

Table S1. The standard curve, validation range, LOD, LOQ, HRF score and coefficient of determination (r²) for sulfur volatile compounds in passion fruit wine.

Standard	HRF score	Formula	M ^a	Mass error (ppm)	Calibrated range (µg/L)	r ²	Slope	Intercept	LOD (µg/L)	LOQ
Benzothiazole	99.628	C ₇ H ₅ NS ⁺	135.0137	0.7021	0.01-43.75	0.9941	217.69	-0.1519	0.001	0.005
			*						6	3
		C ₆ H ₄ S ⁺	108.0029	0.7931						
		C ₄ H ₂ S ⁺	81.9872	0.9022						
Diethyl disulfide	97.0433	C ₄ H ₁₀ S ₂ ⁺	122.0218	0.2315	0.08-41.00	0.9957	45.71	0.1037	0.006	0.020
			*						8	4
		C ₂ H ₆ S ₂ ⁺	93.9906	0.6783						
		CH ₃ S ₂ ⁺	78.9672	0.7022						
3-(Methylthio)propanoic acid ethyl ester	94.9905	C ₆ H ₁₂ O ₂ S ⁺	148.0553	0.1444	0.016-130.00	0.9964	396.81	0.0611	0.003	0.012
			*						9	9
		C ₃ H ₆ S ⁺	74.0185*	0.2424						
		C ₃ H ₇ S ⁺	75.0263	0.2631						
3-(Methylthio)propyl acetate	95.1033	C ₆ H ₁₂ O ₂ S ⁺	148.0553	0.6668	0.88-113.20	0.9955	3069.50	-6.7311	0.006	0.020
			*						8	4
		C ₄ H ₈ S ⁺	88.0341*	0.3762						
		C ₃ H ₅ O ₂ ⁺	73.0285	0.8079						
Methionol	97.0737	C ₄ H ₁₀ OS ⁺	106.0447	0.5426	5.16-1320.00	0.9977	17319.0	-32.435	0.012	0.042
			*						8	8
		C ₄ H ₈ S ⁺	88.0342	0.8896						
		C ₃ H ₅ S ⁺	73.0107	0.8977						
3-Mercaptohexyl acetate	99.7294	C ₄ H ₇ S ⁺	87.0263*	0.2711	0.36-179.04	0.9993	910.40	-1.6925	0.002	0.007
									4	2
		C ₅ H ₉ S ⁺	101.0419	0.3188						
		C ₆ H ₁₂ S ⁺	116.0655	0.4352						
2-Methyltetrahydrothiophen-3-one	100	C ₅ H ₈ OS ⁺	116.0291	0.4785	0.72-46.38	0.9993	1043.00	-1.2723	0.002	0.008
			*						6	6
		C ₄ H ₈ S ⁺	88.0342	0.5219						
		C ₂ H ₄ S ⁺	60.0029	0.7119						
3-Mercaptohexanol	93.3314	C ₆ H ₁₄ OS ⁺	134.0761	0.6841	0.24-30.88	0.9995	1761.80	-0.0445	0.046	0.155
									7	6
		C ₆ H ₁₀ ⁺	82.0777*	0.9026						
		C ₅ H ₇ ⁺	67.0543	0.9502						
S-Ethyl ethanethioate	96.0453	C ₄ H ₈ OS ⁺	104.0291	0.5094	1.60-226.00	0.9984	489.79	0.792	0.012	0.038
									8	4
		C ₂ H ₃ O ⁺	43.0178*	0.4076						
		C ₂ H ₄ S ⁺	60.0028	0.8044						

a HRF (High-Resolution Filtering score); percentage of the spectrum obtained by MS Orbitrap that can be explained by combination of accurate mass, library matching and percentage of explained ions observed.

b Exact mass spectra

c Limit of detection

d Limit of quantification

* Quantitative ion

bold: Molecular ion peak

Table S2. Significant differences of OAV among yeast strain ES488 (ES), BV818 (BV), VIC (VI), and CY3079 (CY).

Odor series	ES	BV	VI	CY
Fruity	1591.78±7.07a	288.68±4.24d	330.57±3.19c	372.9±1.98b
Floral	9017.49±7.78b	7342.91±5.23d	8533.87±6.16c	10333.03±7.44a
Herbaceous (or vegetal)	781.72±21.21a	476.5±3.94b	305.76±3.22c	21.8±1.21d
Caramel	228.24±5.66b	180.04±3.46c	252.07±2.83a	253.25±2.23a
Earthy	2.15±0.09a	1.83±0.08a	2.19±0.13a	2.2±0.14a
Chemical	112.05±1.38c	176.81±2.12a	151.64±1.09b	69.6±1.71d
Fatty	280.57±4.93c	321.65±2.79b	355.7±2.55a	366.22±3.62a

Data are the mean ± standard deviation of duplicate tests. Different letters in each row indicate significant difference at a significant level of 0.05.

Table S3. Mean, standard deviation value and Tukey's test of sensory evaluation.

Attribute	ES	BV	VI	CY
Passion fruit	89.44±0.39a	87.93±0.47a	74.1±0.71b	75±0.71b
Mango	47.38±0.44b	49.92±0.37b	58.62±0.48a	60.13±0.61a
Green apple	45.28±0.51b	32.57±0.3d	39.77±0.87c	50.45±0.39a
Lemon	46.54±0.54b	53.56±0.52a	37.94±0.25c	48.07±0.3b
Floral	1.95±0.04d	6.32±0.06c	12.88±0.08b	37.45±0.46a

Data are the mean ± standard deviation of duplicate tests. Different letters in each row indicate significant difference at a significant level of 0.05.

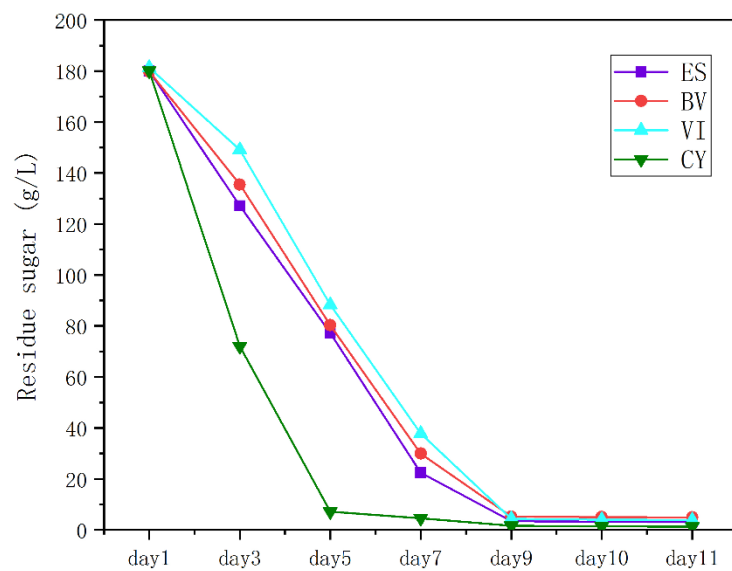


Figure S1. Residual sugar of passion fruit wine fermented by commercial yeast strain ES488 (ES), BV818 (BV), VIC (VI), and CY3079 (CY).