

Supplemental Data for:

Yang R, Qian YL, Feng Y, Huang L, Alcazar Magana A and Qian MC. 2023. Volatile phenols in smoke-exposed Pinot noir wines - Biomarkers and model prediction. *Am J Enol Vitic* 74:0740028. DOI: 10.5344/ajev.2023.22073

Supplemental Table 1 Chemical standards, target ions, internal standards (IS), and calibration curves used to quantify free and total volatile phenols.

Compound	m/z	Linear range (µg/L)	R ²		Equation	
			Free-form	Total	Free-form	Total
Guaiacol- <i>d</i> ₄ (IS)	113, 128					
Guaiacol	124, 109	0.05 - 100	0.9991	0.9999	y = 0.907x + 0.0138	y = 1.056x + 0.0095
4-Methylguaiacol- <i>d</i> ₃ (IS)	141, 126					
4-Methylguaiacol	138, 123	0.05 - 100	0.9998	0.9999	y = 0.935x + 0.0082	y = 0.95x + 0.0088
<i>o</i> -Cresol- <i>d</i> ₇ (IS)	115, 113					
<i>o</i> -Cresol	108, 107	0.05 - 100	0.9997	0.9999	y = 0.973x + 0.0203	y = 0.9987x + 0.0041
<i>p</i> -Cresol- <i>d</i> ₇ (IS)	115, 113					
<i>p</i> -Cresol	108, 107	0.05 - 100	0.9998	0.9998	y = 1.315x + 0.0751	y = 1.357x + 0.0191
<i>m</i> -Cresol- <i>d</i> ₇ (IS)	115, 113					
<i>m</i> -Cresol	108, 107	0.05 - 100	0.9993	0.9999	y = 1.216x + 0.0585	y = 1.357x + 0.0135

Supplemental Table 2 Eigenvalues of each principal component (PC) and cumulative percentage of variance explained. Eigenvalues represent the total variance explained by a given PC expressed as a percentage of the total variation in the data set. The cumulative percent of variance explained sums to one because PCs are orthogonal. For example, PC 1 accounted for 74.6% of the variance. PC 1 and PC 2 explained 83.2% of the total variance of the smoke-exposed group.

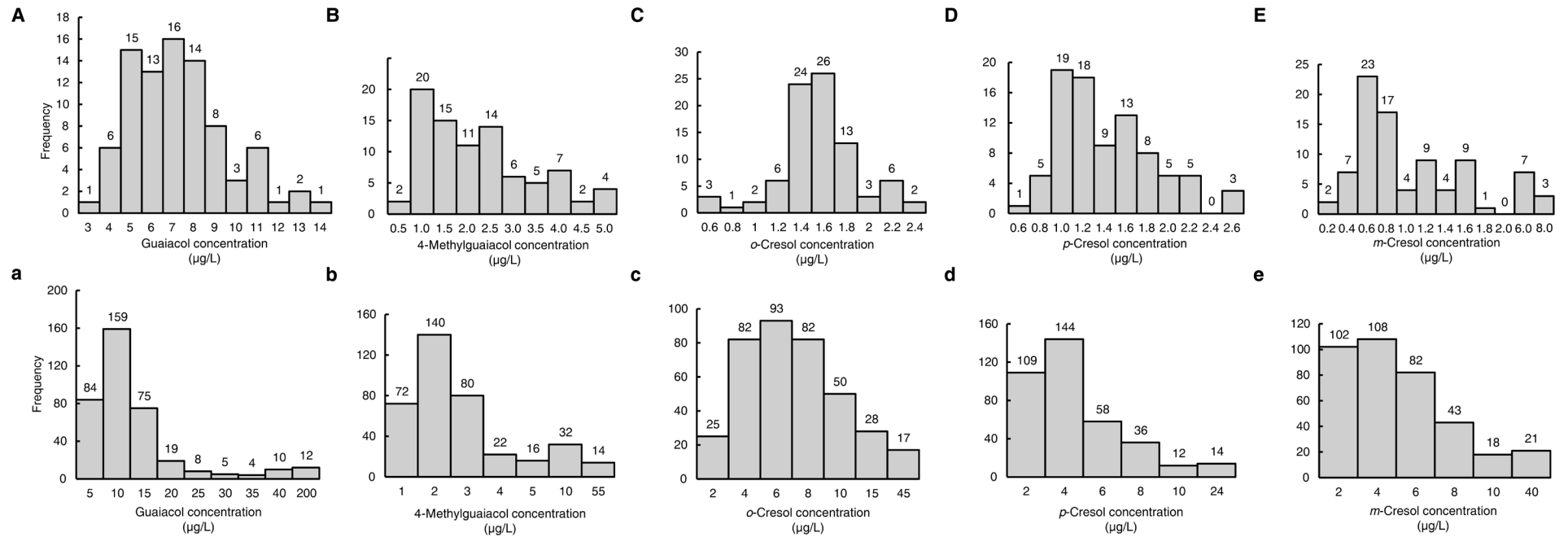
Number	Eigenvalue	Percent	Percentage (cumulative)
1	7.4617	74.617	74.617
2	0.8564	8.564	83.181
3	0.6144	6.144	89.325
4	0.4161	4.161	93.486
5	0.3174	3.174	96.661
6	0.1303	1.303	97.964
7	0.0958	0.958	98.922
8	0.0645	0.645	99.566
9	0.0293	0.293	99.859
10	0.0141	0.141	100.000

Supplemental Table 3 Loading coefficients from principal component analysis (PCA) and common factor analysis. The vectors found by the PCA and factor analysis explain the dominant multivariate variances of the phenols. Principal component (PC) 1 indicates nearly even contributions of the free and total forms. Factor 1 of the factor analyses illustrates more weight in the guaiacols than in the cresols. -F, free form; -T, total of free and bound forms.

Compound	PCA		Varimax rotation		Quartimin rotation	
	PC 1	PC 2	Factor 1	Factor 2	Factor 1	Factor 2
Guaiacol-F	0.35	-0.08	0.85	0.49	0.90	0.12
4-Methylguaiacol-F	0.33	-0.06	0.79	0.43	0.85	0.08
<i>m</i> -Cresol-F	0.34	0.23	0.63	0.75	0.54	0.54
<i>o</i> -Cresol-F	0.32	0.31	0.54	0.76	0.42	0.61
<i>p</i> -Cresol-F	0.24	0.77	0.21	0.79	-0.01	0.83
Guaiacol-T	0.34	-0.30	0.93	0.29	1.06	-0.15
4-Methylguaiacol-T	0.33	-0.32	0.92	0.28	1.06	-0.17
<i>m</i> -Cresol-T	0.24	-0.17	0.51	0.33	0.53	0.11
<i>o</i> -Cresol-T	0.34	-0.10	0.77	0.50	0.80	0.17
<i>p</i> -Cresol-T	0.30	-0.10	0.66	0.38	0.70	0.09

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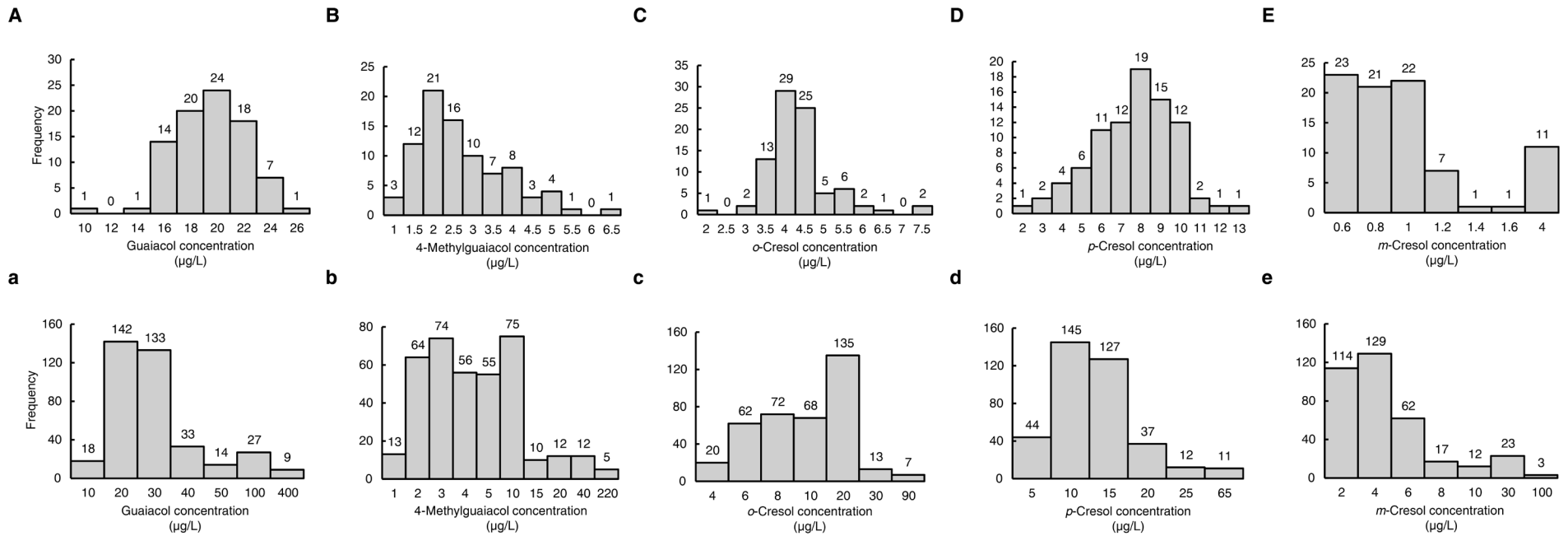
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Supplemental Figure 1 The frequency distribution of free-form volatile phenols in control (panels A to E) and smoke-exposed (panels a to e) wines. The frequency represents the number of samples with ratios within the interval (5:0-5, 10:5-10, 15:10-15, etc.). For example, (a) illustrates that out of the 376 smoke-exposed red wines, 84 and 159 samples had a free guaiacol concentration between 0 and 5 µg/L and between 5 to 10 µg/L, respectively; (b) shows that 140 and 292 samples (140 + 80 + 72) samples had a 4-methylguaiacol concentration between 1 and 2 µg/L and <3 µg/L, respectively.

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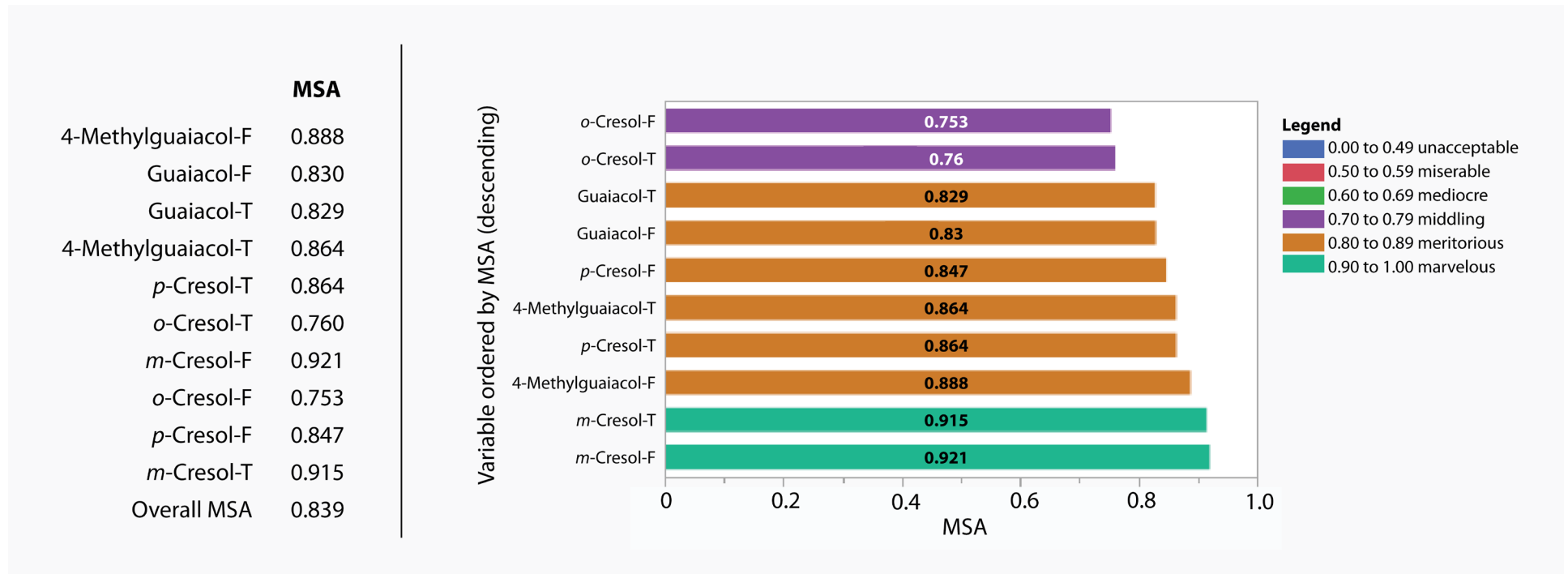
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Supplemental Figure 2 The frequency distribution of the total (free- and bound-form) volatile phenols in control (panels A to E) and smoke-exposed (panels a to e) wines.

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Supplemental Figure 3 A measure of sample adequacy (MSA) by Kaiser-Meyer-Olkin test indicates how suitable the data is for factor analysis, measuring sample adequacy for each variable in the model and for the complete model. A rule of thumb is that the samples are adequate for factor analysis if values are between 0.8 and 1. -F, free form; -T, total of free and bound forms.