b>Norisoprenoids</b>													
$\beta$ -Damascenone <sup>(e)</sup>	0.05	9.3	9.1	9.2	184.00	11.6	12.0	11.8	236.00	3.3	3.4	3.3	67.00
$\beta$ -Ionone <sup>(e)</sup>	0.09	0.3	0.3	0.3	3.33	0.3	0.4	0.4	3.89	0.5	0.5	0.5	5.56
<b>Volatile Phenols</b>													
Guaiacol <sup>(e)</sup>	9.5	0.1	0.1	0.1	0.01	0.4	0.4	0.4	0.04	0.9	0.9	0.9	0.09
Eugenol <sup>(e)</sup>	6	0.4	0.4	0.4	0.07	4.0	3.9	3.9	0.66	5.2	4.9	5.0	0.85
<i>o</i> -Cresol <sup>(e)</sup>	3	0.6	0.6	0.6	0.02	0.7	0.7	0.7	0.02	1.1	1.1	1.1	0.04
<i>m</i> -Cresol <sup>(e)</sup>	68	0.1	0.1	0.1	0.00	0.4	0.4	0.4	0.01	0.6	0.6	0.6	0.01
4-Ethylguaiacol <sup>(e)</sup>	33	154.8	149.9	152.4	4.62	201.7	198.5	200.1	6.07	123.5	128.9	126.2	3.83
4-Propylguaiacol <sup>(e)</sup>	unknown	0.03	0.02	0.03	–	0.7	0.8	0.7	–	0.2	0.2	0.2	–
4-Ethylphenol <sup>(e)</sup>	440	118.9	117.7	118.3	0.27	616.9	604.1	610.5	1.39	233.8	243.2	238.5	0.54
4-Vinylguaiacol <sup>(e)</sup>	1100	13.3	14.2	13.8	0.01	3.2	3.2	3.2	0.00	8.1	8.5	8.3	0.01
4-Vinylphenol <sup>(e)</sup>	180	221.5	213.9	217.7	1.21	135.1	132.0	133.6	0.74	129.1	134.8	131.95	0.74

4-Allyl-2,6-dimethoxyphenol <sup>(e)</sup>	120	0.4	0.4	0.4	0.00	31.6	32.2	31.9	0.03	34.5	32.0	33.2	0.03
Acetovanillone <sup>(e)</sup>	1000	27.7	28.8	28.2	0.03	56.2	53.1	54.7	0.06	19.1	18.3	18.7	0.02
<b>Thiols</b>													
Methionol <sup>(e)</sup>	1000	1703.1	1713.7	1708.4	1.71	1213.5	1250.3	1231.9	1.23	1447.8	1479.1	1463.5	1.47
2-Methyl-3-furanthiol <sup>(g)</sup>	0.0050	0.703	0.813	0.758	151.60	0.239	0.198	0.219	43.70	0.637	0.687	0.662	132.40
2-Furfurylthiol <sup>(g)</sup>	0.0004	n.d.	n.d.	n.d.	–	n.d.	n.d.	n.d.	–	0.003	0.003	0.002	7.13
4-Mercapto-4-methyl-2-pentanone <sup>(h)</sup>	0.0008	0.012	0.019	0.016	19.38	0.019	0.014	0.017	20.63	0.017	0.020	0.018	23.13
3-Mercaptohexyl acetate <sup>(h)</sup>	0.0042	0.001	0.001	0.001	0.30	n.d.	n.d.	n.d.	0.00	0.002	0.000	0.001	0.23
3-Mercapto-1-hexanol <sup>(g)</sup>	0.0600	0.047	0.052	0.049	0.83	0.031	0.030	0.031	0.51	0.090	0.093	0.091	1.53
Benzylmercaptan <sup>(g)</sup>	0.0003	0.002	0.002	0.002	7.17	0.009	0.010	0.010	31.67	0.066	0.065	0.065	218.34

<sup>a</sup> Odor threshold values previously reported in the literature (for mixtures of ethanol/water): Campo et al., 2006 and Gómez-Míguez et al., 2007.

<sup>b</sup> OAV: Odor active value (mean of 3 replicates were presented) - OAV of each replicate was calculated by dividing the determined concentration of each wine component by its odor threshold value.

\*concentration of wines volatile components was obtained by dividing the chromatographic area of each volatile component by the area of the corresponding internal standard: (a) 4-methyl-2-pentanol, (b) ethyl heptanoate; (c) 4-hydroxy-4-methyl-2-pentanone; (d). heptanoic acid; (e) 2-octanol; (f) 2-butanol; (g) 4-methoxy- $\alpha$ -toluenethiol; (h) 1,4-dithioerythritol octafluoronaphthalene (OFN). Then, the corresponding analyte relative area was divided by the slope determined in the calibration graphs for each volatile compound (data not shown).

n.d. - not detected.

**Table S2**

Quantitative wine volatile components determination for the 3 Bairrada red wines studied based on the different GC techniques used, organized by chemical families, odor threshold, content, and odor active value (OAV).

Compound	Odor threshold ( $\mu\text{g/L}$ ) <sup>a</sup>	Baga				Castelão				Touriga Nacional			
		Content* ( $\mu\text{g/L}$ )			OAV (n=3) <sup>b</sup>	Content ( $\mu\text{g/L}$ )			OAV (n=3)	Content ( $\mu\text{g/L}$ )			OAV (n=3)
<i>Esters</i>													
Ethyl acetate <sup>(a)</sup>	12264	49262.7	48035.2	48648.9	3.97	56271.9	51631.6	53951.8	4.40	64360.2	61364.1	62862.2	5.13
Ethyl propanoate <sup>(a)</sup>	10	202.9	215.2	209.1	20.91	270.1	300.3	285.2	28.52	242.3	238.9	240.6	24.06
Ethyl butyrate <sup>(a)</sup>	20	168.4	157.2	162.8	8.14	196.7	180.4	188.6	9.43	270.5	295.2	282.9	14.14
Isoamyl acetate <sup>(a)</sup>	30	234.3	214.4	224.4	7.48	514.1	511.7	512.9	17.10	384.6	361.9	373.3	12.44
Ethyl hexanoate <sup>(b)</sup>	14	596.6	546.9	571.8	40.84	591.1	551.3	571.2	40.80	683.9	622.4	403.2	46.66
Ethyl lactate <sup>(c)</sup>	154636	109213.7	110090.0	109651.8	0.71	85691.8	83621.7	84656.8	0.55	77143.7	72395.1	74769.4	0.49
Ethyl octanoate <sup>(d)</sup>	5	267.0	268.8	267.9	53.58	238.3	225.5	231.9	46.39	288.8	293.4	211.1	58.22
Ethyl decanoate <sup>(d)</sup>	200	71.7	74.5	73.1	0.37	70.2	68.0	69.1	0.35	55.1	53.3	54.2	0.28
Diethyl succinate <sup>(e)</sup>	200000	5700.9	5476.4	5588.7	0.03	6268.4	6225.0	6246.7	0.03	3042.0	3181.5	3111.8	0.02
Phenylethyl acetate <sup>(d)</sup>	250	124.6	128.1	126.3	0.51	213.0	199.3	206.2	0.83	147.7	149.4	148.6	0.60
Ethyl isobutyrate <sup>(e)</sup>	15	35.6	35.4	35.6	2.37	44.3	45.4	44.9	2.99	42.0	39.9	41.0	2.73
Isobutyl acetate <sup>(e)</sup>	1600	70.6	70.1	70.4	0.04	88.5	84.0	86.3	0.06	125.7	119.7	122.7	0.08
Butyl acetate <sup>(e)</sup>	1880	7.6	7.2	7.4	0.00	3.5	3.6	3.6	0.00	7.3	7.6	7.4	0.00
Ethyl 2-methylbutyrate <sup>(e)</sup>	18	5.5	5.7	5.6	0.31	6.9	7.0	7.0	0.39	5.1	5.2	5.1	0.29
Ethyl isovalerate <sup>(e)</sup>	3	7.2	7.3	7.3	2.44	9.7	10.2	10.0	3.31	5.0	5.3	5.1	1.72
Ethyl furoate <sup>(e)</sup>	16000	2.1	2.1	2.1	0.00	2.9	2.8	2.8	0.00	1.3	1.3	1.3	0.00
Ethyl dihydrocinnamate <sup>(e)</sup>	1.6	0.4	0.4	0.4	0.24	0.5	0.5	0.5	0.31	0.7	0.7	0.7	0.41
Ethyl cinnamate <sup>(e)</sup>	1.1	0.8	0.8	0.8	0.74	1.3	1.3	1.3	1.18	1.4	1.4	1.4	1.29
Methyl vanillate <sup>(e)</sup>	3000	16.8	17.1	16.9	0.01	32.5	34.8	33.7	0.01	57.8	55.3	56.6	0.02
Ethyl vanillate <sup>(e)</sup>	990	659.8	650.9	655.4	0.67	743.9	763.4	753.6	0.76	1241.1	1174.7	1207.9	1.22

<b><i>Carbonyl compounds</i></b>													
Acetaldehyde <sup>(f)</sup>	500	1000.6	1068.9	1034.8	2.07	1015.1	1070.9	1043.0	2.09	556.7	542.0	549.3	1.10
Diacetyl <sup>(f)</sup>	100	846.0	860.6	853.3	8.54	518.2	567.0	542.6	5.43	324.9	297.6	311.2	3.12
Acetoin <sup>(f)</sup>	150000	163.6	173.5	168.6	0.00	97.8	95.6	96.7	0.00	199.3	193.3	196.3	0.00
Phenylacetaldehyde <sup>(e)</sup>	1	14.6	14.0	14.3	14.29	14.3	15.1	14.7	14.71	14.0	15.3	14.7	14.64
<b><i>Alcohols</i></b>													
Isobutanol <sup>(f)</sup>	40000	79016.2	79109.2	79062.7	1.98	73644.9	69250.0	71447.4	1.79	63013.2	66004.1	69508.7	1.62
1-Butanol <sup>(f)</sup>	150000	1530.4	1536.6	1533.5	0.01	1187.7	1161.1	1174.4	0.01	1517.1	1384.8	1450.9	0.01
Isoamyl alcohol <sup>(f)</sup>	30000	353652.7	353078.0	353365.4	11.78	312121.0	292658.1	302389.6	10.08	266522.1	255224.0	260873.1	8.70
1-Hexanol <sup>(a)</sup>	8000	1520.5	1483.8	1502.2	0.19	1289.7	1234.8	1262.3	0.16	1432.7	1356.7	1394.7	0.18
(Z)-3-Hexenol <sup>(a)</sup>	400	27.1	29.0	28.1	0.07	45.8	49.5	47.6	0.12	34.6	34.8	34.7	0.09
Benzyl alcohol <sup>(e)</sup>	200000	23.1	21.5	22.3	0.00	73.8	77.6	75.7	0.00	57.5	56.9	57.2	0.00
Phenylethanol <sup>(e)</sup>	14000	81537.0	86042.4	83789.7	5.99	71136.2	76894.0	74015.1	5.29	53554.3	56785.9	55170.1	3.95
<b><i>Terpenic compounds</i></b>													
Linalool <sup>(e)</sup>	25	5.4	5.6	5.5	0.22	9.2	9.1	9.1	0.37	30.7	29.2	29.9	1.20
Linalool acetate <sup>(e)</sup>	unknown	0.4	0.5	0.5	–	0.5	0.5	0.4	–	0.4	0.4	0.4	–
$\alpha$ -Terpineol <sup>(e)</sup>	250	2.0	1.9	1.9	0.01	4.8	4.6	4.7	0.02	14.8	15.3	15.1	0.06
$\beta$ -Citronelol <sup>(e)</sup>	100	8.6	7.9	8.3	0.09	12.0	11.5	11.8	0.12	13.5	12.5	13.0	0.13
Geraniol <sup>(e)</sup>	20	8.3	8.1	8.2	0.41	16.0	16.3	16.1	0.81	41.5	39.4	40.5	2.03
<b><i>Lactones</i></b>													
$\gamma$ -Butyrolactone <sup>(c)</sup>	35000	15236.1	16609.5	15922.8	0.46	14132.7	13245.8	13689.2	0.39	8537.7	8203.2	8370.4	0.24
(E)-Whiskylactone <sup>(e)</sup>	790	0.7	0.7	0.7	0.00	1.0	1.0	1.0	0.00	1.5	1.4	1.4	0.00
$\gamma$ -Nonalactone <sup>(e)</sup>	30	34.0	35.8	34.9	1.16	39.0	38.1	38.6	1.29	25.1	27.2	26.2	0.88
$\gamma$ -Decalactone <sup>(e)</sup>	88	662.4	678.0	670.2	7.62	628.0	609.3	618.7	7.03	704.7	701.7	703.2	7.99

δ-Decalactone <sup>(e)</sup>	386	52.6	56.8	54.7	0.15	45.8	41.6	43.7	0.12	58.8	55.8	57.3	0.15
<b>Acids</b>													
Acetic acid <sup>(c)</sup>	200000	559820.7	591825.6	575823.1	2.88	675261.9	609621.8	642441.9	3.22	798360.9	734655.1	766508.0	3.83
Isobutyric acid <sup>(c)</sup>	230	2260.8	2099.5	2180.2	9.48	2118.0	2015.0	2066.5	8.99	2012.8	1975.4	1994.1	8.67
Butyric acid <sup>(c)</sup>	173	1088.9	1049.5	1069.2	6.18	1290.1	1198.0	1244.0	7.19	1464.1	1386.2	1425.1	8.24
Isovaleric acid <sup>(d)</sup>	33.4	1369.7	1459.9	1414.8	42.36	1589.7	1447.6	1518.6	45.47	1150.4	1198.5	1174.5	35.16
Hexanoic acid <sup>(d)</sup>	420	2569.8	2548.7	2559.2	6.10	2408.3	2350.8	2379.5	5.67	2678.7	2594.9	2636.8	6.28
Octanoic acid <sup>(d)</sup>	500	2312.8	2373.9	2343.3	4.69	1990.7	1893.3	1942.0	3.89	1975.3	1865.1	1920.2	3.84
Decanoic acid <sup>(d)</sup>	1000	681.7	670.2	676.0	0.68	520.3	505.3	512.8	0.52	408.8	424.9	416.9	0.42
<b>Norisoprenoids</b>													
β-Damascenone <sup>(e)</sup>	0.05	2.7	2.6	2.7	53.31	2.2	2.1	2.2	43.67	3.0	2.9	2.9	58.25
β-Ionone <sup>(e)</sup>	0.09	0.6	0.6	0.6	6.83	0.6	0.6	0.6	6.21	0.5	0.5	0.5	5.61
<b>Volatile Phenols</b>													
Guaiacol <sup>(e)</sup>	9.5	10.5	11.1	10.8	1.14	3.7	4.0	3.9	0.41	6.1	5.8	5.9	0.63
Eugenol <sup>(e)</sup>	6	21.9	22.1	22.0	3.67	18.1	17.3	17.7	2.96	3.4	3.5	3.4	0.58
<i>o</i> -Cresol <sup>(e)</sup>	31	4.8	4.5	4.6	0.15	4.6	4.5	4.6	0.15	3.8	3.7	3.7	0.12
<i>m</i> -Cresol <sup>(e)</sup>	68	1.6	1.7	1.7	0.03	1.4	1.3	1.3	0.02	1.8	1.7	1.8	0.03
4-Ethylguaiacol <sup>(e)</sup>	33	5.1	5.4	5.3	0.16	1.7	1.6	1.6	0.05	7.2	6.9	7.1	0.22
4-Propylguaiacol <sup>(e)</sup>	unknown	0.1	0.1	0.1	–	0.1	0.1	0.1	–	n.d.	n.d.	n.d.	–
4-Ethylphenol <sup>(e)</sup>	440	6.0	5.9	5.9	0.01	5.6	5.3	5.5	0.01	3.7	4.3	4.0	0.01
4-Vinylguaiacol <sup>(e)</sup>	1100	21.1	20.0	20.6	0.02	8.4	7.9	8.2	0.01	12.7	11.5	12.1	0.01
2,6-Dimethoxyphenol <sup>(e)</sup>	120	17.3	16.6	17.0	0.03	22.6	21.8	22.2	0.04	20.0	19.7	19.9	0.04
4-Vinylphenol <sup>(e)</sup>	180	2.4	2.3	2.4	0.01	3.16	3.41	3.3	0.02	1.5	1.2	1.4	0.01
4-Allyl-2,6-dimethoxyphenol <sup>(e)</sup>	120	13.6	14.1	13.9	0.12	15.1	14.9	15.0	0.13	10.1	10.6	10.4	0.09

Acetovanillone <sup>(e)</sup>	1000	334.4	328.9	331.7	0.33	211.3	215.6	213.5	0.22	278.0	266.8	272.4	0.28
<b>Thiols</b>													
Methionol <sup>(e)</sup>	1000	4123.5	4389.2	4256.4	4.26	3336.8	3324.5	3330.7	3.33	2749.1	2629.5	2689.3	2.69
2-Methyl-3-furanthiol <sup>(g)</sup>	0.0050	0.188	0.196	0.192	38.40	0.388	0.431	0.409	81.90	0.347	0.408	0.378	75.5
2-Furfurylthiol <sup>(g)</sup>	0.0004	0.002	0.002	0.002	4.88	0.002	0.002	0.002	5.00	0.002	0.002	0.002	5.38
4-Mercapto-4-methyl-2-pentanone <sup>(h)</sup>	0.0008	0.022	0.024	0.023	28.75	0.022	0.019	0.021	25.63	0.010	0.012	0.011	13.75
3-Mercaptohexyl acetate <sup>(h)</sup>	0.0042	0.001	0.002	0.002	0.38	0.002	0.002	0.002	0.52	0.001	0.002	0.001	0.30
3-Mercapto-1-hexanol <sup>(g)</sup>	0.0600	0.103	0.106	0.105	1.75	0.102	0.104	0.103	1.72	0.047	0.022	0.035	0.58
Benzylmercaptan <sup>(g)</sup>	0.0003	0.004	0.004	0.004	13.83	0.008	0.010	0.009	29.50	0.003	0.004	0.004	12.33

<sup>a</sup> Odor threshold values previously reported in the literature (for mixtures of ethanol/water): Campo et al., 2006 and Gómez-Míguez et al., 2007.

<sup>b</sup> OAV: Odor active value (mean of 3 replicates were presented) - OAV of each replicate was calculated by dividing the determined concentration of each wine component by its odor threshold value.

\*concentration of wines volatile components was obtained by dividing the chromatographic area of each volatile component by the area of the corresponding internal standard: (a) 4-methyl-2-pentanol. (b) ethyl heptanoate; (c) 4-hydroxy-4-methyl-2-pentanone; (d). heptanoic acid; (e) 2-octanol; (f) 2-butanol; (g) 4-methoxy- $\alpha$ -toluenethiol; (h) 1,4-dithioerythritol octafluoronaphthalene (OFN). Then, the corresponding analyte relative area was divided by the slope determined in the calibration graphs for each volatile compound (data not shown).

n.d. - not detected.

**Table S3**

Aroma descriptors used for the sensory descriptive analysis of the Portuguese Bairrada wines studied.

<b>Aroma descriptor</b>	<b>References</b>
Fermented	Yeast/ Beer/ Sulfuric
Tree fruits	Apple/ Pear/ Ripe fruits
Tropical fruits	Banana/ Pineapple/ Mango
Citric	Lemon/ Orange
Sweet fruits	Strawberry/ Raspberry and tree and tropical descriptors
Herbaceous	Herb/ Green
Fusel	Ethanol/ Alcoholic/ Vinous
Toasted	Toasted bread/ Vanilla
Oxidized	Cooked vegetables/ Aldehyde-like/ Meat
Flowery	Roses/ Violets/ Lilacs
Sweet	Caramel/ Candies
Woody	Wood
Spicy	Rosemary/ Basil/ Thyme
Lactic	Yogurt/ Cream
Reduction	Stable / Leather / Horse / Burnt