SUPPLEMENTARY DATA
Vasiliki Summerson, Claudia Gonzalez Viejo, Damir D. Torrico, Alexis Pang and Sigfredo Fuentes (2020).
Detection of smoke-derived compounds from bushfires in Cabernet-Sauvignon grapes, must, and wine using Near-Infrared spectroscopy and machine learning algorithms. *OENO One*, *54*(4). https://doi.org/10.20870/oeno-one.2020.54.1.4105

Table S1. Levels of volatile phenols in grape juice (µg/L) and their glycoconjugates in grape homogenate (µg/kg) one day after smoke treatments

		C		CM		LS		HS		HSM	
		Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD
Volatile phenols	guaiacol	2^{c}	0	2^{c}	0	3^{c}	0	25^{a}	9	17^{b}	4
	4MG	4^{b}	0	4^{b}	0	4^{b}	0	5^{a}	1	5^{a}	1
	phenol	2^{b}	0	3^{b}	1	5^{b}	1	12^{a}	3	11^{a}	3
	Syringol	8^{b}	5	21^{ab}	18	6^{b}	1	24^{a}	3	21^{ab}	3
	MSy	2^{bc}	0	2^{c}	0	2^{bc}	0	3^{a}	0	2^{b}	0
	m-cresol	2^{b}	0	2^{b}	0	3^{b}	0	8^{a}	0	8^{a}	0
	p-cresol	0^{b}	0	0^{b}	0	1^{b}	1	12^{a}	6	9^{a}	2
	total m/p cresol	1^{b}	0	1^{b}	0	2^{b}	1	10^{a}	3	10^{a}	4
	o-cresol	2^{b}	0	2^{b}	0	3^{b}	1	12^{a}	4	11^{a}	3
	total cresols	3^{b}	0	3^{b}	0	5^{b}	2	23^{a}	8	21^{a}	7
Glycoconjugate	SyGG	10.8^{c}	6.6	3.6^{c}	0.4	20.8^{bc}	2.8	248.0^{a}	136.0	129.4^{b}	34.0
	SyMG	1.6^{bc}	1.3	0.4^{c}	0.2	3.2^{bc}	0.6	43.4^{a}	21.1	19.4^{b}	5.7
	SyPG	2.0^{c}	0.5	1.2^{c}	0.1	3.4^{c}	0.2	18.9^{a}	6.9	10.7^{b}	2.9
	CrPG	19.1^{b}	1.7	12.4^{b}	0.5	26.9^{b}	0.2	136.6^{a}	55.7	96.0^{a}	23.8
	CrGG	0.6^{bc}	0.2	0.4^{c}	0.1	0.5^{bc}	0.0	1.0^{a}	0.4	0.8^{ab}	0.1
	CrRG	4.9^{b}	1.5	2.3^{b}	0.4	9.2^{b}	0.2	56.0^{a}	23.4	41.8^{a}	9.4
	GuPG	7.3^{bc}	2.4	3.7^{c}	0.4	9.2^{bc}	0.2	114.6^{a}	56.4	55.2^{b}	19.8
	GuGG	0.2^{b}	0.1	0.1^{b}	0.0	0.5^{b}	0.1	5.7^{a}	3.3	3.7^{a}	0.8
	GuRG	0.0^{c}	0.1	0.0^{c}	0.1	0.9^{bc}	0.1	2.7^{a}	1.5	1.9^{ab}	0.1
	GuMG	0.8^{b}	0.3	0.3^{b}	0.1	3.0^{b}	0.3	34.5^{a}	25.7	15.2^{ab}	2.4
	MGuPG	1.7^{c}	0.7	0.8^{c}	0.1	2.5^{c}	0.2	36.2^{a}	17.2	18.2^{b}	6.3
	MGuRG	1.3^{c}	0.4	0.7^{c}	0.1	2.3^{c}	0.1	15.1^{a}	6.4	9.6^{b}	2.0
	MSyGG	2.1^{c}	1.3	0.5^{c}	0.1	3.2^{c}	0.4	44.0^{a}	21.4	21.4^{b}	4.2
	MSyPG	0.1^{c}	0.0	0.1^{c}	0.0	0.3^{c}	0.0	4.2^{a}	1.4	2.4^{b}	0.4
	PhRG	0.8^{b}	0.1	0.6^{b}	0.1	2.3^{a}	0.1	9.8^{a}	4.1	6.8^{a}	1.6
	PhGG	0.1^{c}	0.1	0.0^{c}	0.0	0.2^{c}	0.0	2.4^{a}	1.2	1.3^{b}	0.3
	PhPG	3.7^{b}	0.8	3.5^{b}	0.2	13.0^{b}	1.3	54.5^{a}	22.3	38.3^{a}	10.9
	PhMG	0.1^{b}	0.0	0.1^{b}	0.0	0.6^{b}	0.2	2.6^{a}	2.1	1.2^{ab}	0.3

Abbreviations: C = control without misting; CM = control with misting; LS = low density smoke exposure; HS = high density smoke exposure without misting; HSM = high density smoke exposure with misting. Gu = guaiacol; Cr = cresol; Ph = phenol; Sy = syringol; 4MG = 4-methylguaiacol; MSy = 4-methylsyringol; MG = monoglucoside; GG = glucose-glucoside; PG = pentose-glucoside; R = rutinoside; SD= standard deviation; Min= minimum value; Max= maximum value; nd = not detected. Means followed by different letters are statistically significant based on Fisher's least significant difference (LSD) post hoc test (α= 0.05).

Table S2. Levels of volatile phenols in grape juice (µg/L) and their glycoconjugates in grape homogenate (µg/kg) at harvest

		C		CM		LS		HS		HSM	
		Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD
Volatile phenols	guaiacol	2^{b}	0	2^{b}	0	3^{b}	0	10^{a}	3	8^{a}	2
	4MG	4^{b}	0	4^{b}	0	4^{b}	0	4^{a}	0	4^{a}	0
	phenol	2^{b}	1	2^{b}	0	6^{b}	2	21^{a}	7	17^{a}	5
	Syringol	ns	-	ns	-	ns	-	ns	-	ns	-
	MSy	ns	-	ns	-	ns	-	ns	-	ns	-
	m-cresol	2^{b}	0	2^{b}	0	3^{b}	0	5^{a}	1	5^{a}	1
	p-cresol	0^{b}	0	0^{b}	0	0^{b}	0	1^{a}	1	1^{a}	0
	total m/p cresol	1^{b}	0	1^{b}	0	2^{b}	1	6^{a}	2	6^{a}	1
	o-cresol	2^{b}	0	2^{b}	0	3^{b}	1	7^{a}	2	6^{a}	1
	total cresols	2^{b}	0	3^{b}	0	5^{b}	1	13^{a}	4	12^{a}	3
Glycoconjugate	SyGG	23.1^{c}	13.1	6.7^{c}	0.6	43.0^{c}	8.6	535.0^{a}	209.0	325.0^{b}	26.6
	SyMG	4.8^{c}	0.9	2.7^{c}	0.1	6.5^{c}	1.1	50.1^{a}	15.8	31.9^{b}	6.7
	SyPG	16.2^{c}	8.5	6.8^{c}	0.4	27.3^{c}	7.4	257.5^{a}	96.9	136.0^{b}	9.5
	CrPG	73.4^{c}	20.3	42.7^{c}	1.3	136.3^{c}	37.9	988.0^{a}	353.0	672.9^{b}	109.7
	CrGG	3.0^{c}	0.2	2.9^{c}	0.2	2.2^{c}	0.4	5.5^{a}	0.9	4.2^{b}	0.9
	CrRG	6.3^{c}	1.7	3.3^{c}	0.2	15.0^{c}	1.9	97.8^{a}	22.4	69.4^{b}	8.7
	GuPG	38.4^{c}	18.4	16.7^{c}	1.5	63.1^{c}	19.4	803.0^{a}	373.0	420.5^{b}	55.4
	GuGG	1.9^{b}	1.1	0.7^{b}	0.1	3.6^{b}	1.2	45.3^{a}	19.3	30.2^{a}	5.4
	GuMG	1.8^{c}	0.8	1.9^{c}	1.1	2.3^{bc}	0.5	20.4^{a}	8.6	9.4^{b}	1.5
	GuRG	2.2^{c}	0.8	1.2^{c}	0.1	4.3^{c}	0.5	25.1^{a}	6.0	17.1^{b}	0.8
	MGuPG	10.0^{c}	3.7	6.9^{c}	0.2	15.6^{bc}	4.2	170.8^{a}	83.3	83.3^{b}	9.6
	MGuRG	10.3^{c}	3.8	7.8^{c}	1.5	20.0^{c}	3.4	117.6^{a}	32.0	66.1^{b}	5.9
	MSyGG	10.2^{c}	6.7	2.7^{c}	0.2	14.5^{c}	4.5	220.3^{a}	71.2	114.9^{b}	24.3
	MSyPG	2.8^{c}	0.9	1.7^{c}	0.1	3.7^{c}	0.8	27.3^{a}	6.7	16.4^{b}	2.3
	PhRG	7.3^{c}	3.1	4.4^{c}	0.8	22.9^{c}	4.8	135.4^{a}	35.1	96.5^{b}	21.1
	PhGG	1.0^{c}	0.5	0.1^{c}	0.2	1.3^{c}	0.4	19.8^{a}	7.6	10.7^{b}	2.7
	PhPG	34.8^{c}	6.6	20.0^{c}	3.8	94.1^{c}	28.7	576.0^{a}	207.0	350.8^{b}	38.5
	PhMG	1.6^{c}	0.4	1.4^{c}	0.4	3.0^{bc}	0.7	13.5^{a}	7.7	8.8^{ab}	2.3

Abbreviations: C = control without misting; CM = control with misting; LS = low density smoke exposure; HS = high density smoke exposure without misting; HSM = high density smoke exposure with misting. Gu = guaiacol; Cr = cresol; Ph = phenol; Sy = syringol; 4MG = 4-methylguaiacol; MSy = 4-methylsyringol; MG = monoglucoside; GG = glucose-glucoside; PG = pentose-glucoside; R = rutinoside; SD= standard deviation; Min= minimum value; Max= maximum value; nd = not detected; ns = not significant. Means followed by different letters are statistically significant based on Fisher's least significant difference (LSD) post hoc test (α= 0.05).

Table S3. Levels of volatile phenols and their glycoconjugates (µg/L) in wine

		C		CM		LS		HS		HSM	
		Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD
Volatile phenols	guaiacol	2^{b}	1	1^{b}	1	4^{b}	1	29^{a}	9	23^{a}	1
	4MG	nd	-	nd	-	nd	-	4^{a}	1	3^{b}	0
	Syringol	2^{b}	1	2^{b}	0	3^{b}	1	5^{a}	1	5^{a}	1
	m-cresol	nd	-	nd	-	2^{b}	0	10^{a}	3	10^{a}	1
	p-cresol	nd	-	nd	-	1^{b}	1	7^{a}	2	5^{a}	0
	o-cresol	nd	-	nd	-	3^{b}	1	11^{a}	3	11^{a}	1
Glycoconjugate	SyGG	24.3^{c}	9.5	10.9^{c}	0.7	42.6^{c}	2.7	272.4^{b}	20.8	412.7^{a}	147.0
	SyMG	0.8^{c}	0.2	0.4^{c}	0.0	1.4^{c}	0.1	7.4^{b}	0.1	11.3^{a}	3.1
	SyPG	4.8^{c}	1.5	1.8^{c}	0.1	8.8^{c}	0.8	46.7^{b}	1.1	76.6^{a}	23.7
	CrPG	1.1^{c}	0.2	0.5^{c}	0.1	1.5^{c}	0.1	9.5^{b}	0.9	13.8^{a}	3.4
	CrRG	6.3^{c}	1.5	3.2^{c}	0.3	13.9^{c}	1.7	77.8^{b}	2.3	101.5^{a}	28.1
	GuPG	14.9^{c}	3.8	6.1^{c}	0.8	21.5^{c}	1.6	126.0^{b}	3.3	233.9^{a}	83.7
	GuGG	0.4^{b}	0.1	0.4^{b}	0.1	0.4^{b}	0.1	1.6^{a}	0.3	2.1^{a}	0.6
	GuRG	3.3^{c}	0.7	1.2^{c}	1.1	6.6^{c}	0.8	28.0^{b}	2.2	37.1^{a}	10.0
	GuMG	0.6^{c}	0.2	0.2^{c}	0.0	1.0^{c}	0.2	6.2^{b}	0.4	9.4^{a}	2.8
	MGuPG	2.3^{c}	0.6	1.5^{c}	0.1	3.3^{c}	0.3	19.4^{b}	0.5	37.1^{a}	12.8
	MGuRG	2.0^{c}	0.7	0.9^{c}	0.2	4.4^{c}	0.7	21.4^{b}	1.6	31.1^{a}	8.7
	MSyGG	0.9^{c}	0.5	0.2^{c}	0.1	1.5^{c}	0.2	11.5^{b}	1.5	22.9^{a}	6.8
	MSyPG	0.5^{c}	0.1	0.3^{c}	0.1	0.8^{c}	0.0	4.1^{b}	0.1	6.6^{a}	1.6
	PhRG	3.1^{c}	0.8	1.7^{c}	0.3	9.8^{c}	2.1	43.4^{b}	2.5	59.0^{a}	16.6
	PhGG	0.3^{c}	0.2	0.1^{c}	0.0	0.4^{c}	0.1	3.0^{b}	0.2	4.7^{a}	1.3
	PhPG	1.1^{c}	0.2	0.6^{c}	0.1	2.6^{c}	0.5	10.3^{b}	1.4	17.0^{a}	4.9
	PhMG	1.8^{c}	0.5	1.0^{c}	0.2	3.9^{c}	0.5	21.4^{b}	1.8	31.2^{a}	10.7

Abbreviations: C = control without misting; CM = control with misting; LS = low density smoke exposure; HS = high density smoke exposure without misting; HSM = high density smoke exposure with misting. Gu = guaiacol; Cr = cresol; Ph = phenol; Sy = syringol; 4MG = 4-methylguaiacol; MSy = 4-methylsyringol; MG = monoglucoside; GG = glucose-glucoside; PG = pentose-glucoside; R = rutinoside; SD= standard deviation; Min= minimum value; Max= maximum value; nd = not detected. Means followed by different letters are statistically significant based on Fisher's least significant difference (LSD) post hoc test (α= 0.05).

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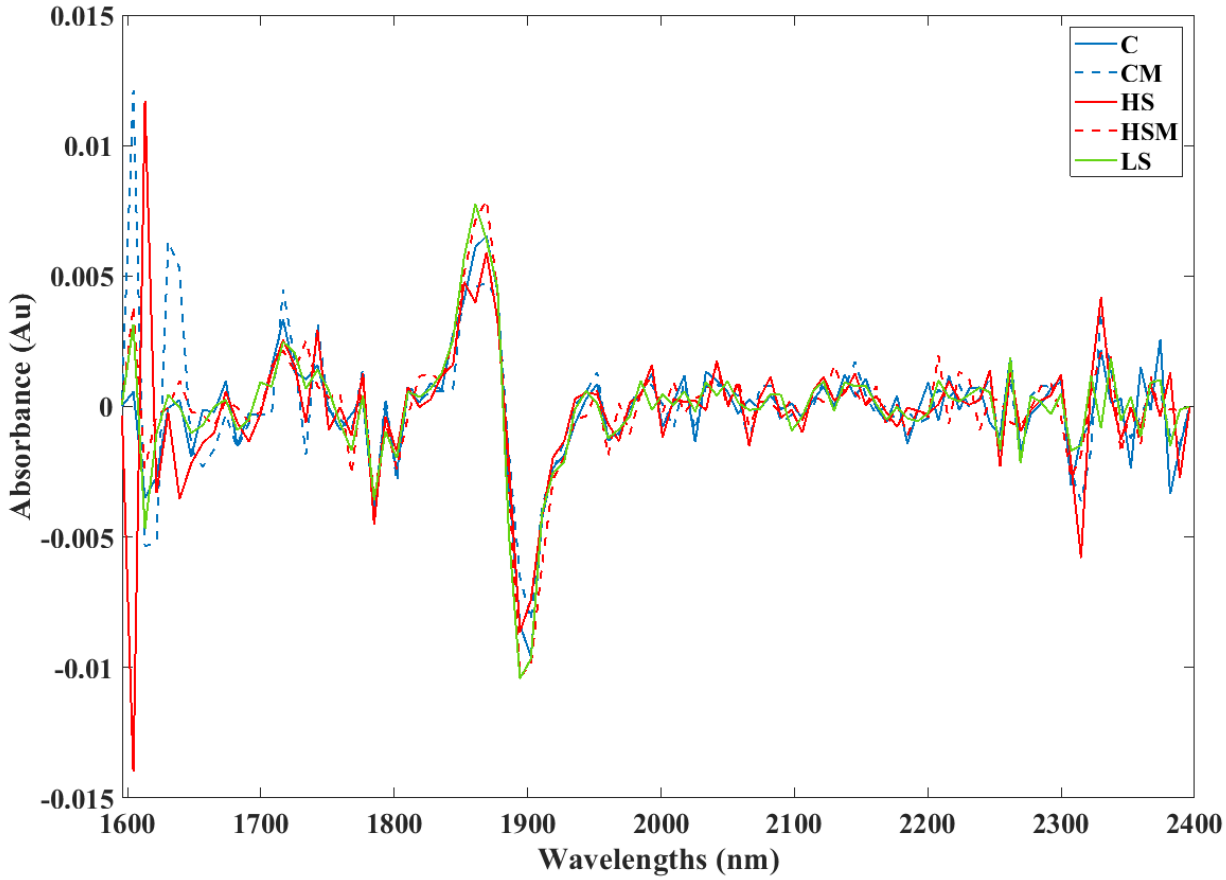

Figure S1. Second derivative berry spectra for the five smoke treatments. Abbreviations: C = control without misting; CM = control with misting; HS = high-density smoke without misting; HSM = high-density smoke with misting; and LS = low-density smoke

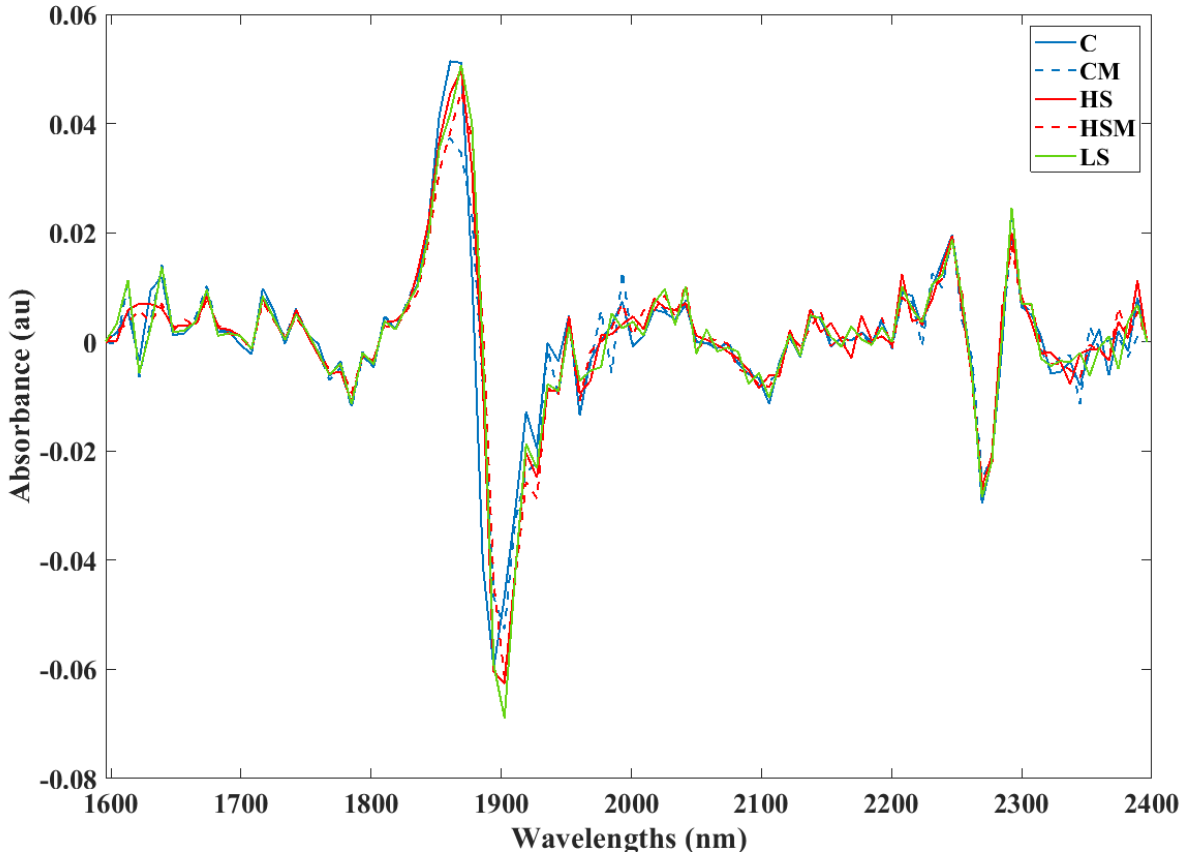

Figure S2. Second derivative must spectra for the five smoke treatments. Abbreviations: C = control without misting; CM = control with misting; HS = high-density smoke without misting; HSM = high-density smoke with misting; and LS = low-density smoke

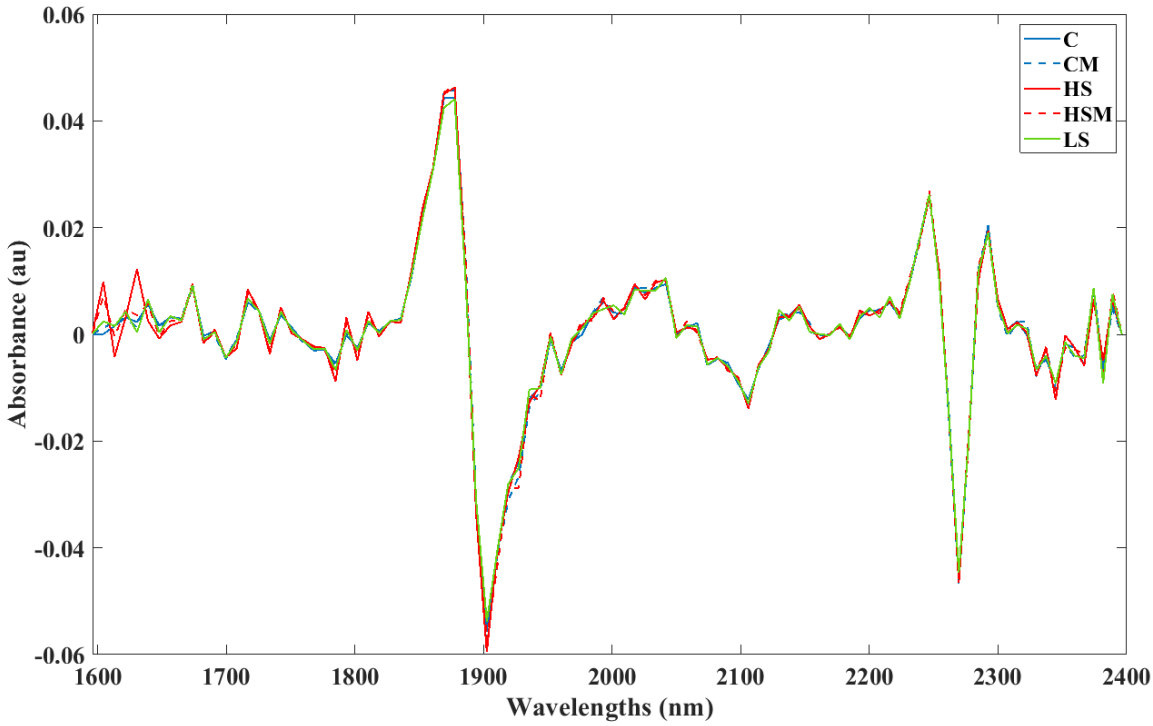

Figure 4. Second derivative wine spectra for the five smoke treatments. Abbreviations: C = control without misting; CM = control with misting; HS = high-density smoke without misting; HSM = high-density smoke with misting; and LS = low-density smoke