

Supplemental Data for:

Sen, I., and F. Tokatli. 2014.

Characterization and classification of Turkish wines based on elemental composition.

Am. J. Enol. Vitic. 65:134-142. doi: 10.5344/ajev.2013.13081.

Supplemental Table 1 Loadings of elements for the established PLS-DA models for regional and varietal discriminations.

Red-regional model			White-regional model			Red-varietal model			White-varietal model		
	w[1] ^a	w[2] ^a		w[1]	w[2]		w[1]	w[2]		w[1]	w[2]
Ca	0.43	-0.25	Mg	0.35	0.17	Ca	0.43	-0.17	K	-0.052	0.347
Sr	0.07	0.51	Sr	-0.63	-0.21	K	-0.38	0.15	Mg	0.400	-0.217
B	0.42	-0.12	Al	-0.23	0.39	B	-0.47	0.22	Na	0.019	-0.319
Al	0.13	0.62	Ba	-0.11	-0.12	Al	-0.07	0.35	Sr	0.361	0.354
Li	-0.15	0.08	Li	0.50	0.01	Ba	-0.26	0.28	Li	0.398	0.502
Ni	-0.48	-0.38	Co	0.28	-0.24	Li	-0.17	-0.32	Mn	0.460	-0.239
Cu	-0.29	0.35	Ni	-0.29	-0.46	Mn	-0.06	-0.52	Co	0.462	-0.092
Pb	-0.53	-0.14	Pb	-0.04	-0.73	Cu	-0.45	-0.12	Cu	0.161	0.406
						Zn	-0.38	-0.56	Pb	0.312	-0.352

^aw[1] and w[2] are the loading weights for components 1 and 2, respectively.

Supplemental Table 2 Prediction sets and membership probabilities of PLS-DA models for regional and varietal discriminations.

Prediction set/ variety-region	Membership probability		Prediction set/ variety-region	Membership probability	
	Red-varietal model	Red-regional model		White-varietal model	White-regional model
Kalecik Karası-Denizli	0.90	0.50	Emir-Cappadocia	0.77	0.61
Kalecik Karası-Denizli	0.29	0.82	Emir-Cappadocia	0.83	0.39
Kalecik Karası-Izmir	0.33	0.17	Chardonnay-Denizli	0.74	0.42
Syrah-Denizli	0.47	0.40	Chardonnay-Izmir	0.98	0.24
Çalkarası-Denizli	0.66	0.31	Narince-Tokat	0.91	0.64
Öküzgözü-Izmir	0.43	0.13	Muscat-Izmir	0.14	0.30
Öküzgözü-Elazığ	0.62	0.84	Muscat-Thrace	0.78	0.47
Öküzgözü-Elazığ	0.76	0.74	Muscat-Denizli	0.66	0.49
Merlot-Izmir	0.57	0.87			
Merlot-Denizli	0.55	0.98			
Cabernet Sauvignon-Tokat	0.45	0.85			
Cabernet Sauvignon-Thrace	0.16	0.99			