Table S1: Pairwise regression vector (RV) coefficients ($p \leq 0.01$) for score configuration using IR raw data vs. its mathematical transformations using multiplicative scatter correction (MSC), first derivative (1st deriv), and their combinations before Principal Component Analysis (PCA).

Data set		1st deriv	1st deriv MSC	MSC	MSC 1st deriv	raw	1st deriv	1st deriv MSC	MSC	MSC 1st deriv	raw
AVN	1st deriv	1	0.99	0.81	0.98	0.83	1	0.97	0.89	0.97	0.84
	1st deriv MSC	0.99	1	0.82	0.99	0.78	0.97	1	0.9	0.99	0.74
	MSC	0.81	0.82	1	0.87	0.88	0.89	0.9	1	0.92	0.83
	MSC 1st deriv	0.98	0.99	0.87	1	0.82	0.97	0.99	0.92	1	0.74
	raw	0.83	0.78	0.88	0.82	1	0.84	0.74	0.83	0.74	1
CDB	1st deriv	1	0.98	0.92	0.98	0.89	1	0.98	0.91	0.98	0.86
	1st deriv MSC	0.98	1	0.94	1	0.78	0.98	1	0.9	0.99	0.76
	MSC	0.92	0.94	1	0.95	0.75	0.91	0.9	1	0.93	0.77
	MSC 1st deriv	0.98	1	0.95	1	0.78	0.98	0.99	0.93	1	0.76
	raw	0.89	0.78	0.75	0.78	1	0.86	0.76	0.77	0.76	1
DTK	1st deriv	1	0.88	0.81	0.89	0.89	1	0.98	0.92	0.97	0.89
	1st deriv MSC	0.88	1	0.95	1	0.89	0.98	1	0.97	1	0.78
	MSC	0.81	0.95	1	0.94	0.95	0.92	0.97	1	0.97	0.7
	MSC 1st deriv	0.89	1	0.94	1	0.88	0.97	1	0.97	1	0.76
	raw	0.89	0.89	0.95	0.88	1	0.89	0.78	0.7	0.76	1
FRV	1st deriv	1	0.97	0.88	0.95	0.88	1	0.95	0.91	0.94	0.9
	1st deriv MSC	0.97	1	0.9	1	0.75	0.95	1	0.93	1	0.72
	MSC	0.88	0.9	1	0.92	0.77	0.91	0.93	1	0.94	0.74
	MSC 1st deriv	0.95	1	0.92	1	0.73	0.94	1	0.94	1	0.71
	raw	0.88	0.75	0.77	0.73	1	0.9	0.72	0.74	0.71	1
KZC	1st deriv	1	0.44	0.37	0.46	0.98	1	0.97	0.91	0.97	0.88
	1st deriv MSC	0.44	1	0.99	0.99	0.38	0.97	1	0.93	1	0.76
	MSC	0.37	0.99	1	0.99	0.31	0.91	0.93	1	0.94	0.73
	MSC 1st deriv	0.46	0.99	0.99	1	0.41	0.97	1	0.94	1	0.76
	raw	0.98	0.38	0.31	0.41	1	0.88	0.76	0.73	0.76	1
PDB	1st deriv	1	0.98	0.82	0.96	0.92	1	0.96	0.91	0.95	0.85
	1st deriv MSC	0.98	1	0.9	0.99	0.89	0.96	1	0.94	1	0.74
	MSC	0.82	0.9	1	0.94	0.86	0.91	0.94	1	0.93	0.76
	MSC 1st deriv	0.96	0.99	0.94	1	0.9	0.95	1	0.93	1	0.73
	raw	0.92	0.89	0.86	0.9	1	0.85	0.74	0.76	0.73	1
Average	overall	0.85	0.88	0.84	0.89	0.79	0.93	0.91	0.88	0.91	0.78
	without KZC	0.91	0.92	0.88	0.92	0.84	---	---	---	---	---
Stdev	Overall	0.17	0.16	0.16	0.15	0.17	0.04	0.1	0.08	0.1	0.06
	without KZC	0.06	0.08	0.06	0.07	0.06	---	---	---	---	---
Overall	min	0.37	0.38	0.31	0.41	0.31	0.84	0.72	0.7	0.71	0.7
	max	0.99	1	0.99	1	0.98	0.98	1	0.97	1	0.9
Without KZC	min	0.81	0.75	0.75	0.73	0.73	---	---	---	---	---
	max	0.99	1	0.95	1	0.95	---	---	---	---	---

Table S2: Cumulative percentage explained variance (%EV) of the first two principal components of the PCA (VCC, ARP, UV-Vis, and IR) and first two dimensions of the CA (sensory) for individual data sets.

| CULTIVAR	DATA SET	VCC	ARP	UV-VIS	INFRA-RED	SENSORY
CHENIN BLANC	AVN	82	84	93	79	65
	CDB	83	80	91	74	78
	DTK	72	85	97	96	66
	FRV	74	83	78	76	71
	KZC	76	94	93	98	76
	PDB	74	92	95	83	72
	average	77	86	91	84	71
	stdev	4	5	6	9	5
SAUVIGNON BLANC	AVN	79	82	92	68	64
	CDB	73	75	97	71	68
	DTK	76	81	80	64	71
	FRV	76	86	99	80	66
	KZC	80	79	97	65	55
	PDB	74	88	82	77	62
	average	76	82	91	71	64
	stdev	2	4	8	6	5
OVERALL	low	72	75	78	64	55
	high	83	94	99	98	78
	average	77	84	91	78	68
	stdev	3	5	7	10	6

The sample sets are identified by three letters corresponding to each winery (i.e., AVN, CDB, DTK, FRV, KZC, PDB).

Table S3: Pairwise RV coefficients (p ≤ 0.01) for the scores of the individual data blocks.

Data set	Data block	Chenin Blanc					Sauvignon Blanc				
		ARP	UV-Vis	IR	Sensory	VCC	ARP	UV-Vis	IR	Sensory	VCC
AVN	ARP	1	0.8	0.38	0.85	0.83	1	0.73	0.31	0.8	0.82
	UV-Vis	0.8	1	0.39	0.73	0.81	0.73	1	0.46	0.63	0.5
	IR	0.38	0.39	1	0.51	0.56	0.31	0.46	1	0.51	0.27
	Sensory	0.85	0.73	0.51	1	0.81	0.8	0.63	0.51	1	0.66
	VCC	0.83	0.81	0.56	0.81	1	0.82	0.5	0.27	0.66	1
CDB	ARP	1	0.79	0.47	0.87	0.63	1	0.93	0.47	0.6	0.5
	UV-Vis	0.79	1	0.39	0.67	0.39	0.93	1	0.31	0.43	0.33
	IR	0.47	0.39	1	0.71	0.54	0.47	0.31	1	0.72	0.75
	Sensory	0.87	0.67	0.71	1	0.72	0.6	0.43	0.72	1	0.85
	VCC	0.63	0.39	0.54	0.72	1	0.5	0.33	0.75	0.85	1
DTK	ARP	1	0.82	0.2	0.79	0.66	1	0.9	0.4	0.82	0.62
	UV-Vis	0.82	1	0.1	0.7	0.48	0.9	1	0.62	0.79	0.62
	IR	0.2	0.1	1	0.38	0.45	0.4	0.62	1	0.55	0.51
	Sensory	0.79	0.7	0.38	1	0.79	0.82	0.79	0.55	1	0.73
	VCC	0.66	0.48	0.45	0.79	1	0.62	0.62	0.51	0.73	1
FRV	ARP	1	0.9	0.71	0.78	0.55	1	0.83	0.38	0.73	0.6
	UV-Vis	0.9	1	0.67	0.73	0.58	0.83	1	0.21	0.46	0.45
	IR	0.71	0.67	1	0.78	0.69	0.38	0.21	1	0.61	0.62
	Sensory	0.78	0.73	0.78	1	0.73	0.73	0.46	0.61	1	0.73
	VCC	0.55	0.58	0.69	0.73	1	0.6	0.45	0.62	0.73	1
KZC	ARP	1	0.78	0.33	0.62	0.57	1	0.72	0.74	0.69	0.58
	UV-Vis	0.78	1	0.56	0.74	0.52	0.72	1	0.79	0.43	0.34
	IR	0.33	0.56	1	0.47	0.41	0.74	0.79	1	0.66	0.46
	Sensory	0.62	0.74	0.47	1	0.6	0.69	0.43	0.66	1	0.66
	VCC	0.57	0.52	0.41	0.6	1	0.58	0.34	0.46	0.66	1
PDB	ARP	1	0.93	0.67	0.63	0.76	1	0.92	0.68	0.71	0.45
	UV-Vis	0.93	1	0.62	0.59	0.66	0.92	1	0.62	0.67	0.51
	IR	0.67	0.62	1	0.86	0.58	0.68	0.62	1	0.66	0.42
	Sensory	0.63	0.59	0.86	1	0.67	0.71	0.67	0.66	1	0.63
	VCC	0.76	0.66	0.58	0.67	1	0.45	0.51	0.42	0.63	1

The sample sets are identified by three letters corresponding to each winery (i.e., AVN, CDB, DTK, FRV, KZC, PDB).

Table S4: Pairwise RV coefficients (p ≤ 0.01) for the PCA scores of the chemistry data blocks vs. low-level PCA fused model.

Data set	Data block	Chenin Blanc		Sauvignon Blanc	
AVN	IR	⬆	0.9	⬈	0.88
	ARP	⬊	0.66	⬊	0.61
	VCC	⬈	0.8	⬇	0.47
	UV-Vis	➡	0.75	⬈	0.82
CDB	IR	⬈	0.88	⬈	0.85
	ARP	➡	0.74	⬈	0.83
	VCC	⬊	0.6	➡	0.72
	UV-Vis	➡	0.78	➡	0.76
DTK	IR	⬈	0.88	⬆	0.94
	ARP	⬊	0.56	⬊	0.67
	VCC	⬊	0.64	⬊	0.63
	UV-Vis	⬊	0.56	⬈	0.85
FRV	IR	⬆	0.95	⬈	0.83
	ARP	⬈	0.85	➡	0.75
	VCC	➡	0.73	➡	0.72
	UV-Vis	⬈	0.86	➡	0.72
KZC	IR	⬆	0.96	⬆	0.95
	ARP	⬊	0.53	➡	0.78
	VCC	⬊	0.51	⬇	0.46
	UV-Vis	➡	0.77	⬆	0.94
PDB	IR	⬆	0.92	⬆	0.93
	ARP	⬈	0.88	⬈	0.86
	VCC	⬊	0.69	⬊	0.54
	UV-Vis	⬈	0.88	⬈	0.86

VCC – volatile compounds composition, ARP – antioxidant-related parameters, UV-Vis – ultraviolet visible spectra, IR – infrared spectra, PCA – principal component analysis. The sample sets are identified by three letters corresponding to each winery (i.e., AVN, CDB, DTK, FRV, KZC, PDB).

Table S5: Pairwise RV coefficients (p ≤ 0.01) between MFA and individual data blocks PCA/CA.

Data set	Data Block	Chenin Blanc	Sauvignon Blanc
AVN	IR	0.9	0.88
	ARP	0.67	0.61
	VCC	0.8	0.45
	UV-Vis	0.76	0.82
	Sensory	0.73	0.68
CDB	IR	0.88	0.86
	ARP	0.75	0.83
	VCC	0.6	0.72
	UV-Vis	0.78	0.76
	Sensory	0.84	0.74
DTK	IR	0.88	0.93
	ARP	0.57	0.68
	VCC	0.65	0.64
	UV-Vis	0.56	0.86
	Sensory	0.66	0.73
FRV	IR	0.95	0.83
	ARP	0.85	0.75
	VCC	0.74	0.72
	UV-Vis	0.86	0.72
	Sensory	0.84	0.71
KZC	IR	0.96	0.96
	ARP	0.53	0.79
	VCC	0.52	0.46
	UV-Vis	0.78	0.93
	Sensory	0.63	0.61
PDB	IR	0.92	0.93
	ARP	0.88	0.86
	VCC	0.69	0.55
	UV-Vis	0.88	0.86
	Sensory	0.82	0.75

The sample sets are identified by three letters corresponding to each winery (i.e., AVN, CDB, DTK, FRV, KZC, PDB).