Heliyon 9 (2023) e12814

Contents lists available at ScienceDirect

Heliyon

journal homepage: www.cell.com/heliyon

Research article

Multidimensional analysis of the interaction of volatile compounds and amino acids in the formation of sensory properties of natural wine

Alexan Khalafyan [a], Zaual Temerdashev [a,*], Aleksey Abakumov [a], Yuri Yakuba [b], Olga Sheludko [b], Anastasia Kaunova [a]

[a] Kuban State University, 149 Stavropol'skaya St., Krasnodar, 350040 Russia
[b] North Caucasian Federal Research Center of Horticulture, Viticulture, Winemaking, 39, 40-let Pobedy St., Krasnodar, 350901, Russia

ARTICLE INFO

Keywords:
Tasting assessment
Correlation relationships
Wine quality
Data analysis

ABSTRACT

The content of free amino acids and aroma compounds present in wine and dependent on the grape variety, conditions of its growing and technology of production form its consumer properties. In this paper, the structure of interactions of amino acids and volatile organic compounds in 150 samples of natural dry red and white wines produced in the Krasnodar region, Russia, (2010–2013) was studied. The aim of this work was to comparatively evaluate the contribution of volatile compounds and amino acids to the sensory properties of wines by using regression, canonical, covariance, factor analyses, as well as principal component analysis. The list of volatile compounds, i.e., acetaldehyde, ethyl acetate, methanol, the total content of higher alcohols, acetic acid, and furfural, and such amino acids as arginine, proline, threonine was selected based on their influence on sensory properties of wines. The concentrations of volatile compounds and amino acids in wines were determined by gas chromatography and capillary electrophoresis, respectively. Sensory evaluation was conducted by experts with professional experience in wine tasting. Application of statistical methods allowed to establish intra- and inter-group correlations among amino acids and volatile compounds as well as between the groups of these compounds, which determined sensory properties of wines. More than 80% of the variability of the sensory assessment of wines is determined by the degree of relationship between the selected amino acids and volatile compounds; the contribution of amino acids to this indicator is 4.5-fold higher. The results obtained can be used to predict the sensory assessment of red and white wines based on the levels of volatile compounds and amino acids.

1. Introduction

According to Jackson [1], wine quality assessment by its composition is not fully objective. The chemical composition affects wine taste characteristics, but it is not entirely clear how they are perceived by the tasting participants, which leads to difficulties in optimizing their sensory perception. Sensory properties are the main wine characteristics determining success among consumers [2,3]. In sensory perception, it is important that all chemical and visual senses are integrated into the orbitofrontal cortex [4]. In the review

* Corresponding author..
E-mail address: temza@kubsu.ru (Z. Temerdashev).

https://doi.org/10.1016/j.heliyon.2023.e12814
Received 21 September 2022; Received in revised form 29 December 2022; Accepted 3 January 2023
Available online 5 January 2023

article [5], Francis and Williamson analyzed current state of knowledge about sensory properties important to consumer preferences and tastes. They also investigated the limitations of the methodology for characterizing consumer perceptions and hedonistic reactions, implications of blind and informed evaluations, and relationship between consumer sensory testing and marketing research.

Despite the presence of numerous studies regulating the sensory evaluation of wines [1,6–10], expert methods for determining their quality have certain disadvantages. The results of wine sensory evaluation are influenced by the composition of experts, their number, physiological characteristics during examination, subjectivity in the perception of organoleptic properties of wines, imbalance of wines, etc. Therefore, processing of expert assessments includes checking the consistency of expert opinions and averaging the expert opinions within an agreed group.

Modern methods of analytical chemistry (gas chromatography-mass spectrometry (GC-MS), gas chromatography with flame ionization detection (GC-FID), quantitative gas chromatography-olfactometry (GC/O)) in combination with statistical modeling methods (descriptive statistics, analysis of variance (ANOVA), principal component analysis (PCA), analysis of compliance (CA), cluster and regression analyses, logistic modeling, design of experiments) expanded the capabilities of specialists in establishing the relationship between the sensory properties and chemical composition of grapes and wines. For these purposes, diverse techniques were used from the statistical software SPSS [11], STATISTICA [12], SAS [13], STATA [14] to modern data analysis tools, e.g., the R programming environment [12,15,16], machine learning [17,18]. Expanding the possibilities of obtaining information related to the concentrations of volatile compounds allows to understand the complexity and, to a certain extent, evaluate some features of the formation of wine sensory properties [5,19–21].

The choice of the list of amino acids and volatile compounds studied in the sensory analysis of wine quality by multidimensional statistical analysis has been justified, first of all, by their contribution to the wine quality index and the maximum permissible concentrations determined by the recommendations of the International Organisation of Vine and Wine (OIV) [22] and the results presented in Refs. [23–29].

Francis and Newton [19] described the possibilities and limitations of assessing the contribution of chemical components to the aroma and taste of wine, analyzed the relationship between sensory properties and the chemical composition of wine. An important aspect of this relationship is the establishment of a list of compounds with the greatest impact on sensory descriptive analysis and related statistical methodologies complementing the data on the chemical composition of aroma compounds. The sensory properties are formed by a number of free amino acids and aroma-forming compounds in wines, the contents of which depend on the grape variety, growing conditions, production technology, type, strain of wine yeast, and batonnage technique [30-32].

There exist studies describing the analysis results of chemical and sensory significance of different compounds in a complex wine matrix [33], influence of volatile compounds on the sensory profiles of wines [23,34], relationship between the sample composition and sensory analysis [24,25].

Significant amount of information on the organoleptic properties and chemical composition of wines in combination with multivariate data analysis methods are a suitable tool for revealing complex relationships associated with the regional origin of wine in terms of the content of volatile compounds [35-39]. Based on the analysis of data on the component composition of wine as well as the relationship between the chemical composition of wines and organoleptic indicators, chemometric methods were used to group them by the region of origin. The regional origin of wines has been emphasized to be a multifaceted concept including volatile substances, other compounds derived from grapes, as well as vinification and storage processes influenced by natural elements and human intervention.

When assessing taste of 150 wine samples produced in the Krasnodar region by correlation analysis, the authors [27] selected arginine, proline, threonine among the amino acids and acetaldehyde, ethyl acetate, methanol, the total content of higher alcohols, acetic acid, and furfural as volatile compounds contributing the most to the sensory assessment results. Arginine was chosen from the group of free amino acids of grape must consumed during alcoholic fermentation and not returning to wine during autolysis [40-42]. Proline was selected from the group of free amino acids consumed during alcoholic fermentation, but then returning to wine due to autolysis of yeast [40,42]. Threonine was selected from the group of free amino acids not digested by yeast, but the concentrations of which increase during wine aging [40–42]. Acetaldehyde, ethyl acetate, higher alcohols (for example, isobutyl and isoamyl alcohols) are related to background components of aroma [43]. Higher alcohols give wines a fullness of taste, so their increased concentrations are desirable. High contents of acetaldehyde, ethyl acetate, acetic acid, and furfural negatively affect the sensory assessment of wine. Methanol is a poison, its content in wine distillates is normalized and mandatory controlled [22].

The aim of the present work is to study intra- and inter-group correlations between amino acids and volatile compounds and assessment of their contribution to the sensory properties of 150 samples of dry red and white grape wines obtained by traditional technologies from European, hybrid grape varieties grown in the Krasnodar region, Russia, (2010–2013) using regression, canonical, covariance, factor analyses, and principal component analysis. The results obtained can be recommended for predicting the sensory evaluation of red and white wines by the content of volatile compounds and amino acids in them.

2. Methods and materials

2.1. The research objects

were 150 samples of dry red (86 samples) and white (64 samples) wines of Russian origin produced according to traditional technologies from European (Cabernet Sauvignon (26 samples), Merlot (29 samples), Aligote (5 samples), Pinot Noir (5 samples), Riesling (4 samples), Saperavi (12 samples), Rkatsiteli (4 samples), Sauvignon Blanc (12 samples), Traminer (4 samples), Chardonnay (23 samples)) and hybrid grape varieties (Bianca (8 samples), Krasnostop (8 samples), Shiraz (6 samples), Viorica (4 samples)). The

analyzed wines were produced in 2010–2013 in the Krasnodar region by the following industrial manufactures: "Myskhako" (Novorossiysk), "Fanagoria Number Reserve" (pos. Sennoy), "Kuban-Vino" (st. Starotitarovskaya), "Southern wine company (SWK)" (st. Vyshestebliyevskaya), "Villa Victoria" (Novorossiysk), "Chateau Tamagne" (st. Taman), "Chateau le Grand Vostock" (khut. Sadovyy). The wine samples were kindly provided by the manufacturers. The wines were poured in dark green glass bottles with screw caps and stored at temperatures up to 10 °C. A detailed information about the studied wines is summarized in Table S1.

2.2. Reagents

To prepare working and calibration solutions, standard sample solutions of threonine, proline (DIA-M, Russia), benzimidazole, arginine, acetaldehyde, ethyl acetate, methanol, acetic acid, furfural as well as the mixture of higher alcohols: 2-propanol, 1-propanol, isobutanol, 1-butanol, isoamylol, 1-hexanol (Sigma-Aldrich, USA), and analytically pure tartaric acid, H_3PO_4, HCl, NaOH, $Na_2B_4O_7 \times 10H_2O$ (Vecton, Russia) were used.

Sets of calibration mixtures for analysis of alcohol-containing liquids by gas chromatography were also applied, namely, certified calibration mixture for the analysis of alcohol authenticity (Ecolan, Russia); certified calibration mixtures for the determination of furfural (Ecolan, Russia) and volatile acids (acetic, propionic, isobutyric, butyric, isovaleric, valeric acids) (Ecolan, Russia) in alcohol.

2.3. Research methods

2.3.1. Chromatographic determination of volatile compounds

Volatile compounds were determined using methods recommended by OIV for the quantification of volatile compounds by GC-FID [44-46] applying standard sample solutions of acetaldehyde, ethyl acetate, methanol, acetic acid, furfural as well as higher alcohols: 2-propanol, 1-propanol, isobutanol, 1-butanol, isoamylene, 1-hexanol.

The influence of the analyzed matrix, i.e., possible degradation products of non-volatile components, was eliminated by direct injection of a wine sample 5-times diluted with distilled water into the chromatograph. Volatile compounds were quantified by GC-FID. A Crystall 2000 M chromatograph (Chromatec, Russia) equipped with an HP-FFAP capillary column (50 m × 0.32 mm, 0.52 μm, Agilent, USA) was used. The analysis conditions were as follows: injector temperature – 200 °C; FID temperature – 220 °C; carrier gas (nitrogen) flow rate – 1.21 mL/min; split ratio 1:33; initial oven temperature – 70 °C with a 7-min isotherm, an increase to 140°C at 5 °C/min followed by a 10-min plateau and an increase to 180°C at 10 °C/min, which was held constant until the end of analysis; injection volume – 1 mm^3; hydrogen flow rate – 20 mL/min; oxygen flow rate – 20 mL/min; analysis time – 40 min.

To construct calibration curves, both standard solutions and certified calibration mixtures for alcohol authenticity analysis as well as furfural and volatile acids determination were applied.

2.3.2. Determination of free amino acids

Target amino acids, namely, arginine, proline, threonine, were selected based on the results of previous studies [26-29]. Free amino acids in wines were determined by capillary electrophoresis [47]. The concentration of free amino acids in wines was determined using a CAPEL capillary electrophoresis system (Lumex, Russia) equipped with a positive polarity power supply, an ultraviolet detector, and a 0.5-m quartz capillary with an inner diameter of 75 μm in a water heating thermostat.

Indirect detection of amino acids was conducted at the wavelength of 254 nm using benzimidazole-phosphoric acid electrolyte. Calibration solutions with concentrations of 10, 50, 100, 200, 500 mg/L were prepared by dilution of chemically pure arginine, proline, threonine standards with 16% ethanol aqueous solution. Wine samples were not diluted prior to analysis. The capillary was conditioned for 3 min with 1 M NaOH followed by a 5-min washing with distilled water and the electrolyte. Between runs, the capillary was equilibrated by a 2-min washing with the electrolyte. Standard solutions and wine samples were introduced into the capillary hydrodynamically for 5 s at 30 mbar. The applied separation voltage was 15 kV with positive polarity at the injection end. Identification was carried out based on the retention times of the components, while quantification was carried out using calibration curves.

2.4. Sensory analysis

All experimental studies related to sensory analysis were conducted in the accredited center for product certification – Federal Research Center of Horticulture, Viticulture, and Winemaking (FSC HVW, Krasnodar, Russia). A total of 15 specialists (9 females and 6 males) aged between 32 and 45 (12 experts) and 55–66 years (3 experts) participated in the sensory assessment procedure. All participants are considered experts in the field of wine making and have professional experience in the field of sensory analysis. The experts participated in general and specific training for the sensory analysis of products in accordance with the OIV documents [48]. The experts were members of the tasting commissions of various levels – the scientific center of FSC HVW, Ministry of Agriculture of the Russian Federation, and federal expert tasters with the appropriate certificates of the Register of Personnel Certification Systems. Wine quality sensory assessment included appearance, aroma (bouquet), taste, and harmony/overall impression (Table S2). Sensory assessment was carried out according to the interstate standard [48] using a 100-point scale. The sensory assessment algorithm is similar to the Parker rating system [6]. The selection, training, and control over the work of experts was carried out in accordance with the requirements [49].

Prior to the sensory assessment, all wine samples were randomly coded. During the sensory assessment, information about the manufacturer and product name was hidden from the experts, the bottle with the tasting wine was placed in an opaque case. The expert was informed only about the code and the year of harvest. A certain sequence of products supply for tasting by categories was followed:

first white, then red wines. The tests were carried out in a well-lit tasting room with controlled temperature conditions. The experts were located in separate test booths, all workplaces were equipped with individual light sources for determining the transparency of the sample, as well as computers for transmitting data to a unified system. Experts were prohibited to communicate during the sensory assessment procedure. The total score was determined by the sum of the single assessments, considering their weight coefficients. For a consolidated assessment of wines, the average values of sensory evaluations were calculated by the computer program.

During the sensory assessment, the wines were served in transparent tulip shape glasses with a volume of 220 mL. Wine samples (50 mL) were poured into each glass and covered with a 5.7-cm diameter Petri dish for 30 min prior to the sensory assessment. The samples were submitted for assessment after preliminary storing at the following temperatures: white wines – from 10 °C to 12 °C, red wines – from 15 °C to 20 °C. The intervals between tasting of each sample were 2 min. During each interval, experts rinsed their mouths with water. Experts evaluated each sample in triplicate during the working week.

2.5. Ethical permission

Informed consent was obtained from each subject. The study was approved by the local ethics committee according to principles of the Helsinki Statement and Public Health Regulations (Clinical Experiments on Humans, including revisions and amendments) of the state budgetary healthcare institution "Research Institute-Regional Clinical Hospital No 1 n. a. Prof. S.V. Ochapovsky, 1 May St. 167, Krasnodar, 350086, Russia", protocol No. 122.

2.6. Data analysis

All statistical analyses were carried out using STATISTICA version 13.3.0 (TIBCO Statistica, 2017, USA. URL https://www.tibco.com/) [50]. The contribution of volatile compounds and amino acids to the sensory properties of wines was assessed by multiple regression and covariance analysis. Canonical analysis was applied to study stochastic relationships between the concentrations of amino acids and volatile compounds. Latent (hidden) factors characterizing the sensory properties of wines were identified by factor analysis and principal component analysis.

For multidimensional analysis, the following symbols corresponding to the concentrations of components were introduced: acetaldehyde – C_A; ethyl acetate – C_E; methanol – C_M; total content of higher alcohols– C_{HA}; acetic acid – C_{AA}; furfural – C_F; arginine – C_{Arg}; proline – C_{Pr}; threonine – C_{Trn}; average value of sensory assessment – *Est*; group of quality (*low, medium, high*) – *GofQ*.

3. Results and discussion

The arithmetic mean, minimum, and maximum values of the obtained concentrations of volatile compounds and amino acids in the studied wine samples, grouped by quality, are summarized in Table 1. More detailed data on the contents of the studied compounds in 150 wine samples can be found in the Supplementary Table S1.

The studied samples of dry red and white wines of 14 varieties were cultivated and produced in 6 grape growth territories of the Krasnodar region. As a result, differences in the contents of amino acids and volatile compounds in the groups were observed. The boxplots for acetaldehyde concentrations in groups based on wine color, grape variety, and region of growth are given in Supplementary Figs. S1–S3.

As can be seen in the figures, mean concentration values of acetaldehyde and their scattering are different in these groups. In the wine color groups, the average concentrations of acetaldehyde and the variations are approximately the same. In the groups based on the region of growth and grape variety, the differences in average values, standard errors, and deviations are more significant.

The scatterplots of canonical values were used to evaluate the homogeneity of the volatile compounds and amino acids based on the color, region of growth, and variety. Scatterplots allowed to transfer objects of a multidimensional space (in our case, the number of dimensions was 9 – by the number of amino acids and volatile compounds) to a plane with Root 1 and Root 2 coordinates while

Table 1
Main statistical characteristics of volatile compounds and amino acids, mg/L.

Variable	Quality								
	High			Medium			Low		
	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max
Volatile compounds									
C_A	35.36	21.00	51.00	166.74	120.00	230.00	36.54	21.00	51.00
C_E	57.18	44.00	77.00	58.46	52.00	77.00	56.42	44.00	74.00
C_M	54.96	40.00	68.00	51.44	41.00	68.00	109.02	88.00	165.00
C_{HA}	245.32	210.00	301.00	241.06	210.00	300.00	562.18	440.00	750.00
C_{AA}	346.72	240.00	405.00	624.30	450.00	850.00	343.60	320.00	401.00
C_F	5.50	3.00	9.00	5.38	2.00	8.00	36.00	18.00	66.00
Amino acids									
C_{Arg}	25.46	21.00	31.00	4.32	1.00	8.00	5.66	1.00	9.00
C_{Pr}	685.44	600.00	788.00	213.22	168.00	255.00	48.78	35.00	59.00
C_{Trn}	49.98	40.00	58.00	5.84	1.00	34.00	14.28	10.00	25.00

preserving the order of the distances between them. Close objects on the plane are also close in a multidimensional space, which means they are similar in terms of a set of features. As can be seen from Supplementary Figs. S4–S6, the geometric figures depicting wine samples of various groups are located arbitrarily on the plane, without forming uniformity classes, i.e., they do not have a cluster structure relative to color, region, and variety.

Despite the differences in the groups, these results allowed to consider dry wine samples as a homogeneous group and to study the contribution of amino acids and volatile compounds to the formation of sensory properties of wines.

In the study [51], three quality groups were proposed for wines, i.e., low, medium, and high, based on the results of sensory assessment of 330 dry red and white wine samples produced from the same grape varieties.

- if furfural content in the wine sample is higher than 9 mg/L, the wine is of low quality;
- if furfural content in the wine sample does not exceed 9 mg/L, acetic acid and methanol contents are more than 430 and 95 mg/L, respectively, the wine is also of low quality,
- if furfural content in the wine sample does not exceed 9 mg/L, acetic acid content is higher than 430 mg/L, and methanol concentration in the wine sample does not exceed 95 mg/L, the wine is of medium quality;
- if furfural and acetic acid contents in the wine sample do not exceed 9 and 430 mg/L, respectively, and higher alcohol concentrations exceed 150 mg/L, the wine is of high quality.

Considering the above approach, the mean, minimum, and maximum values of the initial experimental data on the concentrations of studied volatile compounds and amino acids were combined into quality groups (Table 1). More detailed data on the content of the studied compounds in the wine samples are summarized in Supplementary Table S1.

The analysis of the obtained data has revealed a significant difference both in the average concentrations of compounds as well as in their ranges in different categories of wine quality. For example, mean contents of methanol, furfural, and higher alcohols in the wines of *low* quality significantly exceeded their contents in the wines of *high* quality. High concentrations of amino acids were observed in the wines of *high* quality. Ethyl acetate has the least variability among wine quality groups. The least significant difference (LSD) criterion of ANOVA (Table 2) showed that the differences between all amino acid concentrations were statistically significant ($p < 0.05$ *values are highlighted in bold*) for all three pairs of compared groups of wines. The difference in the concentrations of volatile compounds is statistically significant in at least two pairs of groups, except for ethyl acetate, in which statistical significance has not been achieved due to large differences in the concentrations in wine samples. In more than 70% of cases of paired comparisons, the difference in the concentrations of volatile compounds and amino acids was statistically significant.

The justification for the fact that the wine samples in the groups differ in quality is the statistically significant difference of average sensory assessment values (*Est*) in the *high* (87.76), *medium* (72.14), and *low* (68.72) quality groups according to the LSD criterion. The box plot (Fig. 1) graphically shows the degree of difference in the average values of the sensory assessment in wine quality groups with relatively small variations in sensory assessments.

Discriminant analysis (DA) showed that the combination of the concentrations of amino acids and volatile compounds determines the differences between wine quality groups. The built DA scatterplot of canonical scores (Fig. 2) allowed to transfer wine samples as objects of a multidimensional space of dimension 9 (according to the number of amino acids and volatile compounds) to a plane with coordinates Root 1 and Root 2 while maintaining the order of distances between them. The diagram shows that the wine samples, depicted as different geometric figures depending on the wine quality groups, are localized in certain parts of the plane. Small distances between wine samples of the same quality group indicate their intragroup similarity, and large distances between groups indicate intergroup differences in the concentrations of the selected amino acids and volatile compounds, proving that wine samples have a pronounced cluster structure relative to their quality.

3.1. Covariance analysis of wine groups

Covariance analysis allowed to empirically describe the relationship between the concentrations of volatile compounds and amino acids and sensory properties of analyzed wine groups as a linear regression equation (1) [26]:

$$Est = 64.482 - 0.017 \bullet C_{Arg} + 0.039 \bullet C_{Pr} - 0.101 \bullet C_{Trn} - 3.906 \bullet GofQ_1 + 0.024 \bullet GofQ_2 \quad (1)$$

Table 2
Significance levels p of LSD criteria for the intergroup comparisons.

Variable	$P_{High\text{-}Medium}$	$P_{High\text{-}Low}$	$P_{Medium\text{-}Low}$
C_A	**0.000**	0.785	**0.000**
C_E	0.306	0.542	0.104
C_M	0.166	**0.000**	**0.000**
C_{HA}	0.704	**0.000**	**0.000**
C_{AA}	**0.000**	0.781	**0.000**
C_F	0.929	**0.000**	**0.000**
C_{Arg}	**0.000**	**0.000**	**0.002**
C_{Pr}	**0.000**	**0.000**	**0.000**
C_{Trn}	**0.000**	**0.000**	**0.000**

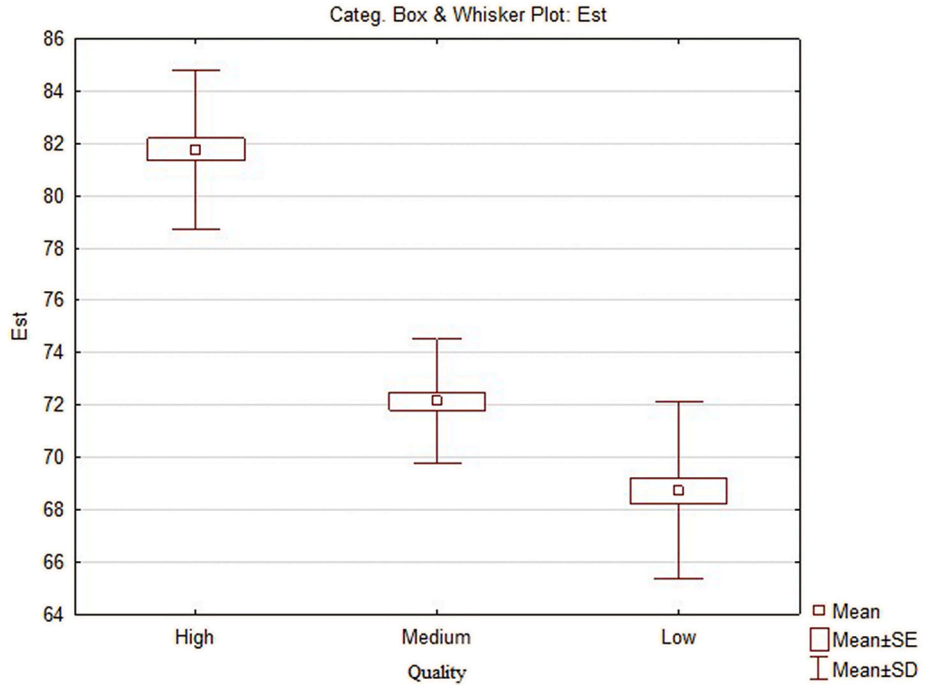

Fig. 1. Box plot of the sensory assessment Est in wine quality groups
*Est– average value of sensory assessment, SE – standard error, SD – standard deviation.

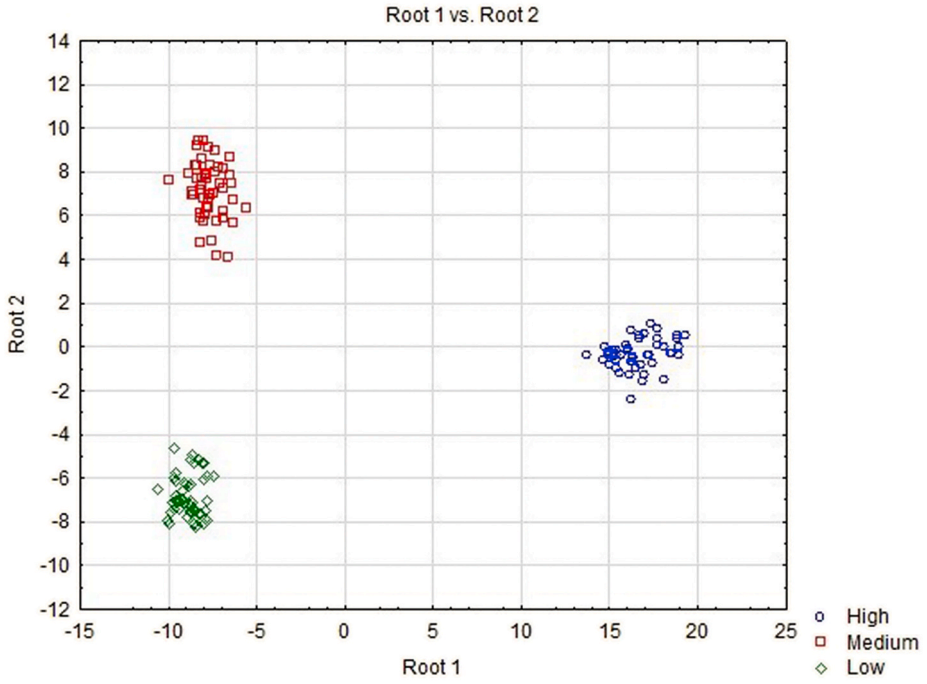

Fig. 2. Scatterplot of canonical scores for wine samples.

In the regression equation, amino acids are represented by predictors C_{Arg}, C_{Pr}, C_{Trn} explicitly, and volatile compounds are implicit through quality predictors $GofQ_1$ and $GofQ_2$; sensory properties of wines are represented by the average value of sensory assessment (*Est*). Quality predictors $GofQ_1$ and $GofQ_2$ are present in the equation in accordance with the principle of sigma-limited parameterization of covariance analysis, in which the categorical predictor *GofQ* can take only 2 values allowing to encode them in the binary

system as 0 and 1. Therefore, the *GofQ* predictor, which takes 3 values, is represented as $GofQ_1$ and $GofQ_2$ predictors with two values each – *high*, *low* and *medium*, *low*. If the wine belongs to the *high* quality group, then $GofQ_1 = 1$, $GofQ_2 = 0$; if the wine belongs to the *medium* quality group, then $GofQ_1 = 0$, $GofQ_2 = 1$; if it belongs to the *low* quality group, then $GofQ_1 = 0$, $GofQ_2 = 0$. Model adequacy indicators (the multiple correlation coefficient $R = 0.906$ and the determination coefficient $R^2 = 0.821$) have values close to 1, which indicates the adequacy of model (1) describing the relationship of the *Est* response with predictors, i.e., contents of amino acids, volatile compounds, and quality groups. Considering the well-known principles of linear regression analysis [52], it can be concluded that 82% of the response variability relative to the average value is determined by the model predictors. Since in the regression equation the response is the sensory evaluation, and model (1) predictors are amino acids and wine quality groups determined by the concentrations of volatile compounds, then 82% of the variability of the sensory properties of the analyzed wine groups falls on the amino acids and volatile compounds.

Using one-dimensional criteria of covariance analysis, the dominant role of amino acids in the perception of wine sensory properties by experts was revealed, when the average value of sensory assessment (*Est*) was used as a generalized indicator (Table 3). This statement follows from the fact that the total variability of the response from the concentrations of amino acids $SS_{total} = 0.19 + 211.223 + 31.954 = 243.367$ is more than 4-times greater than the variability of the response from the quality group *GofQ*, determined by the concentrations of volatile compounds $SS = 59.012$, where SS is the sum of squared deviations of the predicted response values from their average, initiated by this parameter.

3.2. Linear regression analysis of wine groups

In covariance analysis, volatile compounds are present implicitly through the quality predictor *GofQ*; however, in linear regression analysis, where the response is the sensory assessment *Est*, and predictors are the concentrations volatile compounds and amino acids, they are present explicitly. Table 4 shows the values of the multiple correlation ($R = 0.916$) and determination ($R^2 = 0.833$) coefficients, which are close to maximum, indicating a high adequacy of the linear model of the relationship of the sensory assessment with concentrations of volatile compounds, amino acids, and the possibility of its practical application.

The coefficients of the regression equation for the initial and standardized concentrations of volatile compounds and amino acids are shown in columns b and b* of the table. According to the coefficients from column b, the regression equation (2) was compiled, which can be used to predict the average sensory assessment based on the concentrations of amino acids and volatile compounds:

$$Est = 78.048 – 0.143 \bullet C_{Arg} + 0.029 \bullet C_{Pr} – 0.137 \bullet C_{Trn} – 0.023 \bullet C_A – 0.02 \bullet C_E + 0.021 \bullet C_M – 0.009 \bullet C_{HA} – 0.007 \bullet C_{AA} – 0019 \bullet C_F \quad (2)$$

The larger the absolute value of the coefficient in the column b*, the greater the contribution of predictors to the predicted response value will be [52]. Therefore, the largest contribution was observed for proline ($b^* = 1.258$), the smallest – for ethyl acetate ($b^* = -0.2$). The total contribution of proline and threonine concentrations to the formation of the sensory properties was higher than the total contribution of all volatile compounds. The greatest contribution to wine sensory properties among volatile compounds was made by acetaldehyde concentration; its contribution turned out to be 5- and 2-times lower compared to the concentrations of proline and threonine, respectively. The average contribution of amino acids is $(0.226 + 1.258 + 0.431)/3 = 0.638$; for volatile compounds it is $(0.244 + 0.02 + 0.096 + 0.24 + 0.157 + 0.047)/6 = 0.134$. This means that the average contribution of amino acids to the prediction of wine sensory properties is more than 4.5-times higher than for all volatile compounds. More than 83% of the variability of the predicted response, i.e., sensory properties of analyzed wines, was related to the studied amino acids and volatile compounds, which is indicated by the coefficient $R^2 = 0.833$ given in the information part of Table 4.

Thus, regression analysis confirmed the results of covariance analysis on the contribution of volatile compounds and amino acids to the variability of wine sensory properties and showed that the average contribution of amino acids to the prediction of the sensory properties is more than 4-times higher than that of volatile compounds.

Table 3
One-dimensional significance criterion of covariance analysis of the relationship between the concentrations of volatile compounds, amino acids, and sensory properties of the analyzed wine groups.

Effect	Univariate Results for Each DV Sigma-restricted parameterization Effective hypothesis decomposition				
	Est SS	Degr. of Freedom	Est MS	Est F	Est p
Intercept	3446.436	1	3446.436	472.938	0.000
C_{Arg}	0.190	1	0.190	0.026	0.871
C_{Pr}	211.223	1	211.223	28.985	0.000
C_{Trn}	31.954	1	31.954	4.384	0.038
GofQ	59.012	2	29.506	4.049	0.019
Error	1049.368	144	7.287		
Total	5862.593	149			

Table 4
Results of multiple regression analysis modelling the relationship between concentrations of volatile compounds, amino acids, and sensory properties of wines.

N = 150	Regression Summary for Dependent Variable: Est R = 0.916, R^2 = 0.838, Adjusted R^2 = 0.828 F(9,140) = 80.717 p < 0.000; Std.Error of estimate: 2.601					
	b*	Std.Err. of b*	b	Std.Err. of b	t(140)	p-value
Intercept			78.048	4.408	17.706	0.000
C_{Arg}	−0.226	0.138	−0.143	0.087	−1.640	0.103
C_{Pr}	1.258	0.177	0.029	0.004	7.126	0.000
C_{Trn}	−0.431	0.141	−0.137	0.045	−3.063	0.003
C_A	−0.244	0.084	−0.023	0.008	−2.913	0.004
C_E	−0.020	0.038	−0.020	0.038	−0.526	0.600
C_M	0.096	0.075	0.021	0.016	1.277	0.204
C_{HA}	−0.240	0.146	−0.009	0.006	−1.645	0.102
C_{AA}	−0.157	0.080	−0.007	0.004	−1.960	0.052
C_F	−0.047	0.128	−0.019	0.050	−0.370	0.712

3.3. Canonical analysis of correlations between amino acids and volatile compounds

The analysis of correlations within groups of amino acids and volatile compounds, as well as between these groups was equally interesting. Canonical correlation is a generalization of the paired and multiple correlation coefficients, which characterizes the degree of the relationship between two groups of random variables, i.e., volatile compounds and amino acids. The analysis showed that the canonical correlation coefficient ($R = 0.938$) had almost the maximum value (Table 5). This means that there is a strong relationship between the concentrations of amino acids and volatile compounds. A strong relationship is also indicated by large values of the total redundancy of the left (amino acids, 86.1%) and right (volatile compounds, 60.4%) sets, when another set is specified.

Pair correlation coefficients both within and between sets are shown in Tables 6–8. The tables are symmetrical with respect to the diagonal with units, so it is sufficient to interpret the correlation coefficients (r) over the diagonal. It is conditionally accepted that: if $|r| \leq 0.25$ – the relationship is weak, if $0.25 \leq |r| \leq 0.75$ – the relationship is moderate, if $|r| > 0.75$ – it is strong. If the correlation coefficient between the quantitative indicators is positive, an increase in the first indicator leads to an increase in another one, while in the case of negative correlation coefficient, an increase in the first indicator results in a decrease in another one [53]. In the present case, a positive sign means that an increase in the concentration of one of the amino acids in wine, for example, arginine, entails an increase in the concentration of proline and threonine. It is also evidenced from strong positive correlations between all the amino acid concentrations (Table 6).

For volatile compounds, strong positive correlation was observed between the concentrations of acetaldehyde and acetic acid, methanol and higher alcohols, methanol and furfural, higher alcohols and furfural (Table 7). The relationships between the concentrations of ethyl acetate and other volatile compounds were absent or weak. The remaining relationships were moderate.

The relationships between the concentrations of amino acids and volatile compounds are of particular interest (Table 8). There was no correlation between the contents of ethyl acetate and amino acids; the remaining correlations were moderate and negative. Consequently, an increase in the concentrations of volatile compounds is accompanied by a decrease in the concentrations of amino acids in wines, which may be explained by deamination of amino acids and formation of volatile compounds [29].

3.4. Factor analysis of the relationship between sensory properties of wines

The presence of intra- and inter-group correlations of interactions between amino acids and volatile compounds is a prerequisite for their combination into homogeneous groups – factors that explain the connections between the sensory properties of wines. To

Table 5
Results of canonical analysis of the relationship between concentrations of amino acids and volatile compounds.

N = 150		Canonical Analysis Summary Canonical R: 0,938 χ^2 (18) = 525,40 p = 0,000	
		Left Set	Right Set
No. of variables		3	6
Variance extracted		100.0%	81.0%
Total redundancy		86.1%	60.4%
Variable	1	C_{Arg}	C_A
	2	C_{Pr}	C_E
	3	C_{Trn}	C_M
	4		C_{HA}
	5		C_{AA}
	6		C_F

Table 6
Correlation coefficients between amino acid concentrations.

N = 150	Correlations, left set		
	C_{Arg}	C_{Pr}	C_{Trn}
C_{Arg}	1.000	0.921	0.939
C_{Pr}	0.921	1.000	0.879
C_{Trn}	0.939	0.879	1.000

Table 7
Correlation coefficients between volatile compound concentrations.

N = 150	Correlations, right set					
	C_A	C_E	C_M	C_{HA}	C_{AA}	C_F
C_A	1.000	0.031	−0.467	−0.432	0.831	−0.410
C_E	0.031	1.000	−0.061	−0.122	0.174	−0.082
C_M	−0.467	−0.061	1.000	0.815	−0.451	0.817
C_{HA}	−0.432	−0.122	0.815	1.000	−0.459	0.961
C_{AA}	0.831	0.174	−0.451	−0.459	1.000	−0.443
C_F	−0.410	−0.082	0.817	0.961	−0.443	1.000

Table 8
Correlation coefficients between amino acid and volatile compound concentrations.

N = 150	Correlations, left set with right set					
	C_A	C_E	C_M	C_{HA}	C_{AA}	C_F
C_{Arg}	−0.500	−0.060	−0.350	−0.418	−0.489	−0.413
C_{Pr}	−0.261	0.039	−0.592	−0.646	−0.230	−0.631
C_{Trn}	−0.599	−0.078	−0.250	−0.298	−0.582	−0.300

determine the number of homogeneous groups, the scree plot was used, in which the eigenvalues of factors connected by straight line segments were plotted (Fig. 3). Since the decrease in eigenvalues slows down starting from the third eigenvalue, 3 factors were identified – *Factor 1, Factor 2, Factor 3*.

Correlation coefficients between component concentrations and selected factors, i.e., factor loadings, are given in Table 9. If the homogeneous group is successfully identified, the factor loadings should be large with one of the factors and small with the others. Such distribution of factor loadings was achieved by rotating the coordinate axes according to the *Varimax raw* method [53]. As can be seen, the correlations of the concentrations of methanol, higher alcohols, and furfural are strong with *Factor 1* and weak with *Factors 2* and *3*. The correlations of arginine, proline, and threonine concentrations are strong with *Factor 2* and weak or moderate with *Factors 1* and *3*. A strong correlation of *Factor 3* was observed only with ethyl acetate concentration. Therefore, the dominant effect on *Factor 1* was exerted by volatile compounds, and on *Factor 2* – by amino acids. *Factor 3* was dominated by ethyl acetate, which was not associated with other volatile compounds and amino acids.

The sum of the variance proportions given in the bottom raw of table (0.416 + 0.403+0.114 = 0.933) shows that the selected factors describe approximately 93.3% of the variability of the data on the component composition of wines, which indicates a successful factorization.

A plot of factor loadings obtained by principal component analysis is shown in Fig. 4. The horizontal axis corresponds to *Factor 1*, the vertical axis – to *Factor 2*. The concentrations of volatile compounds and amino acids are depicted as points (vectors) of a two-dimensional space with coordinates equal to factor loadings, or correlations of components with factors. The components on the plane localized in the immediate vicinity formed three homogeneous groups identified by factor analysis. The first group includes higher alcohol concentrations, methanol, and furfural, the second – amino acids, the third – acetaldehyde and acetic acid. Ethyl acetate is located separately, away from all identified homogeneous groups. The angles between the vectors determine the nature of the correlation between the components – with the decrease in the angle, the correlation is becoming stronger; sharp angles correspond to positive correlation, obtuse – to negative correlation.

4. Conclusions

The data on the sensory evaluation were analyzed to assess the interactions of amino acids (arginine, proline, threonine) and volatile compounds (acetaldehyde, ethyl acetate, methanol, the total content of higher alcohols, acetic acid, furfural) in 150 dry red and white wine samples. When choosing the list of volatile compounds and amino acids to be determined, we were guided by their greatest influence on the sensory properties of wines. Target volatile compounds and amino acids were selected based on their contribution to the sensory properties of wines. To assess the contribution of volatile compounds and amino acids to the sensory

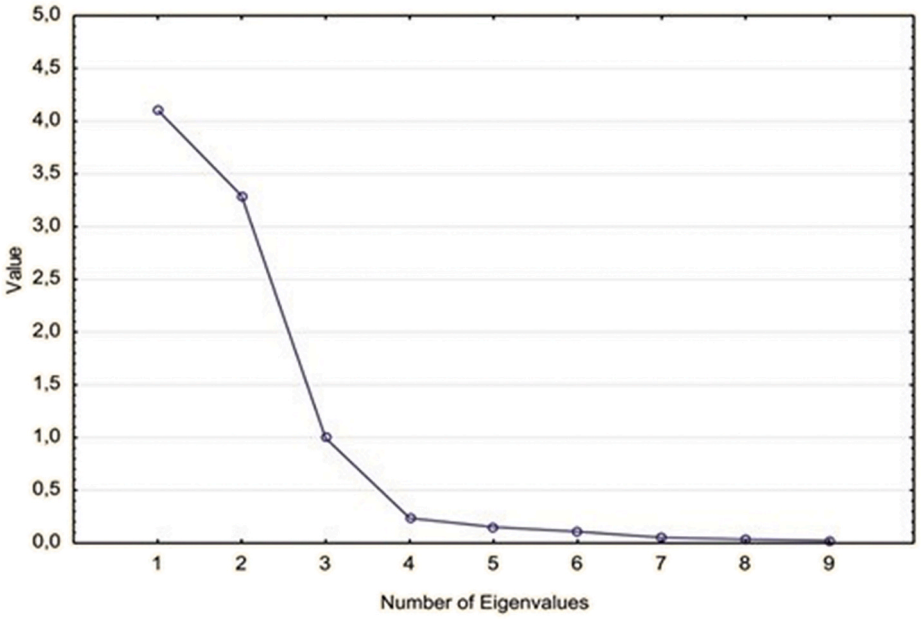

Fig. 3. Scree plot for establishing the number of selected factors.

Table 9
Factor loadings of correlation between component concentrations and selected factors.

Variable	Factor Loadings (Varimax raw) Extraction: Principal components (Marked loadings are >0.700)		
	Factor 1	Factor 2	Factor 3
C_{Arg}	0.259	−0.944	0.038
C_{Pr}	0.525	−0.832	−0.042
C_{Trn}	0.134	−0.970	0.048
C_A	0.619	0.720	0.048
C_E	0.058	0.041	−0.996
C_M	−0.908	0.135	0.003
C_{HA}	−0.946	0.191	0.080
C_{AA}	0.626	0.698	−0.124
C_F	−0.939	0.194	0.040
Expl.Var	3.744	3.624	1.023
Prp.Totl	0.416	0.403	0.114

properties, multidimensional approaches of analysis were applied, which allowed to establish a number of relationships.

- more than 80% of the variability of the sensory evaluation of wines is determined by the data of the covariance analysis of the relationship between the selected amino acids and volatile compounds, and the contribution of amino acids to this indicator is 4-fold higher;
- the contribution of amino acids to the sensory properties is more than 4.5-fold higher than the total contribution of volatile compounds according to the results of multiple regression analysis;
- canonical analysis of stochastic relationships between the concentrations of amino acids and volatile compounds allowed to establish strong positive correlations between the concentrations of amino acids, while for volatile compounds – between the concentrations of acetaldehyde and acetic acid, methanol and higher alcohols, methanol and furfural, higher alcohols and furfural;
- moderately negative correlations between the concentrations of volatile compounds and amino acids in wines may be explained by deamination of amino acids and formation of volatile compounds;
- amino acids and volatile compounds form three homogeneity groups: the first is higher alcohols, methanol, and furfural; the second is amino acids; the third is acetaldehyde and acetic acid.

The limitations of the study are the lack of data on the influence of different territories of grape growth on the ratios of volatile compounds and amino acids, the influence of climatic conditions on the sensory properties of wines. In further studies, we plan to expand the geography of the origin of dry wines as well as the range of compounds affecting sensory properties, since the studies have

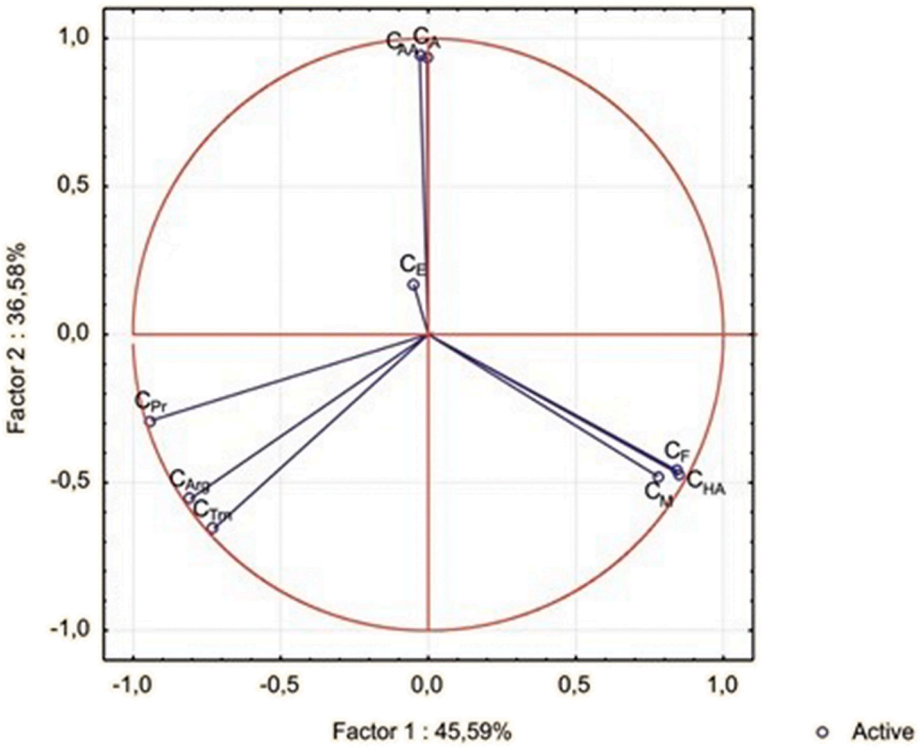

Fig. 4. A plot of factor loadings on the plane.

revealed that the considered compounds determine 80% of the variability of sensory evaluation.

Declarations

Author contribution statement

Alexan Khalafyan, Olga Sheludko: Analyzed and interpreted the data.

Zaual Temerdashev: Conceived and designed the experiments; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Aleksey Abakumov: Performed the experiments; Wrote the paper.

Yuri Yakuba: Performed the experiments.

Anastasia Kaunova: Performed the experiments; Analyzed and interpreted the data.

Funding statement

This work was supported by the Ministry of Education and Science of the Russian Federation (FZEN-2020-0022).

Data availability statement

Data included in article/supp. material/referenced in article.

Declaration of interest's statement

The authors declare no competing interests.

Acknowledgements

The experiments were carried out with the use of scientific equipment of the Environmental Analytical Center of Collective Use at the Kuban State University.

Appendix A. Supplementary data

Supplementary data related to this article can be found at https://doi.org/10.1016/j.heliyon.2023.e12814.

References

[1] R.S. Jackson, Wine tasting, in: R.S. Jackson (Ed.), Oral Sensations (Taste and Mouthfeel), third ed., Academic Press, San Diego, 2017, pp. 103–136, https://doi.org/10.1016/B978-0-12-801813-2.00004-5.
[2] R.S. Jackson, Wine Tasting, third ed., Elsevier Inc., 2008 https://doi.org/10.1016/S1082-0132(08)X0011-1.
[3] P. Ribéreau-Gayon, Y. Glories, A. Maujean, D. Dubourdieu, Handbook of Enology, second ed., John Wiley & Sons, Ltd, Chichester. West Sussex, England, 2006.
[4] Rolls H.D. Et Critchley, J.V. Verhagen, M. Kadohisa, The representation of information about taste and odor in the orbitofrontal cortex, Chemosens. Percept. 3 (2010) 16–33, https://doi.org/10.1007/s12078-009-9054-4.
[5] I.L. Francis, P.O. Williamson, Application of consumer sensory science in wine research, Aust. J. Grape Wine Res. 21 (2015) 554–557, https://doi.org/10.1111/ajgw.12169.
[6] RM Bordeaux Parker, A Consumer's Guide to the World's Finest Wines, 4th., Simon & Schuster, London, 2003.
[7] C. Spence, Perceptual learning in the chemical senses: a review, Int. Food Res. J. 123 (2019) 746–761, https://doi.org/10.1016/j.foodres.2019.06.005.
[8] D. Taladrid, L. Lorente, B. Bartolomé, M.V. Moreno-Arribas, L. Laguna, An integrative salivary approach regarding palate cleansers in wine tasting, J. Texture Stud. 50 (2019) 75, https://doi.org/10.1111/jtxs.12361, 2.
[9] R.S. Jackson, Wines: wine tasting, in: B. Caballero, P. Finglas, F. Toldrá (Eds.), Encyclopedia of Food and Health, Elsevier Inc, 2016, pp. 577–584, https://doi.org/10.1016/B978-0-12-384947-2.00757-1.
[10] Q.J. Wang, C. Spence, Wine complexity: an empirical investigation, FQAP 68 (2018) 238, https://doi.org/10.1016/j.foodqual.2018.03.011, 4.
[11] R. Perestrelo, C. Silva, P. Silva, J.S. Câmara, Rapid spectrophotometric methods as a tool to assess the total phenolics and antioxidant potential over grape ripening: a case study of Madeira grapes, J. Food Meas. Charact. 12 (2018) 1754, https://doi.org/10.1007/s11694-018-9790-8, 2.
[12] I. Kapusta, T. Cebulak, J. Oszmiański, The anthocyanins profile of red grape cultivars growing in south-east Poland (Subcarpathia region), J. Food Meas. Charact. 11 (2017) 1863, https://doi.org/10.1007/s11694-017-9568-4I, 3.
[13] L.G. Llobodanin, L.P. Barroso, I.A. Castro, Prediction of the functionality of young South American red wines based on chemical parameters, Aust. J. Grape Wine Res. 20 (2014) 15, https://doi.org/10.1111/ajgw.12057, 4.
[14] A.K. Baker, C.F. Ross, Sensory evaluation of impact of wine matrix on red wine finish: a preliminary study, J. Sens. Stud. 29 (2014) 139, https://doi.org/10.1111/joss.12089, 8.
[15] L. Vidal, L. Antúnez, A. Giménez, G. Ares, Evaluation of palate cleansers for astringency evaluation of red wines, J. Sens. Stud. 31 (2016) 93, https://doi.org/10.1111/joss.12194, 0.
[16] A. Rinaldi, L. Moio, Effect of enological tannin addition on astringency subqualities and phenolic content of red wines, J. Sens. Stud. (2018), https://doi.org/10.1111/joss.12325 e12325.
[17] Y. Gupta, Selection of important features and predicting wine quality using machine learning techniques, 2, Procedia Comput. Sci. 125 (2018) 305. ttps://doi.org/10.1016/j.procs.2017.12.041.
[18] G. Leonardi, L. Portinale, Applying Machine Learning to High-Quality Wine Identification. Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics). 10640 LNAI, 2017, pp. 31–33, https://doi.org/10.1007/978-3-319-70169-1_3.
[19] I.L. Francis, J.L. Newton, Determining wine aroma from compositional data, Aust. J. Grape Wine Res. 11 (2005) 114–126.
[20] P. Abbal, et al., A Decision Support system for vine Growers based on a Bayesian Network, J. Agric. Biol. 21 (2016) 131–151, https://doi.org/10.1007/s13253-015-0233-2.
[21] Y.-B. Lan, et al., Characterization and differentiation of key odor-active compounds of'Beibing hong 'ice wine and dry wine by gas chromatography-olfactometry and aroma reconstitution, 6, Food Chem. 287 (2019) 186, https://doi.org/10.1016/j.foodchem.2019.02.074, 6.
[22] The International Organisation of Vine and Wine, Maximum acceptable limits, Retrieved from, https://www.oiv.int/public/medias/3741/e-code-annex-maximum-acceptable-limits.pdf/, 2015. (Accessed 15 August 2021).
[23] K. Tang, Y.R. Xi, Y. Ma, H.N. Zhang, Y. Xu, Chemical and sensory Characterization of Cabernet Sauvignon wines from the Chinese loess plateau region, Molecules (2019), https://doi.org/10.3390/molecules24061122, 24061122.
[24] M. Vilanova, Z. Genisheva, A. Masa, J.M. Oliveira, Correlation between volatile composition and sensory properties in Spanish Albariño wines, Microchem. J. 95 (2010) 240–246, https://doi.org/10.1016/j.microc.2009.12.007.
[25] M. Vilanova, A. Escudero, M. Graña, J. Cacho, Volatile composition and sensory properties of Vitis vinifera red cultivars from North West Spain: correlation between sensory and instrumental analysis, Anal. Chim. Acta 720 (2012) 104, https://doi.org/10.1016/j.aca.2012.01.026, 1.
[26] Z.A. Temerdashev, A.A. Khalafyan, Y.F. Yakuba, Comparative assessment of amino acids and volatile compounds role in the formation of wines sensor properties by means of covariation analysis, Heliyon. e02626 (2019), https://doi.org/10.1016/j.heliyon.2019.e02626.
[27] Y.F. Yakuba, A.A. Khalaphyan, Z.A. Temerdashev, V.V. Bessonov, A.D. Malinkin, Flavouring estimation of quality of grape wines with use of methods of mathematical statistics, Voprosy Pitaniia 85 (2016) 93–99.
[28] A. Vilela, A. Inês, F. Cosme, Is wine savory? Umami taste in wine, J. Food Sci. Technol. 1 (3) (2016) 1–6.
[29] P. Hernández-Orte, J.F. Cacho, V. Ferreira, Relationship between varietal amino acid profile of grapes and wine aromatic composition. Experiments with model solutions and chemometric study, J. Agric. Food Chem. 50 (10) (2002) 2891–2899, https://doi.org/10.1021/jf011395o.
[30] L. Pekka, Determination of amines and amino acids in wine - a review, Am. J. Enol. Vitic. 47 (1996) 127–133.
[31] B. Zoecklein, K. Fugelsang, B. Gump, F. Nury, Wine Analysis and Production, Springer, New York, 1995, pp. 101–104.
[32] R. Del Barrio-Galán, M. Bueno-Herrera, P. López de la Cuesta, S. Pérez-Magariño, Stepwise linear discriminant analysis to differentiate Spanish red wines by their protected designation of origin or category using physico-chemical parameters, Oeno One 1 (2020) 86–99, https://doi.org/10.20870/oeno-one.2020.54.1.2588.
[33] J. Ruiz, et al., Effects on varietal aromas during wine making: a review of the impact of varietal aromas on the flavor of wine, Appl. Microbiol. Biotechnol. 103 (2019) 7425–7450, https://doi.org/10.1007/s00253-019-10008-9.
[34] Y. Bouzas-Cid, E. Falqué, I. Orriols, J.M. Mirás-Avalos, Effects of irrigation over three years on the amino acid composition of Treixadura (Vitis vinifera L.) musts and wines, and on the aromatic composition and sensory profiles of its wines, Food Chem. 240 (2018) 707, https://doi.org/10.1016/j.foodchem.2017.08.013, 6.
[35] R. Urvieta, G. Jones, F. Buscema, R. Bottini, A. Fontana, Terroir and vintage discrimination of Malbec wines based on phenolic composition across multiple sites in Mendoza, Argentina, Sci. Rep. 11 (1) (2021) 2863, https://doi.org/10.1038/s41598-021-82306-0.
[36] W. Pearson, et al., Regionality in Australian Shiraz: compositional and climate measures that relate to key sensory attributes, Aust. J. Grape Wine Res. 27 (4) (2021) 458–471, https://doi.org/10.1111/ajgw.12499.
[37] M. Kustos, et al., A matter of place: sensory and chemical characterisation of fine Australian Chardonnay and Shiraz wines of provenance, Int. Food Res. J. 130 (2020), 108903, https://doi.org/10.1016/j.foodres.2019.108903.
[38] S. Li, J.W. Blackman, L.M. Schmidtke, Exploring the regional typicality of Australian Shiraz wines usinguntargeted metabolomics, Aust. J. Grape Wine Res. 27 (2021) 378–391, https://doi.org/10.1111/ajgw.12493.

[39] L. Souza Gonzaga, D.L. Capone, S.E.P. Bastian, L. Danner, D.W. Jeffery, Sensory typicity of regional Australian Cabernet Sauvignon wines according to expert evaluations and descriptive analysis, Int. Food Res. 138 (2020), 109760, https://doi.org/10.1016/j.foodres.2020.109760.
[40] E.C. Scutaraşu, C.E. Luchian, I.B. Cioroiu, L.C. Trincă, V.V. Cotea, Increasing amino acids content of white wines with Enzymes Treatments, Agronomy 12 (2022) 1406, https://doi.org/10.3390/agronomy12061406.
[41] A.P. Stines, J. Grubb, H. Gockowiak, P.A. Henschke, P.B. Høj, R. Heeswijck, Proline and arginine accumulation in developing berries of Vitis vinifera L. in Australian vineyards: influence of vine cultivar, berry maturity and tissue type, Aust. J. Grape Wine Res. 6 (2) (2000) 150–158. https://doi:10.1111/j.1755-0238.2000.tb00174.x.
[42] J.M. Mirás-Avalos, Y. Bouzas-Cid, E. Trigo-Córdoba, I. Orriols, E. Falqué, Amino acid profiles to differentiate white wines from three Autochtonous Galician varieties, Foods 9 (2020) 114, https://doi.org/10.3390/foods9020114.
[43] B. Nemzer, D. Kalita, A.Y. Yashin, Y.I. Yashin, Chemical composition and Polyphenolic compounds of red wines: their antioxidant Activities and effects on human Health-A review, Beverages 8 (1) (2022), https://doi.org/10.3390/beverages8010001.
[44] The International Organisation of Vine and Wine, OIV-MA-AS315-27 Analysis of volatile compounds in wines by gas chromatography, Retrieved from, https://www.oiv.int/public/medias/5159/oiv-ma-as315-27.pdf/, 2016. (Accessed 2 December 2022). Accessed.
[45] The International Organisation of Vine and Wine, OIV-MA-AS312-03A methanol, Retrieved from, https://www.oiv.int/public/medias/2492/oiv-ma-as312-03a-en.pdf/, 2015. (Accessed 2 December 2022). Accessed.
[46] The International Organisation of Vine and Wine, OIV-MA-BS-14 Determination of the principal volatile substances of spirit drinks of viti-vinicultural origin, Retrieved from, https://www.oiv.int/public/medias/2674/oiv-ma-bs-14.pdf/, 2009. (Accessed 2 December 2022). Accessed.
[47] Y.F. Yakuba, Z.A. Temerdashev, Chromatography methods in the analysis and identification of grape wines, Analytic and Control 19 (2015) 288–301, https://doi.org/10.15826/analitika.2015.19.4.013.
[48] GOST 32051-2013 Sensory analysis - wine products. Methods of organoleptic analysis, Retrieved from, https://docs.cntd.ru/document/1200103859.
[49] ISO 8586:2012. Sensory analysis. General guidelines for the selection, training and monitoring of selected assessors and expert sensory assessors, Retrieved from, https://www.iso.org/standard/45352.html.
[50] T. Hill, P. Lewicki, Statistics Methods and Applications, StatSoft., Tulsa, OK, 2007.
[51] Y.F. Yakuba, Z.A. Temerdashev, A.A. Khalafʹyan, Application of ranging analysis to the quality assessment of wines on a nominal scale, J. Anal. Chem. 71 (2) (2016) 205–214, https://doi.org/10.1134/S1061934816020155.
[52] N.R. Draper, H. Smith, Applied Regression Analysis, third ed., John Wiley, 1998.
[53] R. Nisbet, r G. Mine, K. Yale, Handbook of Statistical Analysis and Data Mining Applications, Elsevier Inc., 2009, https://doi.org/10.1016/B978-0-12-374765-5.X0001-0.