Characterization of Boğazkere wines from different locations in Turkey relating aroma and sensory properties using chemometrics

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Abstract. Boğazkere (BG) is one of the primary grape varieties that Turkey utilizes to produce premium red wine. Using chemometrics, this research was to investigate the aroma composition and sensory attributes of BG wines from various vintages and locations (Çermik/Diyarbakır, Güney/Denizli, and Pendore/Manisa). Using GC/MS/FID, GC-O, and Descriptive Analysis, aroma, aroma-active compounds, and sensory evaluations were identified and quantified, respectively. To determine the relationship between chemical result and sensory perception, PLS Regression (PLSR) was used. Principal component analysis (PCA) was used to evaluate the sensory results. There have been identified 93 aroma compounds, 29 of which are aroma-active compounds for which modified frequency (MF%) values have been determined. Compounds with high MF% values in BG wines include ethyl-3-methyl-butanoate/ethyl-2-methyl-butanoate (86), ethyl-2-methyl-propanoate (83), isoamylalcohol (82), ethylhexanoate (80), diethylsuccinate (77), and 2-phenylethylalcohol (75). The most prominent attributes associated to these compounds are those of black-fruit, red-fruit, strawberry, raspberry, banana, dry-fruit, cheery and spicy. PCA indicated that the most prevalent aroma descriptors for BG wines are black fruit, dried fruit, red fruit, confectionery, and spicy. Although dry-fruit, black-fruit, and spicy notes are more prevalent in wines from Diyarbakır, red-fruit and confectionary odours are more prevalent in wines from Denizli and Manisa. Red-fruit attributes in wines were positively correlated with diethyl-dl-malate, ethyl-butanoate, ethyl-hexanoate, ethyl-octanoate, ethyl-decanoate, ethyl-3-methylbutanoate, and ethyl-2-methylbutanoate, depending on PLSR. Ethyl-2-hydroxy-methylpentanoate, 4-ethoxycarbonyl-gamma-butyrolactone, gamma-nonalactone, pantolactone, and ethyl-2-methyl-propanoate were positively correlated with the dark fruit attribute of wines. Ethyl-2-hydroxy-4-methyl-pentanoate and gamma-nonalactone compound, which gives the odours of black fruit (blackberry), is particularly noticeable in Diyarbakır wines.

1 Introduction

Boğazkere grapes are one of the primary indigenous red wine varieties. Turkey is one of the earliest regions where Vitis vinifera was domesticated and is the origin of numerous grape varieties [1]. Boğazkere (BG) varieties produce one of the most widely consumed and well-known red wines in Turkey. It is a medium-sized, round grape with thick skin that naturally originates from Eastern Anatolia such as Diyarbakır and Elazığ plateaus [2]. However, the variety has also lately begun to be planted in Western Anatolia's Güney and Pendora districts on the Denizli and Manisa plateaus, respectively.

The term of wine quality is complex and hard to evaluate and varies between vineyard locations. Still, numerous studies have been conducted to identify the factors that influence quality [3,4]. Aroma is a crucial factor that influences the character of wine. The presence of numerous aroma compounds contributes to the complexity of wine. Due to this complexity, the wine's quality increases [5]. The importance of aroma in sensory perception, which plays an essential part in wine consumer preference, cannot be overstated. One of the most notable characteristics of aroma compounds is that they may have a significant impact on quality despite being perceptible even in small amounts [6].

Numerous research [5,7,8] have been conducted to figure out the specific aromas components that give each wine its unique flavour. In some instances, a single aroma compound can impart an odour to the entire wine, while in other instances, a single odour can be caused by multiple aroma compounds [9]. The aroma components of wines are identified and quantified using gas chromatography-mas spectrophotometry [10].

Furthermore, descriptive analysis is widely used for defining the sensory attributes of wine [10-13]. Therefore, the wine's distinctive characteristics are determined. Due to the association between aroma compounds and sensory attributes, characterization of the wine's aroma provides insight into which aroma compounds are associated with particular attributes. The results of instrumental analysis should be associated with those of sensory evaluation and supported by chemometric methods. So, chemometric approaches may be very beneficial in defining the quality category or geographical indication of a wine by proving its distinctive aroma composition and sensory descriptors [14]. Numerous studies [15-18] have utilized chemometric techniques such as PCA (principal component analysis) and PLSR (Partial Least Squares Regression) to investigate the relationship between analytical results and sensory perception and to enhance modelling.

In recent years, Boğazkere wines have evolved into the trademark of Turkey internationally. But, there are a limited number of studies that have linked the aroma characterization and sensory evaluation of Boğazkere wines [2]. The objectives of the research were aimed at (1) characterize the aroma compounds, aroma-active compounds of Boğazkere wines throughout different grape growing locations, and (2) describe the relationship between the sensory attributes and aroma components of these wines.

2 Material and methods

2.1 Samples

Twelve Boğazkere red wines from three distinct locations were collected. They were selected from the foremost wine company in Turkey based on their premium quality, single variety, and limited grape yields, free-run and aging potential. The sampling consisted of three replications. All of the supplied wine samples are included in Table 1, along with additional information.

2.2 Chemical analysis

Alcohol, density, total acidity, pH, dry matter, total phenolic compounds, antosiyanin, tannin, and total and free sulphur dioxide were analysed [19]. Table 1 provides the details of the composition of the wines.

2.3 Aroma Compounds Analysis by Solid Phase Extraction (SPE)

The solid phase extraction (SPE) techniques provided by [20]. were used for analysing aroma compounds. This analysis was performed three times. 50 mL of wine containing an internal standard (3000 g/mL 4-nanonol) was run through a 200 mg LiChrolut EN (Merck, Darmstadt, Germany) cartridge at a flow rate of approximately 2 mL/min. After the flow of 2 millilitres of water, the absorbent was dried out under air (-0.6 bar,

Table 1. Sample information and general analysis of Boğazkere wines.

Codes	*Variety*	*Vintage*	*Location*	*Region*	*Alcohol (%h/h)*	*Titratable Acidity (g/L)**	*pH*	*Total Phenolic Compound (mg/L)*	*Anthocyanins (mg/L)*	*Tannins (g/L)*	*Free SO_2 (mg/L)*	*Total SO_2 (mg/L)*	*Reducing Sugar (g/L)*	*Hue (º)*	*Croma (C*)*
C1	100% BG	2012	Çermik/Diyarbakır	Eastern Anatolia	13.7+0.1	5.4+0.1	3.6+0.1	3219.1+161	200.2+9	5.3+0.3	10.2+1.3	32.0+3.2	2.8+0.1	15.14+0.5	11.60+0.6
C2	100% BG	2013	Çermik/Diyarbakır	Eastern Anatolia	12.4+0.1	5.1+0.1	3.4+0.1	2700.9+135	317.0+12	4.1+0.2	17.9+1.2	40.0+4.1	2.7+0.2	17.75+0.4	10.24+0.4
C3	100% BG	2011	Çermik/Diyarbakır	Eastern Anatolia	13.5+0.1	5.0+0.1	3.5+0.1	3028.2+151	145.9+8	4.8+0.3	9.6+1.3	22.4+2.1	3.1+0.1	15.58+0.3	13.33+0.3
C4	100% BG	2012	Çermik/Diyarbakır	Eastern Anatolia	13.7+0.1	5.6+0.1	3.6+0.1	3355.43+160	189.3+10	5.0+0.1	6.4+1.1	24.0+2.3	3.4+0.2	15.65+0.2	9.19+0.4
C5	100% BG	2011	Çermik/Diyarbakır	Eastern Anatolia	13.9+0.2	5.2+0.1	3.6+0.1	2972.6+145	87.3+4	4.5+0.0	14.7+1.2	40.0+3.5	2.5+0.2	16.62+0.3	23.22+1.1
C6	100% BG	2012	Çermik/Diyarbakır	Eastern Anatolia	13.9+0.2	5.1+0.1	3.5+0.1	2437.3+121	102.4+6	3.9+0.1	11.5+1.1	22.4+3.1	2.7+0.1	17.38+0.1	29.65+1.2
C7	100% BG	2011	Çermik/Diyarbakır	Eastern Anatolia	13.5+0.1	6.0+0.1	3.7+0.1	2446.4+122	107.5+6	4.3+0.2	14.1+1.3	24.0+2.1	2.4+0.2	16.24+0.2	14.59+0.5
C8	100% BG	2012	Çermik/Diyarbakır	Eastern Anatolia	11.6+0.1	5.2−0.1	3.2−0.1	1837.3−93	160.2−7	3.8−0.1	15.4+1.0	108.8+10.1	3.0+0.1	16.01+0.3	23.93+0.9
P1	100% BG	2011	Pendore/Manisa	Western Anatolia	13.2+0.1	5.7−0.2	3.4−0.0	2682.7−131	73.3−3	4.1−0.2	12.8+1.0	33.6+4.0	3.1+0.1	16.21+0.4	18.59+0.2
P2	100% BG	2012	Pendore/Manisa	Western Anatolia	14.1+0.1	6.0−0.2	3.4−0.0	3091.8−157	114.5−6	3.7−0.1	16.0+1.1	32.0+3.1	2.4+0.2	17.61+0.3	29.39+0.9
G1	100% BG	2012	Güney/Denizli	Western Anatolia	13.9+0.2	4.9−0.2	3.6−0.0	2546.4−123	254.5−12	3.5−0.1	12.8+0.9	30.4+2.9	2.7+0.2	15.73+0.5	15.39+0.2
G2	100% BG	2012	Güney/Denizli	Western Anatolia	12.9+0.1	6.0−0.2	3.5−0.0	2073.6−102	105.3−5	3.4−0.4	12.8+0.8	30.4+2.5	3.3+0.1	15.51+0.4	15.26+0.3

Each data is the mean of triplicate determinations; ±standard deviation; † In terms of tartaric acid; ‡ In terms of Gallic acid; § In terms of Malvidin-3-glucoside

10 minutes). The components were recovered through elution via 1.6 mL of dichloromethane 1% methanol. The extract was subsequently analysed with GC/MS/FID. GC/MS/FID conditions have been completely described in a previous study [13]. The aroma compounds were identified by comparing their retention index and mass spectra on the DB-Wax column with those of a commercial spectra database (W10N14, NIST11, NBS75k) and the instrument's internal library, which was compiled from previous laboratory studies. The injection of chemical standards into the GC-MS system confirmed a number of the identified compounds. Utilizing an n-alkane series, the retention indices of the compounds were determined. After identifying aroma compounds, the internal standard method was used to quantify the aroma compounds [13,21]. The ratio of peak area was corrected using response factors for each compound, which were calculated using the intensity ratio of each compound to the internal standard. Then, the mean values of GC analyses conducted in triplicate were calculated.

2.4 Aroma-active compounds analysis by Olfactometry and mass spectrometry

Purge-trap systems applying the dynamic headspace approach [22,23]. were used to extract the aroma-active compounds of wine. In the extraction, a cartridge containing 400 mg of LiChrolut EN resin with an inner diameter of 0.8 cm and an inner volume of 3 ml was used. This resin was selected because it can effectively extract aroma compounds from wine [20]. 80 ml of wine sample was placed in the 37 °C-heated glass container and whirled with a magnetic stirrer prior to the cartridge being set on top of the glass container. 500 ml/min of nitrogen gas was then passed through the system for 100 minutes. In this procedure, the cartridge retains the aroma-active compounds released in the headspace of the glass container. 3.2 ml of dichloromethane containing 5% methanol was then passed through the cartridge to elute the retained aroma compounds. The extract was then concentrated to 200 µL under a flow of purified nitrogen gas. The extract was then utilized to generate the olfactometric profile. The extracted samples were analysed by GC/MS-Olfactometry. GC/MS-O conditions have been entirely described in a previous study [13].

2.4.1 Olfactory Sniffing

Six trained assessors who were a part of the research staff and ranged in age from 23 to 55 conducted the olfactometric analysis. To prevent fatigue, each olfactometry analysis was carried out in two sessions. The sniffing duration for each assessor was maintained at approximately 20 minutes per session. The assessors rated the overall intensity of each odour on a seven-point scale (including half values: 0 = undetectable; 1 = weak, scarcely discernible odour; 2 = clean but not intense odour; and 3 = intense odour). Ferreira et al. [24] have validated the quantitative sufficiency of this technique. Modified Frequency (%) values were calculated from the scores (detection intensity and frequency) to determine the aroma-active compounds. The modified frequency value was computed utilizing the formula suggested by Dravnieks [25].

$$MF\ (\%) = \sqrt{F(\%) x\ I\ (\%)} \qquad (1)$$

In this formula, F (%) represents the percentage of an odorant's detection frequency, and I (%) represents the average intensity as a percentage of the maximum intensity. Subsequently, these compounds were identified by comparing their retention index and mass spectra on the DB-Wax column with those of a commercial spectra database (W10N14, NIST11, NBS 75k) and the instrument's internal library, which was created during the preceding research. The injection of chemical standards into the GC-MS system confirmed a number of the identified compounds.

2.5 Quantitative descriptive analysis (QDA)

Quantitative Descriptive Analysis (QDA), as described by [26], were evaluated by research staff, consisting of eight females and four males aged 25-55. Academic personnel have a minimum of 200 hours of training and experience in descriptive analysis, and they routinely participate in the university's sensory evaluation of research. The assessors participated in seven 2-hour sessions. Assessors participated in an open session to discuss and develop descriptors for the wines during the first and second sessions. According to the open session, the reference standards for each attribute were developed for the following sessions. Assessors presented prepared reference standards during the third and fourth sessions, and a discussion on the reference standards took place during the entire session. In the fifth session, one visual, three taste, four mouthfeel, five aroma and six flavour attributes were selected using a consensus-based approach to define the attributes for descriptive analysis. The sixth, and seventh sessions, assessors used a 15-cm scale to evaluate the intensity of each attribute. Wine (30 mL at 20 °C) was served in random order in International Standard Organization (ISO) wine glasses covered with petri dishes during sessions.

2.6 Statistical analysis

The aromatic constituents that are quantified in the wines were subjected to a two-way Anova analysis using XLSTAT software (Addinsoft version 2021.2, France) to determine the effect of both location and year. Year and location interactions were also evaluated. The Tukey's HSD pairwise comparison test was then used to determine the statistical significance of the differences. A principal component analysis was performed on the sensory data to show the outcome. To determine the relationship between chemical and sensory evaluation results, partial least squares regression (PLSR) analysis was performed with the XLSTAT software (Addinsoft version 2021.2, France) and the sensory descriptors associated with these compounds revealing the characteristics of the wines were identified.

3 Results and Discussion

3.1 Aroma compounds of Boğazkere wines

The aroma characteristics of Boğazkere wines from three different locations and different vintages were evaluated. Table 2 compares the minimum, maximum, effect of the location, and location-year interaction of the aroma compositions of Boğazkere wines from the locations of Diyarbakır, Manisa, and Denizli. In generally, 93 aroma compounds were identified in Boğazkere wines, including 19 higher alcohols, 27 ester, 7 lactones, 20 volatile phenols, 1 norisoprenoids, 2 terpenes, 9 carbonyl compounds, and 8 volatile acids. The average total amount of aroma substances is 162.7 mg/L in Diyarbakır, 148.3 mg/L in Manisa, and 142.67 mg/L in Denizli, based on the locations. Comparing the total number and amount of aroma compounds identified and quantified in the locations, it was discovered that Diyarbakır wines contained a greater number and amount of aroma compounds. Cabaroglu et al. [2] identified 40 aroma constituents in Boğazkere wines and reported the total aroma substance concentration to be 164.3 mg/L.

The esters are the most significant group of aroma substances in wine. Esters, which are the secondary products of yeasts produced during the fermentation of ethyl alcohol, are generally responsible for the wine's fruity aroma and play a vital role in determining the sensory characteristics of young wines. Although esters are hydrolysed over time, the amount of major esters in aged wines exceeds the detection thresholds [27,28]. Boğazkere wines have been identified with 27 ester compounds. Maximum ester amounts have been determined at 55.7 mg/L in Diyarbakır, 46.9 mg/L in Manisa, and 40.5 mg/L in Denizli. Ethyl octanoate, ethyl hexanoate, ethyl butanoate, and ethyl decanoate were the most abundant ethyl esters of fatty acids that affect the fruit aroma of red wines in Boğazkere wines from the all locations. It has been reported that the detection threshold of these compounds in wine matrix is 14 µg/L for ethyl hexanoate, 5 µg/L for ethyl octanoate, 20 µg/L for ethyl butanoate, and 200 µg/L for ethyl decanoate [15,9,30] Table 2 indicates that the concentrations of these compounds in Boğazkere wines are well above the detection threshold. There was a statistically significant difference between the amounts of ethyl octanoate, ethyl hexanoate, and ethyl butanoate in the wines from the locations (p<0.001 and p<0.01). However, a location-year interaction was observed for these compounds (Table 2). It has been reported that the amounts of ethyl hexanoate, ethyl octanoate, and ethyl butanoate compounds in Boğazkere wines reach the detection threshold [2]. Other significant esters found in Boğazkere wines include those with branched chain structures, such as ethyl-2-methyl-propanoate, ethyl-2-methyl-butanoate, ethyl-3-methyl-butanoate, ethyl-3-hydroxy-butanoate, ethyl-4-hydroxy-butanoate, and ethyl-2-hydroxy-4-methyl-pentanoate. It has been reported that the detection threshold value of these compounds in wine matrix is 15 µg/L for ethyl-2-methyl propanoate, 18 µg/L for ethyl-2-methyl-butanoate, 3 µg/L for ethyl-3-methyl-butanoate and ethyl-2-hydroxy-4-methyl-pentanoate for 300 µg/L [7,31] Table 2 shows that the amounts of ethyl-2-methyl propanoate, ethyl-2-methyl butanoate, and ethyl-3-methyl butanoate in Boğazkere wines are well above the detection threshold. According to Ugliano and Henschke [27] and Falcao et al. [31], branched chain esters such as ethyl-2-methyl-propanoate, ethyl-2-methyl-butanoate, ethyl-3-methyl-butanoate, and ethyl-2-hydroxy-4-methyl-pentanoate contribute red and blackberry fruit aromas to wine. It has been reported that ethyl-2-hydroxy-4-methyl pentanoate, in particular, gives a fresh blackberry aroma, has a significant effect on the aroma of wines despite being below the detection threshold value, and exhibits a synergistic perception interaction with ethyl butanoate. The amounts of ethyl-2-methyl-butanoate, ethyl-3-methyl-butanoate, and ethyl-4-hydroxy-butanoate varied significantly among the wines (p<0.05, p<0.01, p<0.001). Higher amounts of ethyl-2-methyl-butanoate and ethyl-3-methyl-butanoate have been detected in wines coming from Manisa. Table 2 indicates that only ethyl-3-methyl-butanoate and ethyl-4-hydroxybutanoate did not exhibit location-year interactions. According to Camara et al. [32] and Reboredo et al. [33], diprotic acid esters such as monoethyl succinate, diethyl succinate, and ethyl lactate play a significant role in the aroma of aged wine, and these compounds increase with age and oxidation. Diethyl succinate, mono-ethyl succinate, and ethyl lactate are three of the most prominent esters found in Boğazkere wines. Diethyl succinate was the only compound for which the difference was statistically significant (p<0.01). These compounds were found in higher concentrations in Manisa wines than in wines from other locations.

The majority of lactones are generated by yeast activity. As the most important lactone group in wines, gamma lactones are typically present in all wines [6]. In Diyarbakır, Manisa, and Denizli Boğazkere wines, seven and five lactone compounds have been identified, respectively. The total amount of lactones in Diyarbakır, Manisa, and Denizli was determined to be 1 mg/L, 0.79 mg/L, and 0.94 mg/L, respectively. In all locations, 4-ethoxycarbonyl-gamma-butyrolactone and gamma-butyrolactone were the predominant lactone compounds. Although gamma-butyrolactone is the most well-known lactone, it does not appear to contribute significantly to the organoleptic properties of wine [6]. The compound 4-ethoxycarbonyl-gamma-butyrolactone, which does not show a year-location interaction between the different locations, was found to have a higher range in Diyarbakır. According to Rocha et al. [34], the 4-ethoxycarbonyl-gamma-butyrolactone compound gives a red fruit aroma to wines. Cabaroglu et al. [2] determined that Boğazkere wines consist of 4-ethoxycarbonyl-gamma-butyrolactone and gamma-butyrolactone compounds.

Boğazkere wines from Diyarbakır contained 20 volatile phenol compounds, whereas wines from Denizli and Manisa contained 12 volatile phenol compounds. compounds, Manisa 5.0 mg/L, and Denizli 6.7 mg/L.

Table 2. The aroma composition of Boğazkere wines from three different locations.

Aroma Compounds (µg/L)	LRI	Çermik/Diyarbakır				Pendore/Manisa				Güney/Denizli				ID	F^{L}	F^{yxL}
		Mean	Min	Max	SE	Mean	Min	Max	SE	Mean	Min	Max	SE			
Higher Alcohols																
1-Propanol	1014	3845.7 b	2765.0	5460.0	30.1	5094.6 a	3430.1	6749.0	274.9	3770.5 b	247.6	5490.2	309.6	MS.LRI.R	**	**
Isobutyl alcohol	1059	2519.0 b	1599.3	3394.7	27.1	1765.0 a	1713.0	1878.2	10.6	2228.6 b	2156.7	2301.7	8.8	MS.LRI.R	*	ns
Butanol	1112	103.8 b	82.8	129.3	0.6	151.5 a	142.9	173.1	1.9	122.2 b	117.2	134.2	1.2	MS.LRI.R	***	ns
Isoamyl alcohol	1176	72866.8 b	60948.9	87540.3	364.4	63804.4 a	60239.1	70249.7	621.3	69760.6 b	66347.4	74423.2	564.6	MS.LRI.R	ns	ns
1-Pentanol	1215	6.0	0.0	49.8	0.7	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI.R	ns	ns
4-Methyl-pentanol	1276	32.5 b	0.0	43.9	0.5	35.4 a	32.2	38.1	0.3	43.4 b	36.8	50.9	1.1	MS.LRI	ns	ns
3-Methyl-pentanol	1288	66.1 b	47.6	92.6	0.6	71.2 a	61.5	81.7	1.5	80.3 b	72.4	87.1	1.1	MS.LRI	ns	ns
1-Hexanol	1314	1322.5 b	880.4	2121.7	16.7	872.3 a	771.2	975.5	14.6	1089.5 b	925.1	1266.6	28.2	MS.LRI.R	*	ns
trans-3-Hexanol	1320	72.8 b	43.7	131.4	1.1	47.4 a	38.2	52.1	0.8	56.3 b	52.5	61.5	0.6	MS.LRI.R	ns	ns
3-etoxhy-1-Propanol	1325	1.6 b	0.0	12.8	0.2	51.4 a	0.0	110.5	9.4	50.1 b	28.1	69.9	3.4	MS.LRI	***	***
cis-3-Hexanol	1336	133.4 b	52.2	274.0	3.4	111.2 a	70.0	154.0	6.9	164.2 b	139.1	188.3	3.8	MS.LRI.R	***	ns
1-Heptanol	1413	nd	nd	nd	nd	nd	nd	nd	nd	40.5 b	0.0	85.8	7.4	MS.LRI.R	***	ns
2-Ethyl hexanol	1451	nd	nd	nd	nd	61.5 a	55.6	69.4	0.9	33.7 b	0.0	77.2	6.2	MS.LRI	***	ns
2.3-Butanediol	1500	89.6	229.9	0.0	3.6	58.8	126.1	0.0	10.8	74.5	158.6	0.0	13.6	MS.LRI	ns	ns
1.3-Butanediol	1526	134.1 b	0.0	489.5	7.7	0.0 a	0.0	0.0	0.0	253.9 b	49.4	473.4	36.7	MS.LRI.R	ns	ns
Methionol	1555	159.7 b	113.0	242.1	1.4	121.1 a	91.5	155.6	4.9	158.3 b	140.4	181.5	2.7	MS.LRI.R	*	ns
Benzyl-alcohol	1815	102.1 b	65.9	182.2	1.6	102.1 a	72.8	136.2	5.1	103.1 b	91.3	112.0	1.6	MS.LRI.R	ns	ns
2-Phenylethanol	1864	28907.7 b	23273.0	34277.8	140.6	16462.1 a	15506.4	18008.2	149.8	11910.3 b	46.1	23884.0	2165.0	MS.LRI	***	ns
3.4.5-Trimethoxybenzyl alcohol	2944	94.8	0.0	340.3	5.4	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI	ns	ns
Total		110458.3 a	96860.0	123395.0	380.3	88809.9 b	83896.0	93724.0	1158.2	89940.0 ab	81648.0	98232.0	1954.4		*	ns
Esters																
Ethyl propanoate	696	49.3 b	0.0	143.9	1.8	66.4 a	0.0	141.2	12.2	29.6 b	0.0	63.7	5.4	MS.LRI.R	**	**
Ethyl 2-methylpropanoate	916	109.4 b	27.0	208.0	2.1	88.7 a	80.0	96.0	1.3	88.7 b	52.6	138.0	5.9	MS.LRI	ns	ns
Ethyl butanote	992	333.3 b	265.5	435.0	2.0	537.2 a	429.2	653.2	18.3	446.9 b	372.9	531.4	11.9	MS.LRI.R	***	***
Ethyl-2-methyl butanoate	1018	47.8 b	33.9	57.9	0.2	61.2 a	56.2	74.6	1.1	59.8 b	57.1	63.0	0.3	MS.LRI.R	***	***
Ethyl-3-methyl butanoate	1026	42.0 b	32.3	52.4	0.3	52.2 a	49.7	56.6	0.4	42.6 b	38.2	48.8	0.8	MS.LRI.R	***	ns
Isoamyl acetate	1119	456.9 b	242.4	720.5	6.7	518.9 a	251.0	826.1	48.1	423.2 b	357.5	491.9	11.0	MS.LRI.R	**	***
Ethyl hexanoate	1241	492.9 b	262.0	761.9	7.1	681.2 a	541.7	857.4	24.7	395.4 b	296.1	500.8	17.5	MS.LRI.R	**	*
Ethyl lactate	1310	3112.9 b	2301.7	4259.9	26.4	2358.4 a	1614.8	3092.7	124.3	3288.8 b	3083.6	3541.0	33.8	MS.LRI.R	***	ns
Ethyl octanoate	1398	507.3 b	327.3	661.2	5.2	816.1 a	706.1	961.4	19.4	465.0 b	330.2	603.2	23.5	MS.LRI.R	***	*
ethyl-3-hydroxybutanoate	1460	64.2 b	27.1	103.1	1.1	54.7 a	43.5	69.3	2.0	79.6 b	42.4	117.9	6.4	MS.LRI	ns	ns
Ethyl-2-hydroy-4-methyl pentanoate	1488	147.4 b	80.6	213.5	2.2	85.6 a	80.8	93.2	0.7	144.9 b	51.5	259.4	17.2	MS.LRI	ns	ns
Isoamyl lactate	1544	214.1 b	109.3	346.2	2.8	101.4 a	77.3	125.7	3.8	245.2 b	140.4	331.5	15.3	MS.LRI.R	***	ns
Ethyl methyl succinate	1572	51.2 b	21.6	101.4	1.1	58.4 a	33.3	84.6	3.5	44.1 b	30.1	62.2	2.5	MS.LRI	ns	ns
Ethyl decanoate	1654	115.6 b	33.6	222.9	2.3	219.8 a	169.1	278.7	8.1	73.5 b	69.2	77.9	0.6	MS.LRI.R	***	ns
Diethyl succinate	1651	4574.4 b	1054.6	9047.1	116.1	8293.6 a	6366.1	10280.0	316.3	4040.7 b	3581.1	4506.5	79.1	MS.LRI.R	**	ns
Ethyl glutarate	1715	28.3 b	0.0	61.1	0.8	53.1 a	45.9	61.5	0.9	39.9 b	24.0	57.9	2.9	MS.LRI	*	ns
Ethyl-4-hydroxybutanoate	1737	163.1 b	93.1	332.9	2.8	87.7 a	63.4	110.5	2.9	167.9 b	116.4	216.0	8.5	MS.LRI	*	ns
2-Phenylethyl acetate	1757	73.1 b	31.3	125.7	1.2	67.7 a	49.6	86.7	3.1	77.7 b	71.6	82.2	0.7	MS.LRI.R	ns	ns
Diethyl-2-hydroxy-2-methylsuccinate	1781	8.4 b	0.0	49.7	0.7	77.1 a	53.8	98.5	3.3	30.6 b	0.0	77.9	5.8	MS.LRI	***	ns
Diethyl dl-malate	2141	206.1 b	112.9	402.1	3.6	535.6 a	180.9	921.7	61.3	273.2 b	159.1	388.9	19.3	MS.LRI	***	***
Diethyl-2-hydroxy-3-methylsuccinate	2395	780.0 b	416.0	1096.2	8.0	1029.8 a	874.1	1186.0	22.4	1002.0 b	800.0	1224.2	35.0	MS.LRI	*	*
Ethyl-2-hidroxy-3-phenyl propanate	2537	122.0 b	61.5	174.4	1.3	121.9 a	102.6	142.6	3.0	124.5 b	93.6	154.8	4.8	MS.LRI	ns	ns
Ethyl hexadecanoate	2583	0.0 b	0.0	0.0	0.0	46.5 a	0.0	102.9	8.6	0.0 b	0.0	0.0	0.0	MS.LRI	***	***
Diethyl tartrate	2603	118.8 b	0.0	365.3	4.4	318.7 a	191.5	614.5	26.3	28.9 b	0.0	68.0	5.4	MS.LRI	***	***
Mono-ethyl succinate	2646	23330.6 b	10199.5	39517.0	345.6	27661.4 b	25047.6	29835.6	335.7	27540.3 b	26600.9	29072.2	176.8	MS.LRI.R	ns	ns
N-Acetyl-dl-methionine ethyl ester	2853	92.3 a	0.0	147.7	2.3	nd	nd	nd	nd	54.1 b	0.0	110.3	9.9	MS.LRI	***	ns
Ethyl- 3-(4-OH-3methoxyphenyl)propionate	2912	41.0 b	0.0	105.1	1.4	53.2 a	42.0	63.6	1.4	43.3 b	23.1	58.9	2.3	MS.LRI	ns	ns
Total		35395.1 a	18052.0	55731.0	500.7	44046.4 b	41170.0	46922.0	677.9	39250.5 ab	37973.0	40528.0	301.1		ns	ns
Lactones																
gamma-Butyrolactone	1588	289.7 b	149.7	686.4	6.3	167.1 a	98.3	275.9	12.1	285.4 b	245.8	356.4	7.7	MS.LRI.R	ns	ns
cis-Whiskey lactone	1807	18.8 a	0.0	102.1	1.4	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI.R	ns	ns
trans-Whiskey lactone	1932	95.0 a	0.0	267.9	3.7	nd	nd	nd	nd	135.5 a	98.2	174.1	6.5	MS.LRI.R	**	ns

Pantolactone	2107	33.3 b	21.2	56.7	0.3	31.9 a	27.6	38.0	0.6	22.8 b	20.1	26.5	0.4	MS.LRI.R	*	ns
gamma-Nonalactone	2116	25.4 b	0.0	44.3	0.5	21.3 a	15.0	25.7	0.6	0.0 b	0.0	0.0	0.0	MS.LRI.R	***	ns
gamma-decalactone	2146	2.6 b	0.0	31.5	0.3	0.0 a	0.0	0.0	0.0	0.0 b	0.0	0.0	0.0	MS.LRI	ns	ns
4-Ethoxycarbonyl-gamma-butyrolactone	2171	536.8 b	419.3	715.9	3.3	567.8 a	543.4	608.4	4.0	496.0 b	294.2	598.5	17.7	MS.LRI	ns	ns
Total		1001.6 a	769.0	1205.0	6.7	788.1 b	735.0	841.0	12.5	939.7 ab	932.0	947.0	1.8		ns	ns
Volatile phenols																
4-Ethylquaiacol	2113	56.9 b	0.0	471.9	6.4	0.0 a	0.0	0.0	0.0	166.8 b	105.4	233.9	9.8	MS.LRI.R	***	ns
4-Ethylphenol	2404	61.1 b	0.0	468.0	6.3	0.0 a	0.0	0.0	0.0	669.9 b	250.0	1086.9	72.5	MS.LRI.R	***	ns
4-hydroxy-3-methyl-acetophenone	2430	nd	nd	nd	nd	nd	nd	nd	nd	9.2 a	0.0	23.0	1.7	MS.LRI	***	ns
2-Methoxy-4-vinylphenol	2435	712.3 b	300.1	1181.9	10.8	410.7 a	221.9	584.8	28.6	105.1 b	73.3	127.9	4.1	MS.LRI	***	**
2.6-Dimethoxy phenol	2520	170.3 b	98.4	315.8	2.5	155.5 a	122.7	186.4	4.4	115.0 b	84.0	151.1	4.8	MS.LRI.R	**	ns
2.6-Dimethoxy-4-methylphenol	2608	12.1 a	0.0	64.5	0.9	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI	ns	ns
4-Vinylphenol	2643	63.4 a	0.0	514.9	7.1	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI.R	ns	ns
Vanillin	2777	92.6 b	0.0	317.1	4.5	35.3 a	0.0	84.5	6.6	76.8 b	0.0	171.8	14.2	MS.LRI.R	ns	ns
Ethyl vanilate	2823	62.8 a	0.0	339.4	4.8	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI.R	ns	ns
Acetovanillone	2825	327.2 b	173.1	510.6	3.7	431.3 a	294.3	565.8	20.1	352.3 b	205.8	552.5	25.5	MS.LRI.R	**	***
Zingerone	2907	50.4 a	0.0	229.0	2.5	50.1 b	0.0	122.8	9.4	nd	nd	nd	nd	MS.LRI	**	ns
Propiovanillone	2915	146.4 b	50.9	307.9	3.6	55.9 a	51.3	60.0	0.7	109.9 b	86.5	140.8	3.2	MS.LRI	ns	ns
Homovanillic alcohol	2928	204.6 b	73.2	412.2	4.7	95.6 a	67.0	121.1	3.8	144.2 b	101.6	188.8	5.9	MS.LRI	*	**
Homosyringic acid	2948	60.5 a	0.0	540.7	5.7	58.6 b	0.0	130.0	10.8	nd	nd	nd	nd	MS.LRI	ns	ns
Vanillic acid	2996	138.5 a	0.0	574.7	8.3	163.4b	125.5	284.3	10.2	nd	nd	nd	nd	MS.LRI.R	*	***
Isovanillic acid	2992	18.2 a	0.0	166.1	2.1	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI	ns	ns
Syringaldehyde	2970	73.7 a	0.0	615.2	8.3	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI	ns	ns
Homovanillic acid	2992	178.1 b	84.4	347.5	3.5	75.0 a	69.3	88.5	1.2	235.2 b	152.7	294.1	10.9	MS.LRI	**	ns
Tyrosol	3004	4842.9 b	3263.2	6179.3	31.1	2834.4 a	2619.2	3376.2	48.5	4597.6 b	4046.9	5184.4	84.4	MS.LRI	***	ns
p-Cumaric acid ethyl ester	3074	1316.5 b	573.9	2124.2	21.0	621.2 a	521.3	749.2	13.2	103.8 b	0.0	242.7	19.2	MS.LRI	***	ns
Total		8588.5 a	7436.7	10701.1	42.4	4986.9 b	4977.2	4996.6	2.3	6685.9 ab	5809.2	7562.5	206.6		**	ns
Norizoprenoids																
3-oxo-alpha-ionol	2830	80.3 a	0.0	150.2	1.7	58.4b	0.0	127.6	10.8	nd	nd	nd	nd	MS.LRI.R	***	***
Terpenes																
6.7-dihydro-7-hydroxy linalool	2012	3.8 b	0.0	32.0	0.4	22.5 a	0.0	48.6	4.1	nd	nd	nd	nd	MS.LRI	***	***
Hydroxy citronellol	2478	4.1 b	0.0	35.0	0.5	13.7 a	0.0	28.6	2.5	nd	nd	nd	nd	MS.LRI.R	**	***
Total		7.9 ab	.0	35.0	0.6	36.2 a	26.3	48.6	0.4	nd	nd	nd	nd		*	ns
Carbonyl Compounds																
Diacetyl	952	133.3 b	45.2	254.8	2.7	207.4 a	122.8	283.8	12.8	61.5 b	0.0	123.6	11.2	MS.LRI.R	***	***
Acetoin	1231	56.2 b	28.1	112.3	1.1	42.9 a	25.1	60.2	3.0	37.2 b	12.6	63.1	4.4	MS.LRI.R	ns	ns
2-Butylfuran	1245	2.0 a	0.0	20.4	0.2	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI	ns	ns
2-Methyl-3-thiolannone	1458	9.2 b	0.0	29.6	0.5	35.9 a	20.2	54.3	2.8	20.0 b	0.0	42.7	3.7	MS.LRI	***	ns
5-Methyl furfural	1497	8.6 a	0.0	73.7	1.0	nd	nd	nd	nd	nd	nd	nd	nd	MS.LRI	ns	ns
Furfuryl alcohol	1589	20.8 a	0.0	161.5	2.1	nd	nd	nd	nd	25.4 a	0.0	51.2	4.6	MS.LRI	**	ns
4-Hydroxy-2-methyl-2-cyclopentenone	2015	14.9 b	0.0	59.8	0.9	17.9 a	0.0	37.6	3.3	15.6 b	0.0	32.0	2.8	MS.LRI	ns	ns
3-Hydroxy-4-phenyl-2-butanone	2513	29.0 b	0.0	59.8	0.6	39.6 a	27.2	55.4	1.9	20.0 b	0.0	48.7	3.9	MS.LRI	*	ns
Phenylacetaldehyde	2530	105.5 b	19.9	129.2	1.0	52.6 a	47.6	56.4	0.5	51.8 b	34.2	59.6	1.7	MS.LRI	***	ns
Total		379.5 a	268.0	598.0	4.5	396.3 b	299.9	492.8	22.7	231.5 ab	168.1	294.8	14.9		ns	ns
Volatile Acids																
Acetic acid	1394	239.4 b	141.0	308.8	1.6	189.6 a	157.0	215.2	3.2	202.2 b	141.6	265.9	9.7	MS.LRI.R	ns	ns
Propanoic acid	1479	32.7 b	18.0	46.2	0.3	50.2 a	48.6	52.8	0.3	37.0 b	35.7	40.0	0.3	MS.LRI.R	***	***
2-Methyl propanoic acid	1508	240.0 b	98.1	394.9	5.1	122.4 a	117.7	133.4	0.9	176.7 b	135.2	215.0	6.4	MS.LRI	ns	ns
Butanoic acid	1565	174.5 b	91.8	274.7	2.5	217.2 a	191.1	255.4	3.9	133.3 b	123.9	149.6	1.5	MS.LRI.R	*	ns
3-Methyl-butanoic acid	1630	467.5 b	304.7	651.3	4.6	317.5 a	303.8	354.1	3.1	328.3 b	165.4	428.7	16.1	MS.LRI	**	ns
Hexanoic acid	1775	2072.2 b	1149.1	2843.5	24.8	3038.0 a	2523.8	3692.5	86.4	1803.6 b	1470.5	2167.4	60.5	MS.LRI.R	***	**
Octanoic acid	2025	2913.5 b	1675.8	3773.6	31.6	4257.6 a	3888.3	4777.6	57.0	2494.7 b	2043.4	2947.1	77.3	MS.LRI.R	***	ns
Decanoic acid	2550	669.8 b	356.7	985.4	9.9	1011.2 a	945.3	1122.3	10.7	449.2 b	354.9	544.4	16.6	MS.LRI.R	***	ns
Total		6809.5 a	4570.0	8611.0	62.7	9203.6 b	8391.0	10017.0	191.6	5624.8 ab	4690.0	6560.0	220.4		ns	ns

Mean, average amount of Boğazkere wines from Diyarbakır, Manisa and Denizli locations; Min, is the minimum value within the data; Max, Is the maximum value within the data; LRI. Kovats index value determined in DB-Wax column; SE. Standard Error; nd. not detected; ID; Identification. MS: identification by comparison with the mass spectrum from NIST library. LRI: identification by comparison with data from previous literature. R: identification with the injection of reference compounds. F^{L}: the effect of the location according to the two-way analysis of variance; F^{Lxy}: location-year interaction; ns: not significant. $^{*}p<0.1$ $^{**}p<0.05$ $^{***}p<0.01$

Diyarbakır contained 8.6 mg/L of volatile phenol Comparing the locations revealed that Diyarbakır wines had a higher total amount of volatile phenol, with the difference being statistically significant without any effect by location-year interaction

3-oxo-ionol is one of the norisopronoids that are varietal aroma compounds present in wines. In grapes and wines, the amount of the compounds present is measured in micrograms [35]. When the locations were compared, it was determined that 3-oxo-ionol was statistically significantly higher in the Diyarbakır location. Cabaroglu et al. [2] observed seven norisopronoid components in Boğazkere wine and characterised the 3-oxo-alpha-ionol compound as a bonded aroma compound.

3.2 Aroma-active compounds of Boğazkere wines

The aroma-active compounds, linear retention indices (LRI), modified frequency (MF%) values, and sensory descriptors are presented in Table 3. Boğazkere wines contained 29 aroma-active compounds. A total of 13 esters, 7 higher alcohols, 1 C6 compound, 1 carbonyl compound, 6 volatile acids, and 3 lactones were identified in Boğazkere wines. The MF% values of the compounds detected in wines range from 8% to 89%. As is well-known, when the MF% value of aroma-active compounds rises, the compounds' perception also improves [23].

It was determined that compounds and odours with MF% values greater than 75% were, in order: ethyl-2-methyl propanoate associated with red apple odour; ethyl-3-methyl butanoate/ethyl-2-methyl butanoate associated with strawberry odour; isoamyl acetate associated with banana odour; isoamyl alcohol associated with whey/alcohol-like odour; It is observed that the majority of active compounds in Boğazkere wines arise from esters, which provide potent odours of red and black berries. As previously mentioned, ethyl esters of fatty acids and branched-chain esters give red wines their fresh red and blackberry odours [31, 36].

Upon comparing the locations, the compounds isoamyl acetate, isoamyl alcohol, 2-phenylethyl alcohol, ethyl 2-hydroxy-4-methyl-pentanoate, and mono-ethyl succinate displayed significant differences. Specifically, blackberry-associated ethyl 2-hydroxy-4-methyl-pentanoate had significantly higher value in the wines of Diyarbakır and Manisa. Moreover, Manisa and Denizli wines had significantly higher mono-ethyl succinate associated with dried fruit odour, a compound known to increase with ageing and oxidation [32,33]

3.3 Sensory evaluation of Boğazkere wines

Descriptive Analysis (DA) was used in order to evaluate the sensory characteristics of Boğazkere wines. Twelve assessors performed sensory analyses of the wines. The assessors evaluated the wines with 23 distinct attributes using a 15-cm scale to determine the intensity of each attribute in DA. One visual attribute (colour), three taste attributes (sweetness, sourness, bitterness), four mouthfeel attributes (astringency, body, complexity, aftertaste, overall flavour intensity), five aroma attributes (N-red fruit, N-black fruit, N-dry fruit, N-confectionery, N-woody, N-chocolate, N-spicy), and six flavour attributes (P-red fruit, P-black fruit, P-dry fruit, P-confectionery, P-woody, P-chocolate, P-spicy) were assessed. Figure 1 displays the principal component analysis (PCA) of sensory evaluation data for Boğazkere wines with two dimensions. According to PCA, PC1 explains 38.7% of the variance, PC2 explains 21.2% of the variance, PC3 explains 12.6% of the variance, and PC4 explains 8.9% of the variance, for a total of 4 components explaining 81.4% of the variance. The PC3 and PC4 have not been included for the purpose of simplicity, as they have little impact on the outcome.

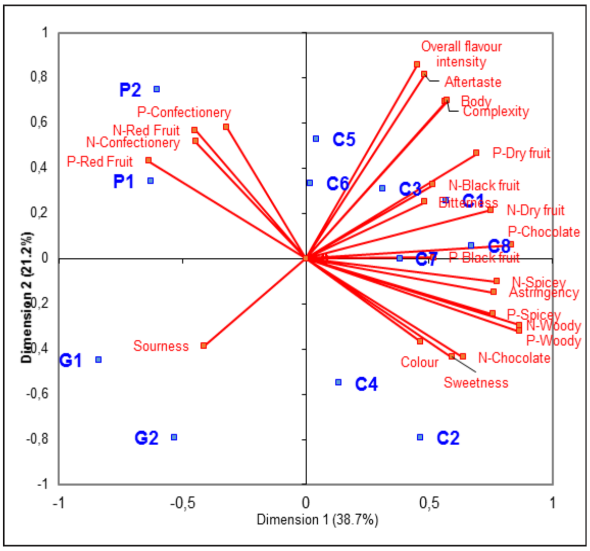

Figure 1. Principal component analysis of the dataset featuring descriptive analyses of wines. PC1 and PC2 dimensions. C, indicates wines from Çermik/Diyarbakır, P, indicates wines from Pendore/Manisa, and G, indicates wines from Güney/Denizli.

Overall flavour intensity descriptors display a positive correlation with aftertaste ($r = 0.92$), body ($r = 0.90$), and complexity ($r = 0.89$) according to the PCA correlation matrix. Descriptors of red fruit on the palate were positively correlated with descriptors of confectionery on the palate ($r = 0.84$) and red fruit on the nose ($r = 0.72$), whereas sourness and dry fruit on the palate were negatively correlated ($r = -0.73$). The first component (PC1) explains the descriptors of dried fruit, astringency, spicy, black fruit, chocolate, and woody, while Diyarbakır wines show a positive correlation in terms of dry fruit, black fruit, spicy, woody, and astringency attributes. The 2nd component (PC2), on the other hand, explains the descriptors of red fruit, confectionery, body, aftertaste, complexity, and overall flavour intensity, whereas Manisa wines demonstrate a positive correlation with the descriptors of red fruit and confectionery. The PC2 component distinguished Diyarbakır wines from those of Manisa and Denizli, whereas the PC1 component separated Manisa and Denizli wines.

Table 3. Aroma-active compounds of Boğazkere wines detected by GC-O, with related descriptors, identification, and %MF values.

LRI	Descriptor	Çermik/Diyarbakır			Güney/Denizli			Pendore/Manisa			F^L	ID	Identification
		%MF	Min	Max	%MF	Min	Max	%MF	Min	Max			
916	red apple	82	75	89	81	77	84	82	75	89	ns	MS,LRI,R	Ethyl 2-methyl propanoate
992	fruit, apple	73	71	76	72	68	75	70	68	71	ns	MS,LRI,R	Ethyl butanoate
987	sweet	18	8	31	33	24	41	12	12	12	ns	MS,LRI	1-Propanol
1018	strawberry, raspberry	88	86	91	82	80	84	86	82	88	ns	MS,LRI,R	Ethyl-2-methyl-butanoate+Ethyl-3-methyl-butanoate
1058	whey, lactic	73	71	75	62	54	71	66	66	66	ns	MS,LRI,R	Isobutyl alcohol
1119	banana	66^b	61	71	77^a	77	77	85^a	84	86	**	MS,LRI,R	Isomayl acetate
1176	cheese, chemical, alcohol	80^b	80	82	82^b	82	82	87^a	85	88	**	MS,LRI,R	Isoamyl alcohol
1241	strawberry, raspberry	79	75	82	80	80	80	82	80	84	ns	MS,LRI,R	Ethyl hexanoate
1310	milky, fruity	39	28	48	43	41	45	40	40	40	ns	MS,LRI,R	Ethyl lactate
1314	grass	31	16	41	28	24	32	20	20	20	ns	MS,LRI,R	1-Hexanol
1394	vinegar	45	41	48	55	45	66	64	62	66	ns	MS,LRI,R	Acetic acid
1398	ripe fruit	49	43	55	56	52	61	43	40	45	ns	MS,LRI	Ethyl octanoate
1460	fruity	35	28	48	20	16	23	37	35	40	ns	MS,LRI,R	Ethyl-3-hydroxy butanoate
1544	Blackberry-whey	47^a	43	54	30	28^b	32	45^a	43	47	*	MS,LRI	Ethyl 2-hydroxy-4-methylpentanoate +2-Methyl propanoic acid
1588	caramel	56	43	63	57	52	63	48	45	50	ns	MS,LRI	Gamma butyrolactone
1630	burned, caramel	49	40	58	48	46	49	53	50	55	ns	MS,LRI,R	3-methyl butanoic acid
1651	ripe fruit, caramel	79	71	88	75	68	82	77	77	77	ns	MS,LRI,R	Diethyl succinate
1654	dry fruit	71	62	77	67	63	71	75	73	77	ns	MS,LRI,R	Ethyl decanoate
1757	flowery, rose, spicy	63	61	66	57	52	63	49	45	52	ns	MS,LRI,R	2-phenylethyl acetate
1813	sweet spice	25	14	43	20	14	26	31	31	31	ns	MS,LRI,R	Hexanoic acid
1815	dry flowery, dry rose	31	16	50	16	16	16	nd			ns	MS,LRI,R	Benzyl alcohol
1864	dry flower, honey, spicy	82^a	75	86	66^a	63	68	73^{ab}	71	75	*	MS,LRI,R	2-Phenylethyl alcohol
1934	sweet cherry, grape molasses	10	0	31	34	31	37	28	26	30	ns	MS,LRI,R	trans-whiskey lactone
1956	sour cherry juice, tobacco	51	35	61	55	42	68	77	77	77	ns	MS,LRI	p-Anisaldehyde
2025	boiled grape juice	40	40	40	49	32	66	40	40	40	ns	MS,LRI	Octanoic acid
2091	flower, cherry, boiled grape juice	nd			26	0	52	16	16	16	ns	MS,LRI	2-Phenoxyethyl alcohol
2151	boiled grape juice, burnt, tobacco	17	0	26	26	26	26	33	31	35	ns	MS,LRI	Nonanoic acid
2171	sour boiled grape juice-dry fruit	43	28	54	28	28	28	28	28	28	ns	MS,LRI	4-Ethoxycarbonyl gamma-butyrolactone
2646	cherry-dried fruit	43^b	37	47	64^a	58	71	63^a	62	64	*	MS,LRI	Mono-ethyl succinate

LRI, Kovats index value determined in DB-Wax column; %MF, Modified Frequency value of detected odour; %MF, average value of Boğazkere wines from Diyarbakır, Manisa and Denizli locations; Min. is the minimum value within the data; Max. is the maximum value within the data; F_L: effect of location according to variance analysis; ns, not significant, * $p < 0.1$ ** $p < 0.05$; ID, Identification; MS: identification by comparison with the mass spectrum from NIST library. LRI: identification by comparison with data from previous literature. R: identification with the injection of reference compounds.

PC1 and PC2 components were divided into three groups, and the majority of Diyarbakır wines were gathered in the upper right section. Black fruit, dry fruit, red fruit, confectionary, and spicy have been considered to be the most prominent aroma descriptors of Boğazkere wines. Although dried fruit, black fruit, and chocolate aromas are prominent in Diyarbakır wines, Denizli and Manisa wines have more red fruit and confectionery odours. Assessors referenced the odours of strawberry, raspberry, and red cherry as descriptors of red fruit; black mulberry, blackberry, and black cherry as descriptors of black fruit; and prune, raisin, and dried figs as descriptors of dried fruit. Yıldırım et al. [37] reported that Boğazkere wines are characterised by raisin, woody, and astringency descriptors.

3.4 Relating between aroma compounds and sensory attributes of Boğazkere wines

The relationship between aroma compounds, chemical composition, and sensory attributes has been further investigated using partial least squares regression (PLSR) analysis. According to Jaeger et al. [38], the PLSR method is frequently used to correlate different data groups in sensory analysis studies. In PLSR analysis, the aroma compounds (mostly aroma-active) determined in the wines and the general composition of the wines were defined as X data, whereas sensory attributes were defined as Y data with standardised results. In order to provide a better explanation of the model, some aroma compounds were eliminated from the X data as these did not fit well with the model as determined by VIPs (lower than 0.8). The PLSR analysis consisted of two-dimensional components. The regression model contained 21 aroma-active compounds, 12 aroma compounds, 5 general compositions, and 19 sensory descriptors. Figure 2 indicates the component charts for PLS1 and PLS2. The PLS1 component (X: 31.3%, Y: 31.5%), PLS2 component (X: 34.8%, Y: 39.5%) collectively explained 71.0% of the variance in the Y data.

PLS1 and PLS2 components separated Diyarbakır wines (C1 to C8) from Manisa and Denizli wines (P1, P2, G1, G2), which were grouped together on the top left side of the coordinate system based on the PLSR analysis of Boğazkere wines (Fig. 1). Figure 1 indicates a positive correlation between the red fruit and confectionary attributes of the wines and ethyl butanoate, ethyl octanate, ethly decanoate, diethyl dl-malate, and ethyl-2-methylbutanoate. In addition, these compounds were associated with the wines P1, P2, G1, and G2. On the contrary, ethyl-2-hydroxy-methyl-pentanoate, 4-ethoxycarbonyl-gamma butyrolactone, gamma nonalactone, pantolactone, and ethyl-2-methyl-propanoate were found to be positively correlated with black fruit and dry fruit attributes found in wines from Diyarbakır. Black fruit (nose and palate) had a significant positive correlation with gamma-nonalactone, whereas P-black fruit had a significant negative correlation with ethyl-2-methyl butanoate. Dry fruit has a significant positive correlation with pantolactone and isomaly alcohol on the nose. In addition, the spicy attribute on the nose correlated positively with propiovanillone, and the spicy attribute on the palate correlated positively with 2-methoxy-4-vinylphenol and propiovanillone.

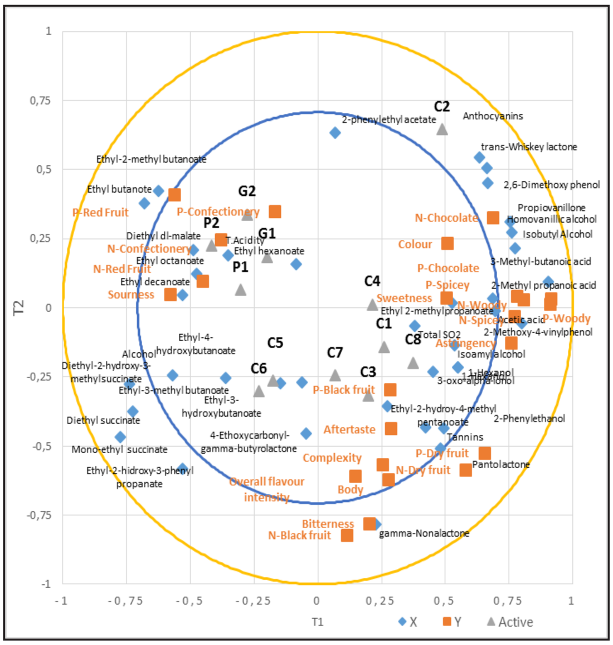

Figure 2. PLS-R loading for sensory attributes (Y variables) and aroma and aroma-active compounds with general composition of Boğazkere wines (X variables) from three locations.

In Bordeaux wines, it has been reported that blackberry fruit odour is associated with ethyl propanoate, ethyl-2-methylpropanoate, and ethyl-2-methyl butanoate compounds, and redberry fruit odour is associated with ethyl butanoate, ethyl hexanoate, ethyl octanoate, and ethyl 3-hydroxybutanoate compounds [39]. Robinson et al. [40] reported that the compounds ethyl-2-methyl propanoate, ethyl-2-hydroxy 3-methyl butanoate, and benzene propyl acetate were positively correlated with red berry fruit odours in Cabernet Sauvignon wines. According to studies conducted by Falcao et al. [31], ethyl-2-hydroxy-4-methylpentanoate has a substantial impact on the overall odour of red wines and has been associated with the aroma of fresh blackberries. In addition, it has been reported that ethyl-2-hydroxy-4-methylpentanoate has a considerable effect on aroma even at levels below the detection threshold (300 g/L in model wine) and that it has a synergistic perception effect with ethyl butanoate [31]. Sensory features may exhibit synergistic formation as a consequence of the interaction of various aroma compounds with one another [41]. According to the olfactory threshold, the concentration of different ethyl esters had no direct effect on the fruit aroma of red wines. However, an overall sensory effect of the red and black berry odours was clearly determined because of the cumulative effect of these esters (ethyl propanoate, ethyl 2-methylpropanoate, and ethyl 2-methylbutanoate for black-berry aromas; ethyl butanoate, ethyl hexanoate, ethyl octanoate, and ethyl 3-hydroxybutanoate for red-berry aromas) [39]. In addition, it is known that the non-volatile wine matrix plays an important role in the perception of aroma compounds [40,42].

4 Conclusion

This study used chemometrics to highlight the relationships between the chemical analyses and the sensory evaluation results for Boğazkere wines produced in Turkey's various viticultural locations and in two different vintages. Esters, higher alcohols, and lactones were identified as three of the majority of significant compounds responsible for the distinctive wine aroma across both vintages and locations. Oenological factors such as maceration techniques, fermentation activators, yeast, and barrel ageing can be investigated further to learn how wine odour evolves over time. In addition, the further research aims to study the microclimate effect on the vineyards of the original locations for the Boğazkere such as sub region of Diyarbakır and Elazığ.

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