

Table S1. Mean concentration and standard deviation of volatile sulfur compounds in Shiraz wines according to the type of closure.

		H ₂ S ^a (µg/L)	MeSH ^a (µg/L)	EtSH ^a (µg/L)	2ME ^a (µg/L)	DMS ^b (µg/L)	DMSP ^a (µg éq. DMS/L)	DES ^b (µg/L)	SMTA ^b (µg/L)	DMDS ^b (µg/L)	ETA ^b (µg/L)	DEDS ^b (µg/L)
0 month												
CR1	Closure 1	172 ± 13	5.1 ± 0.1	1.8 ± 0.1	58.6 ± 2.2	33 ± 2	155	nd	13.5 ± 1.6	nd	7.7 ± 1.2	nd
	Closure 2	188 ± 2	5.4 ± 0.1	1.9 ± 0.1	60.9 ± 1.0	36 ± 2		nd	14.3 ± 0.6	nd	8.1 ± 1.1	nd
	Closure 3	186 ± 7	5.3 ± 0.3	1.9 ± 0.2	60.6 ± 0.8	34 ± 1		nd	12.5 ± 0.7	nd	8.4 ± 0.3	nd
	Closure 4	180 ± 10	5.1 ± 0.2	1.9 ± 0.0	60.1 ± 0.7	33 ± 3		nd	14.3 ± 0.6	nd	4.9 ± 2.2	nd
CR2	Closure 1	37 ± 1	5.1 ± 0.2	0.0 ± 0.0	1.7 ± 0.1	75 ± 7	304	nd	2.4 ± 0.1	nd	nd	nd
	Closure 2	38 ± 1	5.3 ± 0.3	0.0 ± 0.0	1.7 ± 0.1	84 ± 6		nd	2.3 ± 0.2	nd	nd	nd
	Closure 3	36.4 ± 0.4	5.0 ± 0.1	0.0 ± 0.0	1.68 ± 0.04	71 ± 16		nd	2.2 ± 0.3	nd	nd	nd
	Closure 4	38.3 ± 0.4	5.4 ± 0.2	0.0 ± 0.0	1.76 ± 0.02	77.0 ± 0.2		nd	2.0 ± 0.1	nd	nd	nd
LR1	Closure 1	35.3 ± 0.3	5.8 ± 0.2	0.0 ± 0.0	7.6 ± 0.1	109 ± 70	958	nd	0.9 ± 0.1	nd	nd	nd
	Closure 2	36.4 ± 0.2	5.6 ± 0.3	0.0 ± 0.0	7.3 ± 0.0	315 ± 20		nd	1.0 ± 0.1	nd	nd	nd
	Closure 3	37 ± 1	5.9 ± 0.7	0.0 ± 0.0	7.7 ± 0.3	311 ± 1		nd	0.907 ± 0.001	nd	nd	nd
	Closure 4	35 ± 1	5.4 ± 0.3	0.0 ± 0.0	7.4 ± 0.1	311 ± 14		nd	0.91 ± 0.02	nd	nd	nd
LR2	Closure 1	183 ± 6	5.3 ± 0.1	1.2 ± 0.1	36.9 ± 0.7	77 ± 17	283	nd	2.30 ± 0.04	nd	nd	nd
	Closure 2	183 ± 4	5.0 ± 0.1	1.2 ± 0.0	36.8 ± 0.4	106 ± 23		nd	2.8 ± 0.5	nd	nd	nd
	Closure 3	180 ± 1	5.0 ± 0.3	1.2 ± 0.1	36.6 ± 1.0	103 ± 20		nd	2.9 ± 0.3	nd	6.7 ± 0.2	nd
	Closure 4	173 ± 4	4.6 ± 0.2	1.1 ± 0.1	35.7 ± 0.8	83 ± 18		nd	2.7 ± 0.4	nd	nd	nd
LR3	Closure 1	119 ± 6	3.8 ± 0.1	0.0 ± 0.0	14.0 ± 0.3	73 ± 7	400	nd	17.8 ± 2.6	nd	8.7 ± 1.3	nd
	Closure 2	119 ± 2	3.7 ± 0.1	0.0 ± 0.0	13.8 ± 0.4	35 ± 1		nd	19.7 ± 1.8	nd	7.8 ± 0.8	nd
	Closure 3	121 ± 2	3.8 ± 0.1	0.0 ± 0.0	13.9 ± 0.3	59 ± 26		nd	19.0 ± 2.4	nd	9.6 ± 0.4	nd
	Closure 4	119 ± 8	3.5 ± 0.1	0.0 ± 0.0	13.9 ± 0.6	41 ± 7		nd	21.2 ± 4.0	nd	9.9 ± 0.9	nd
LR4	Closure 1	30 ± 2	2.6 ± 0.4	0.0 ± 0.0	2.1 ± 0.1	7.4 ^{a,*}	119	nd	2.9 ± 0.3	nd	nd	nd
	Closure 2	30 ± 1	2.6 ± 0.1	0.0 ± 0.0	2.2 ± 0.1	4.1 ^{a,*}		nd	2.8 ± 0.2	nd	nd	nd
	Closure 3	32.1 ± 0.2	2.7 ± 0.2	0.0 ± 0.0	2.0 ± 0.1	4.8 ^{a,*}		nd	3.0 ± 0.7	nd	nd	nd
	Closure 4	31.3 ± 0.3	2.3 ± 0.2	0.0 ± 0.0	2.4 ± 0.2	4.8 ^{a,*}		nd	3.3 ± 0.2	nd	nd	nd
3 month												
CR1	Closure 1	169 ± 5	18.3 ± 1.7	2.2 ± 0.3	42.9 ± 1.2	180 ± 21	122 ± 7	nd	14.2 ± 0.5	nd	8.7 ± 0.2	nd
	Closure 2	166 ± 3	15.9 ± 0.5	2.2 ± 0.1	45.1 ± 2.5	118 ± 19	115.3 ± 0.3	nd	12.0 ± 0.6	nd	8.9 ± 0.1	nd
	Closure 3	173 ± 2	14.4 ± 0.7	2.5 ± 0.3	45.8 ± 1.1	152 ± 6	118 ± 7	nd	12.3 ± 1.2	nd	8.9 ± 0.1	nd
	Closure 4	169 ± 2	14.0 ± 1.1	2.2 ± 0.2	45.3 ± 1.0	139 ± 4	117 ± 1	nd	13.3 ± 1.1	nd	8.5 ± 1.2	nd
CR2	Closure 1	84 ± 6	24.4 ± 1.7	nd	4.3 ± 0.1	481 ± 54	216 ± 1	nd	nd	nd	7.5 ± 0.1	nd
	Closure 2	76 ± 2	18.9 ± 1.3	nd	4.1 ± 0.1	458 ± 11	203 ± 5	nd	nd	nd	nd	nd
	Closure 3	69 ± 2	20.3 ± 0.7	nd	4.0 ± 0.2	444 ± 16	212 ± 4	nd	nd	nd	7.40 ± 0.01	nd
	Closure 4	83 ± 6	18.9 ± 0.9	nd	4.2 ± 0.2	371 ± 19	209 ± 1	nd	nd	nd	nd	nd
LR1	Closure 1	50 ± 1	26.1 ± 0.8	nd	9.6 ± 0.2	770 ^{**} ± 88	523 ± 6	nd	0.84 ± 0.04	nd	nd	nd

	Closure 2	47.1	±	0.3	27.2	±	1.9	nd		9.5	±	0.1	752**	±	183	525	±	24	nd	1.0	±	0.1	nd	nd		nd
	Closure 3	47	±	1	24.7	±	0.7	nd		9.5	±	0.3	684**	±	97	534	±	36	nd	1.0	±	0.1	nd	nd		nd
	Closure 4	48	±	1	25.7	±	1.1	nd		9.5	±	0.3	521**	±	124	509	±	2	nd	1.00	±	0.04	nd	nd		nd
LR2	Closure 1	135	±	4	23.6	±	2.6	nd		11.7	±	0.5	329	±	7	247	±	2	nd	2.57	±	0.02	nd	nd		nd
	Closure 2	130	±	1	23.3	±	0.6	nd		12.08	±	0.05	277	±	44	235	±	3	nd	2.6	±	0.1	nd	nd		nd
	Closure 3	132	±	9	22.8	±	1.3	nd		11.8	±	0.2	560**	±	6	246	±	3	nd	2.6	±	0.1	nd	nd		nd
	Closure 4	130	±	3	24.6	±	1.7	nd		11.9	±	0.1	555**	±	60	234	±	4	nd	2.5	±	0.1	nd	nd		nd
LR3	Closure 1	179	±	12	43.8	±	2.5	1.4 ± 0.1		33.3	±	1.8	533**	±	11	191	±	27	nd	20.1	±	0.7	nd	9.7 ± 0.4		nd
	Closure 2	193	±	5	39.9	±	0.3	1.49 ± 0.02		37.2	±	1.2	516**	±	21	180	±	5	nd	10.7	±	0.8	nd	8.9 ± 0.2		nd
	Closure 3	187	±	1	38.9	±	1.1	1.6 ± 0.1		35.1	±	0.6	313	±	44	174	±	4	nd	19.0	±	4.8	nd	8.9 ± 1.6		nd
	Closure 4	181	±	6	40.6	±	1.8	1.42 ± 0.05		34.1	±	1.2	353	±	25	169	±	1	nd	10.8	±	0.2	nd	8.7 ± 0.7		nd
LR4	Closure 1	51	±	5	9.6	±	2.0	nd		9.8	±	0.7	91 ^a	±	2	95	±	1	nd	nd			nd	nd		nd
	Closure 2	46	±	1	10.7	±	1.2	nd		10.3	±	0.3	83 ^a	±	3	96	±	4	nd	nd			nd	nd		nd
	Closure 3	47	±	1	9.4	±	0.8	nd		10.4	±	0.2	60 ^a	±	1	95	±	5	nd	nd			nd	7.5 ± 0.3		nd
	Closure 4	46	±	2	11.4	±	1.5	nd		10.1	±	0.2	60 ^a	±	1	91.7	±	0.2	nd	nd			nd	nd		nd

*data obtained with n=1. **extrapolated values (obtained for concentrations superior to the calibration curve).

Table S2. Retention time (RT) and detection conditions by tandem mass spectrometry.

Compound structure	RT (min)	Precursor ion (<i>m/z</i>)	Collision energy (eV)	Daughter ion (<i>m/z</i>)
Ethanethiol (EtSH)	4.82	62 [M] ⁺	15	29 [M-SH] ⁺
		62 [M] ⁺	10	47 [M-CH ₃] ⁺
Dimethyl sulfide (DMS)	5.04	62 [M] ⁺	15	47 [M-CH ₃] ⁺
Diethyl sulfide (DES)	11.08	90 [M] ⁺	10	62 [M-H ₂ C=CH ₂] ⁺
		90 [M] ⁺	15	75 [M-H ₂ C=CH ₂] ⁺
		75 [M-H ₂ C=CH ₂] ⁺	10	47 [M-C ₂ H ₄ -CH ₃] ⁺
Thiophene (Internal Standard)	16.35	84 [M] ⁺	25	45 [M-C ₃ H ₃] ⁺
		84 [M] ⁺	20	58 [M-C ₂ H ₂] ⁺
S-methyl thioacetate (SMTA)	17.07	90 [M] ⁺	5	43 [M-S-CH ₃] ⁺
Dimethyl disulfide (DMDS)	17.66	94 [M] ⁺	35	64 [M-CH ₃ -CH ₃] ⁺
		94 [M] ⁺	15	79 [M-CH ₃] ⁺
S-ethyl thioacetate (ETA)	17.96	104 [M] ⁺	10	43 [M-S-CH ₂ -CH ₃] ⁺
		104 [M] ⁺	10	61 [M-H ₃ C-C=O] ⁺
Diethyl disulfide (DEDS)	20.69	122 [M] ⁺	2	94 [M-H ₂ C=CH ₂] ⁺
		94 [M-H ₂ C=CH ₂] ⁺	2	66 [M-H ₂ C=CH ₂ -H ₂ C=CH ₂] ⁺