

Table S1. Mean values \pm standard error of the volatile aromatic compounds identified in the shiraz wine samples using gas chromatography mass spectroscopy.

VAC	RT	S00	S07	S08	S10	S13	S14	S15	S16	S17	S18	S19	S20	S21
VAC1	4.01	0.00	0.00	0.00	0.00	582,586.00	0.00	498,953.50	446,518.00	585,792.33	0.00	0.00	584,646.00	561,489.00
		± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	97,846.09	75,102.17	89,434.04	± 0.00	± 0.00	± 0.00	59,373.27
VAC2	4.94	0.00	0.00	0.00	0.00	0.00	0.00	0	0	0.00	9,545,274.00	0	0	0
		± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	2,192,038.98	773,588.05	± 0.00	± 0.00	± 0.00	769,212.93	690,670.38
VAC3	5.43	0.00	0.00	7,941,351.00	0.00	0	0.00	0.00	4,188,088.50	0.00	0.00	5,822,721.00	0.00	0.00
		± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	2,590,621.59	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00
VAC4	8.78	982,166.50	0.00	1,132,349.00	0.00	939,663.00	0.00	0.00	0.00	793,795.00	220,739.50	857,331.00	2,034,833.00	908,769.50
		591,141.48	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	398,201.30	10,689.16	52,576.66	1,105,489.83	87,646.42
VAC5	9.01	335,953.50	1,146,852.50	970,497.00	1,441,732.33	1,193,805.50	1,461,028.67	1,361,862.00	1,372,108.00	1,997,121.00	0.00	2,429,892.67	2,955,596.67	2,932,314.50
		3205.16	11,076.18	267,996.35	75,017.59	19,150.52	89,458.74	213,343.70	± 0.00	398,201.30	10,689.16	52,576.66	1,105,489.83	87,646.42
VAC6	9.44	231,666.00	0.00	0.00	0.00	0.00	0.00	386,889.00	0.00	0.00	266,816.00	0.00	783,791.00	0.00
		± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	110,580.58	± 0.00
VAC7	9.83	0.00	357,272.00	329,264.00	197,814.00	421,547.00	0.00	729,797.67	719,603.00	396,677.00	0.00	1,442,898.00	0.00	0.00
		± 0.00	± 0.00	± 0.00	± 0.00	10,535.26	± 0.00	105,343.62	26,593.29	± 0.00	± 0.00	920,915.88	± 0.00	± 0.00
VAC8	10.01	222,010.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00
VAC9	12.07	0.00	0.00	0.00	8,692,493.00	0.00	3,539,349.00	0.00	0.00	0.00	6,610,292.00	751,574.67	1,438,496.50	0.00
		± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	236,635.19	463,449.58	± 0.00
VAC10	14.56	13,103,126.6	11,383,975.3	11,164,952.0	24,037,713.0	14,528,443.3	25,882,878.5	11,864,755.5	18,596,746.3	11,732,983.3		16,487,631.0		
		8,972,259.50	7	3	0	3	0	0	3	3	8,498,525.67	0	9,143,593.00	
VAC11	14.69	1,202,514.53	1,164,270.70	5,533,833.16	215,424.08	± 0.00	665,781.36	2,182,322.67	6901.44	392,427.51	1,488,539.82	440,216.09	± 0.00	610,361.40
		12,962,094.0	20,654,426.0			24,463,542.5		28,570,558.0						
VAC12	15.69	0	0.00	0	0.00	0	0.00	0	0.00	0.00	0.00	0.00	0.00	0.00
		± 0.00	± 0.00	± 0.00	± 0.00	1,303,889.11	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00
VAC13	15.80	267,392.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	757,989.00	468,579.33	409,202.00	0.00
		± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00
VAC14	15.99	541,715.00	1,149,514.33	1,148,721.00	514,861.00	1,046,087.00	489,810.00	1,661,054.33	575,559.00	0.00	7,569,626.33	0.00	0.00	0.00
		48,540.72	109,677.50	144,074.70	50,148.40	224,827.22	86,850.74	903,747.93	28,971.93	± 0.00	7,109,565.07	± 0.00	± 0.00	± 0.00
VAC15	16.28	21,654,569.0	25,275,779.0	29,564,922.3	16,243,744.6	28,715,803.0	29,116,271.3	29,364,413.3	16,732,809.3	147,224,51.3	17,146,253.5	8,529,746.33	8,739,812.00	11,333,319.0
		0	0	3	7	0	3	3	3	3	0		0	
VAC16	19.15	2,765,495.95	1,228,298.65	2,026,217.88	236,712.83	688,330.55	1,901,106.08	1,180,889.78	984,914.65	117,849.23	530,321.47	635,978.01	432,328.84	858,891.99
		11,206,982.3	25,981,961.0	16,442,085.3	13,146,117.3	11,952,724.6		22,508,215.3	20,536,964.3	29,478,570.0	17,613,437.0	14,171,785.6		34,620,343.3
VAC17	16.28	3	0	3	3	7	8,679,119.33	3	3	0	0	7	7,805,214.67	3
		1,964,176.76	1,847,601.53	1,252,407.93	524,850.98	334,335.74	844,133.81	10,345,381.17	1,424,460.34	318,485.70	769,690.10	7,463,365.72	420,043.55	6,444,760.82
VAC18	19.15	977,434.00	1,558,497.67	3,415,396.67	457,376.00	0.00	383,650.00	886,740.50	444,177.67	0.00	0.00	390,456.00	0.00	0.00
		277,627.97	101,526.60	405,921.31	161,982.49	± 0.00	4707.10	67,030.70	11364.34	± 0.00	± 0.00	± 0.00	± 0.00	± 0.00

VAC17	19.41	635,074.00	2,655,743.67	1,615,585.00	797,998.33	386,986.00	1,151,424.33	4,586,270.33	5,480,612.67	9,867,656.00	2,210,302.00	12,144,151.6	4,325,683.67	15,814,294.6
		193,473.09	458,800.92	98,104.91	57,207.30	±0.00	73,753.54	1,634,257.09	395,886.55	603,043.47	33,7654.00	1,984,404.32	661,647.50	1,105,565.92

Abbreviation: VAC: volatile aromatic compounds, as shown in Table 3; RT: retention time; Vintage: as shown in Table 1.

Table S2. Statistical parameters resulting from the machine learning models.

Model	Epoch	Gradient	Mu	Validation checks	Effective number of parameters	Sum squared parameters
Model 1	1000	6.16×10^{-5}	500	NA	169	1.02×10^4
Model 2	13	1.36	1.00×10^{-5}	6	NA	NA
Model 3	259	3.23×10^{10}	5.00×10^{10}	NA	233	1.42×10^3

NA: not applicable.