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How distinctive are 'Gewürztraminer' vineyard terroirs in South Tyrol for wine production? A metabolomics-based approach

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ABSTRACT

Vitis vinifera L. 'Gewürztraminer' produces distinctive, aromatic wines that are strongly influenced by their terroir. This metabolomic study used a data-driven approach, including Principal Component Analysis (PCA) and Multifactorial Analysis (MFA), to correlate a quali-quantitative multivariate concept of terroir (including soil characteristics, and altitude) with sensory, phenolic, antioxidant, and volatile profiles of wines. The study analyzed wines from seven 'Gewürztraminer' vineyards, chosen to minimize the variability due to climate differences. Based on the soil data, the vineyards were clustered into two distinct groups: clay silicate (Group A) and dolomitic (Group B) soils. Group A exhibited lower levels of aromatic compounds such as linalool and higher levels of phenolic compounds such as gallocatechin than Group B. These findings indicate that even small changes in terroir within the same region can significantly impact the chemical, functional (antioxidant), and sensory properties of 'Gewürztraminer' wines, highlighting the importance of terroir in wine production. Statistical analyses confirmed the significance of these correlations ($p < 0.05$), highlighting the need for further research into the intricate relationship between terroir and wine quality.

1. Introduction

Vitis vinifera L. 'Gewürztraminer' is an aromatic variant of pink-skinned 'Savagnin' ('Traminer'), likely originating in Germany in the 19th century [1]. It is also a historical grape variety of South Tyrol (Alto Adige – Südtirol), Northern Italy, where 617 ha are currently planted, making it the second most planted grape in the region. This variety is widely cultivated around Termeno sulla Strada del Vino – Tramin an der Weinstraβe (Tramin), the village it is named after. Substantial plantings also exist in Alsace (France), Austria, Australia, Germany (where 'Roter Traminer' refers to both Gewürztraminer and non-aromatic 'Savagnin Rose'), New Zealand, and the Pacific Northwest of the USA, with smaller plantings in numerous other countries [1].

'Gewürztraminer' is early ripening but frost sensitive, and produces small bunches with lower yields compared to other cool climate cultivars. 'Gewürztraminer' vines are prone to viral infections, and rot can occur in wetter climates [1,2]. Although early ripening, full maturity is required to observe varietal characteristics. Wines from early-harvested grapes can lack character and be excessively tannic [2,3]. 'Gewürztraminer' wines often have high-potential alcohol levels (often more than 14 %) and low acidity, making the cultivar unsuitable for warm climates [1,2]. In Alsace, it is categorized as a "cépage de haut de gamme" (high-quality cultivar) [3].

'Gewürztraminer' produces distinctive, highly aromatic wines that are strongly influenced by the terroir of the vineyard sites where they are grown [4]. Terroir is officially defined as an "area in which collective knowledge of the interactions between the identifiable physical and biological environment and applied viti viticulture practices develops,

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providing distinctive characteristics for the products originating from this area", which include "specific soil, topography, climate, landscape characteristics and biodiversity features" [5]. Consequently, wine can be considered a "molecular kaleidoscope integrating signatures from grapes, yeasts, the winemaking, and the environment, reflected in the variety of compounds, including primary (e.g., sugars, organic acids, amino acids) and secondary metabolites (e.g., phenolics, volatile compounds, and other minor compounds)" [6]. These complex interactions illustrate the direct links between terroir, wine composition, and wine character [7].

The geological environment of a vineyard is an important abiotic stressor influenced by factors such as water availability, salinity, sun exposure, extreme temperature, and excessively acidic or alkaline soil. These conditions significantly affect grapevine ecophysiology. The primary environmental drivers of terroir expression are climate and soil conditions [8–10]. To better understand the impact of soil on wine quality, it is essential to define the measurable parameters that characterize vineyard soils and to assess their effects on soil behavior and plant-soil interactions. Inorganic soil components, such as minerals constituting the parent material, play specific roles in soil composition. Mineral content is fundamental for vine health [11,12], with clays being the most reactive inorganic components, warranting specific attention and research. A previous study by one of the authors used a codified analytical procedure [4] to obtain precise and globally comparable mineralogical information to classify not only the terroir but also the geopedological identity of each vineyard.

Numerous studies have demonstrated the global influence of terroir on the chemical and sensory properties of wine [6,12–20], thus vineyard maps have been produced based on pedological and geological surveys [21,22]. However, fewer studies concentrate on 'Gewürztraminer' specifically [3,4,23–27]. Methods have been proposed to delineate individual terroirs objectively. Laville defined *Natural Terroir Units* based on stable factors, such as topography, soil, climate, and biodiversity [22,28]. More recently, Ferretti proposed both *Vineyard Geological Identity* (VGI) [4,25] and *Solar Radiation Identity* (SRI) [24]. The VGI system uses geological, pedological, and mineralogical data [4], whereas the SRI system focuses on microclimate, altitude, and soil aspects using a detailed digital terrain model [24]. The VGI system has also been successfully applied in the USA [12]. These complementary methods can be combined to achieve a comprehensive understanding of terroir [25]. The present study uses data from the VGI system.

Several studies have examined the impact of terroir on 'Gewürztraminer' grown in the Alsace region of eastern France [3,23,26,29]. The geology of Alsace is particularly complex, and hence its terroirs are distinctive [3,29]. The vineyards of that region differ due to factors such as soil and geology, soil hydrometry and permeability, climate, and pedoclimatic [26]. South Tyrol is also geologically complex, with more than 150 rock types and ten rock formations [4]. Seasonal temperatures in the region are mainly influenced by solar radiation, which is related to altitude and terrain [24,30,31]. The Tramin area in South Tyrol is a small region where environmental differences between vineyards are negligible, but vineyards differ considerably in terms of geopedological characteristics [24].

Previous studies conducted in other regions have shown the influence of both climate and geopedological factors but have been less effective in distinguishing between the effects of climate, geography, and geopedology. This study builds on the work of Ferretti [4,24,25], who examined the differences in 'Gewürztraminer' wines due to geopedological differences in South Tyrol. Ferretti [4] conducted a detailed geopedological and topoclimate survey of several 'Gewürztraminer' vineyards near Tramin using the VGI system. Later studies employed the SRI system to predict ripeness levels and biosynthetic activity [24]. Both VGI and SRI systems have also been used in combination resulting in the classification of vineyards into three soils groups based on parent geology: dolomitic, mixed terrigenous, and silicate, each showing distinct differences in wine and grape compositions [25].

In one of the few other studies conducted in South Tyrol, Pedri & Pertoll [27] examined 'Gewürztraminer' in the Überetsch region, bordering the village of Tramin. They found that sites on limestone rubble (St Josef am See, Planitzing "Garnellen", and Kaltern Dorf) clustered together, with the exception of the higher altitude Eppan "Berg" site (572 m vs. 247–482 m, a.s.l.). The Girlan "Schreckbichl" site was distinct and characterized by humic loamy sandy soil from lake deposits. The remaining sites included acidic soils from moraine deposits (Girlan "Doos", Kaltern "Mazzon", and St Pauls "Feld") and Eppan "Berg", which lacked common features. Sensory profiles showed Eppan "Berg" clustered with other limestone soil sites, with soil exerting a strong influence. Wines from limestone soils exhibited increased acidity and distinct apple and cinnamon notes, whereas wines from other soils had citrus, nutmeg, and clove notes, along with typicity, fullness, and intensity [27]. Compared to the current study, that study examined fewer vineyards across more villages and did not take into account molecular profiles obtained by ultrahigh-performance liquid chromatography (UHPLC) or two-dimensional gas chromatography-mass spectrometry (GC × GC-MS), resulting in less analysis of the impact of terroir on wine. Likewise, previous soil analyses, particularly those focused on mineral content, have primarily been qualitative rather than quantitative at high resolution. This study addresses these gaps, introducing also the VGI method for detailed quantitative soil minerals analysis.

This study aims to investigate how variations in terroir, including soil and geology, relate to the sensory, chemical, and antioxidant capacity characteristics of 'Gewürztraminer' wine. Seven different vineyards in the Tramin area of South Tyrol, Italy were used for this purpose. The hypothesis is that even small changes in terroir can result in observable differences in wine quality. This research could provide insights into the effect of terroir on wine characteristics, with potential implications for agronomic and winemaking practices for 'Gewürztraminer' wines.

2. Materials and methods

2.1. Geographical sites

Vitis vinifera L. 'Gewürztraminer' grapes were collected from seven vineyards near Tramin, in the subregion of Basse Atesina – Unterland, South Tyrol, northern Italy (46° 20′ 40″ N, 11° 14′ 30″ E), which is within the central-eastern part of the Alps (Fig. 1 a and b).

Table 1 and Supplementary Table 3 list the components of the geopedological classification of vineyard soil sediments in Tramin. This highlights their lack of homogeneity due to the complex and varied geological evolution of this portion of the Alpine territory. The soil is characterized by dolomite, limestone, and ancient sedimentary rocks mixed with porphyry. Metamorphic deposits from the north of the region are also present in the southernmost part of South Tyrol [24,25]. Soil types are classified using a modified Sheppard's soil classification, as per Ferretti & Febbroni [25]. Geological domain and mineral composition were also determined and used for the multifactorial analysis (MFA; section 3.5). Soil pH varied from 8.1 to 8.6, and there were no groundwater sources in any of the vineyards.

Near the village of Tramin, there are fine soils of fluvial-glacial origin from ancient sedimentary rocks, with a substantially silty-clayey component colored by iron oxides such as hematite. Calcium carbonate and dolomite minerals result in soils with a pH ranging from slightly alkaline (pH 8.1) to strongly alkaline (pH 8.6) [24,25].

2.2. Vineyard soil and geology

Geological research was conducted on the seven vineyards, based on analyses of 22 soil and subsoil samples. There were at least three replicate samples from each vineyard. The geological aspects related to the seven vineyards were analyzed using the VGI method for analysis of vineyard geopedological conditions [4].

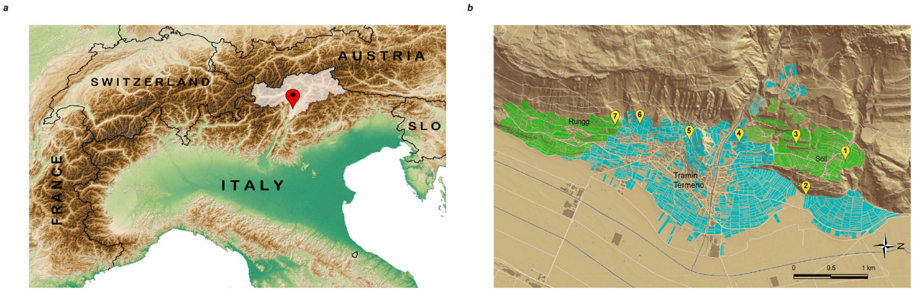

Fig. 1. A, Geographical location of Tramin an der Weinstraβe within the Alps; b, Geographical location of the 'Gewürztraminer' vineyards, Group A (vineyards 1, 3, and 7, as defined by the PCA of soil data detailed in section 3.1) is colored green and Group B (vineyards 4, 5, and 6) and Group C (Vineyard 2) are colored blue. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

Table 1
Vineyard data, adapted from Ferretti & Febbroni (2022). Weight fractions (wt %) of crystalline phases identified by Rietveld refinements in the 22 soil and subsoil samples.

Vineyard code	NRCS-USDA soil	Sheppard soil	SRI	Altitude ASL	Prevalent parent rock	Sedimentary process	Domain
Vineyard 1	loam	sandy silt	78.61	435.0	Metamorphic and ancient sedimentary	Undifferentiated till deposit	siliciclastic
Vineyard 2	silt loam	silt - gravelly silt	75.50	222.4	Dolomite	Mixed fan: stream flow	dolomitic
Vineyard 3	loam	loam	79.02	463.3	Metamorphic and ancient sedimentary	Glacial lodgment till deposit	siliciclastic
Vineyard 4	sandy loam	sandy gravel	76.47	361.7	Dolomite	Ancient mixed fan deposit	dolomitic
Vineyard 5	Loam	silty gravel	78.29	315.3	Dolomite	Ancient mixed fan deposit	mixed
Vineyard 6	Loam	silty gravel	72.65	323.0	Ancient sedimentary and Dolomite	Mixed fan: stream flow and debris flow	mixed
Vineyard 7	silt loam	loam	68.16	346.3	Ancient sedimentary	Gravity driven deposit	terrigenous

2.2.1. *Geo-mineralogical analyses*

Geo-mineralogical analyses were performed to investigate soil sediment origin, soil mineralogy, and bulk soil chemistry. The following analyses were conducted on all soil samples to investigate the site-specific mineralogical characteristics of each vineyard: thermogravimetric analysis, differential thermal analysis, geo-mineralogical microanalysis of soil composition using X-ray diffraction, and X-ray fluorescence. These analyses can provide representative information about different geological environments and soil parent materials.

For X-ray diffusion, a D8 Advance Da Vinci (Bruker, Billerica, MA, USA) with CuKα1.2 radiation equipped with a 1-D LYNXEYE XE detector was used. The sample was mounted on a side-loaded Plexiglass baseplate, and the measurement conditions were as follows: variable slits with fixed illuminated area of 15 mm, angular range: 3–90° 2q, step-size: 0.019°; time/step "0-D equivalent": 12 s; sample spin during measurement. Quantitative modal phase analysis by Rietveld method was carried out using Bruker TOPAS calculation software. Structural models of the crystalline phases found by qualitative analysis were used in the simulation procedure of the observed diffractogram.

For X-ray fluorescence, an ARL Advanta XP X-ray spectrometer (Thermo Fischer Scientific, Waltham, MA, USA) with a Rhodium tube and front window was used. A counting time on peaks of 10 s for major elements and 40 s for trace elements was used, and 3.0 kW of applied power. The results were accurate to more than 3 % relative for Si, Ti, Ca, and K and more than 7 % relative for Al, Mn, Mg, Na, and P, with a detectability limit of 0.01 % for all elements. Correction for the matrix and for inter-elementary effects was as per Lachance & Traill [32].

These methods were used to determine the petrophysical properties of the soils by combining the calculation of the structural formulas of variable composition minerals with a statistical distribution of trace elements over all the minerals present for the entire sample set. Application of the accurate Rietveld method to Quantitative Phase Analysis allowed the large mixture mineralogy of vineyard soils to be fully quantified. The bulk-rock analysis was normalized to 100 wt.%. Soil organic matter content (OM) was also measured (section 2.2.3). The wt.% of OM was not combined with the bulk mineral quantitative results and refers to the whole soil sample. OM is not a measurement that can be summed with the bulk mineral quantitative results, since the minerals were cleaned and measured without the organic fraction.

Diethylenetriaminepentaacetic acid (DTPA) and ethylenediaminetetraacetic acid (EDTA) soil testing were used to provide qualitative and quantitative analysis of soil heavy metals. Trace elements in soils were measured using inductively coupled plasma-mass spectrometry (ICP-MS) using an Agilent 7500ce ICP-MS (Agilent Technologies, Santa Clara, CA, USA) with a ASX-520 autosampler (CETAC Technologies Inc., Omaha, NE, USA), with detection limits of <0.1 mg kg^{-1} for lead, silver, barium, beryl, cerium, lanthanum, manganese, rubidium, and strontium, <0.2 mg kg^{-1} for boron and copper, 0.5 mg kg^{-1} for calcium and zinc, 1.0 mg kg^{-1} for sodium, 20 mg kg^{-1} for sulfur, and 0.5 g kg^{-1} for iron [33,34].

2.2.2. *Soil texture analysis*

Soil texture analysis of all soil samples (grain size <10 cm) was conducted according to DIN ISO 17892-4 standard [35]. Unlike the soil texture test based on the USDA system, which measures the 0–2 mm material fraction, this geotechnical test provides more complete and substantial data on parent material. In many terroir studies, a full-range granulometric analysis is essential to investigating the geopedological identity of each vineyard. This allows for complete evaluation of the depositional processes of sediments, as well as their agronomic and geotechnical behaviors, making it easier to classify soil types of different origins.

The bulk-rock analyses were normalized to 100 wt.%; the wt.% of OM were not combined with the bulk-rock quantitative results and refers to the whole soil sample. The availability of these data can improve the interpretations of ecological soils sub-factors.

2.2.3. *Agrochemical soil tests*

Agrochemical soil tests are conventionally used to classify soils and land plots. Therefore, additional soil classification parameters like texture (using wet sieving and densitometry methods, as per Italian regulation DM September 13, 1999 No. 185 GU No. 248 October 21, 1999 Met II.6 [33] and UNI-CEN IDO/TS 17892–4 [36]), pH (using the potentiometric method with a soil-to-water ratio of 1.0:2.5, as per Italian regulation DM September 13, 1999 n°185 GU No. 248 October 21, 1999 Met III.1 [33]), OM content (using elemental analysis of organic carbon, as per Italian regulation DM September 13, 1999 No. 185 GU No. 248 October 21, 1999 Met VII.1 [33]), and cation exchange capacity (CEC) (via titration in barium chloride and triethanolamine, as per Italian regulation DM September 13, 1999 n°185 GU n°248 October 21, 1999 Met XIII.2 [33]) were determined for all samples.

2.3. Winemaking procedure

'Gewürztraminer' grapes were harvested from the seven vineyards (harvest dates and vineyard areas are shown in Supplementary Table 1) at optimal ripeness (specific gravity between 1.1078 and 1.1124, i.e., 25.47 °Brix to 26.47 °Brix, see Supplementary Table 1) and with yields of 6000 kg ha^{-1}. The vineyards are planted with several clones (Lb 14, Lb 20, 47, 48, and 643) and rootstocks (SO4 and 125AA). Vineyard 2 was harvested slightly earlier, due to problems with the rootstock. The chemical parameters of grape must at harvest (measured in the must) are shown in Supplementary Table 1.

Winemaking procedures were identical for all vineyards. Two replicate fermentations were carried out for each vineyard. Musts were cold soaked at ambient temperatures (15–20 °C) with Cytolyses macerating enzyme (DSM, Maastricht & Heerlen, Netherlands) for two to 3 h, and then pressed for 3 h as whole bunches without destemming in a Bucher pneumatic press (Bucher Vaseline, Chalonnes-sur-Loire, France) using an automatic program with a maximum pressure of 1.8 bars. During pressing, an addition of Uvagen (Bioenologia 2.0, Oderzo, TV, Italy), a commercial blend of tannins, sulfur dioxide, and ascorbic acid, was added to protect the must. The must was racked at approximately 120–170 Nephelometric Turbidity Units.

Fermentations were inoculated with *Saccharomyces cerevisiae* strain EM2 (Institut La Claire/Perdomini-IOC, S. Martino Buon Albergo, VR, Italy). Nitrogen was added as a nutrient for the yeast in the form of diammonium phosphate at 10 g hL^{-1} and in the form of commercial yeast derivatives Springferm and Springferm Xtrem (Fermentis, Marquette-lez-Lille, France), Activit O (Institut Œnologique de Champagne, Epernay, France), and Proteofast (Bioenologia 2.0, Oderzo, TV, Italy). Fermentation took place over 14–19 days in stainless steel. Ageing subsequently took place in stainless steel. Sulfur dioxide was added before bottling. The wines did not undergo cold stabilization and metatartaric acid was not added.

2.4. Sensory analysis

For sensory analysis, a group of 14 panelists was selected from enology students and industry experts (the group consisted of eight women and six men, ranging in age from 23 to 34). The panelists were all from an Italian background, to prevent regionality effects from influencing the panel. This study was conducted in accordance with the Declaration of Helsinki for studies on human subjects [37]. Written informed consent was obtained from each participant.

In the first qualitative phase, panelists were asked to analyze a sample of Gewürztraminer wine and find at least two or three visual, olfactory, and gustatory descriptors, respectively (qualitative session). These data were analyzed using qualitative textual analysis to highlight the highest frequencies of descriptors and create the sensory descriptor table.

Next, the panelists participated in a 2 h training session in which they were instructed in the recognition of the major descriptors shown in Supplementary Table 2.

Sensory analysis was carried out by sorting methodology [38], which is a method based on panelist criteria for dividing samples into groups. There were seven groups allowed, derived from the seven vineyards of Gewürztraminer analyzed. Each panel member was then asked to subdivide the samples into as many groups as they deemed necessary, based on the similarity of the samples. In addition, the panelists were asked to explain the subdivision by some descriptors already selected during the previous qualitative session (Supplementary Table 2).

Training and data collection of the test was carried out using the Cysensy web app, a paperless sensory analysis software developed by the Oenolab group (Free University of Bozen-Bolzano, Bolzano, BZ, Italy) in collaboration with the Faculty of Computer Science and Technology (Free University of Bozen-Bolzano).

2.5. HPLC-PDA-HRMS: characterization of phenolic compounds

The phenolic profile of wines was analyzed using an Ultimate 3000 ultrahigh performance liquid chromatography (UHPLC system, Thermo Fischer Scientific, Waltham, MA, USA) with a Kinetex Biphenyl 2.6 μm 100 Å 100 × 2.1 mm ID column (Phenomenex, Torrance, CA, USA) and photodiode array (PDA) detector. The column temperature was maintained at 30 °C. Wine samples were diluted 1:100 with mobile phase A before analysis. Samples were analyzed in randomized order to avoid bias, with two technical replicates per wine.

The mobile phases consisted of Milli-Q water with 6.5 mM ammonium formate and 0.1 % of formic acid (phase A) and acetonitrile with 6.5 mM ammonium formate and 0.1 % of formic acid (phase B). The applied gradient was as follows: 0–8 min at 2 % phase B, 8–9 min to 10 % phase B, 9–26 min from 10 to 40 % phase B, 26–27 min to 95 % phase B, 27–30 min maintained at 95 % phase B, 30–31 min from 95 to 2 % phase B, followed by a reconditioning step from 31 to 35 min at 2 % phase B. The solvent flow rate was 0.3 mL min^{-1}, and the injection volume was 5 μL. The autosampler was set to 5 °C to refrigerate the samples before and during analysis. The PDA detector measured signals at 280, 320, 365, and 420 nm.

The compounds were identified using a QExactive Orbitrap high-resolution mass spectrometer (Thermo Fischer Scientific, Waltham, MA, USA). Acquisition was done in full-MS mode at a resolution of 70,000 with data-dependent MS-MS fragmentation using an inclusion list of compounds of interest in both positive and negative ionization modes. The scan range was 135–650 *m/z*. The sheath gas flow was set to 20 arbitrary units, and auxiliary gas to 5 arbitrary units. The spray voltage was 3.5 kV, the capillary temperature was 320 °C, and the *S*-lens RF level was 65. Compounds were identified using analytical standards and Phenol Explorer v3.0 [39–41].

2.6. Antioxidant capacity of samples by coulometric array detector (CAD)

The antioxidant capacity of samples was analyzed using a CAD detector. An Agilent 1260 Infinity HPLC system (Agilent, Santa Clara, CA, USA) was coupled to a Dionex CoulArray coulometric array detector (Thermo Fischer Scientific, Waltham, MA, USA), consisting of 16 porous graphite cells with applied potentials from +50 mV to +850 mV with 50 mV increments. The applied potentials of each electrochemical detector were relative to a palladium pseudo-reference electrode with a 360-mV shift difference compared to the Ag/AgCl electrode [42]. The mobile phases and gradients were the same as those in the HPLC-PDA-HRMS analysis. Two technical replicates were measured for each wine. The current signal (μA) over time was measured for each CAD channel. For each sample, the total charge was calculated as the sum of the integrated peak areas of all peaks detected at channels ranging from +50 to +650 mV. The calculated area represents all redox compounds and was used to express the antioxidant capacity of the wine samples. Data acquisition was performed using ESA CoulArray 3.1 software (Dionex. Thermo Fisher Scientific). The data integration and export were performed using Chromeleon CDS software (Thermo Fisher Scientific).

2.7. GC × GC-MS: characterization of volatile aroma compounds

Aroma profile analysis was performed using headspace extraction (HS) with the solid phase microextraction (SPME) technique and two-dimensional gas chromatography (GC × GC) coupled with time-of-flight mass (ToF) spectrometry (HS-SPME-GC × GC-ToF/MS). The system used was a Pegasus BT 4D GC × GC-ToF MS (LECO, St Joseph, MI, USA).

The wine samples (4 mL) were placed in 10 mL vials, and each vial was spiked with 0.5 g of sodium chloride and 5 μL of a 2-methyl-3-pentanol solution as the internal standard (internal standard, IS, 103 mg L^{-1}), previously diluted 1:100 (v/v), to obtain a semi-quantitative evaluation. Wine samples were analyzed in a randomized sampling order, and with two experimental replicates to estimate standard deviations and allow comparisons between the samples. The wines were analyzed immediately after opening the bottles to avoid any modification to the volatile profiles due to the contact with the atmosphere. Samples were kept refrigerated at 5 °C in the autosampler before analysis. For SPME, each sample was heated for 15 min at 40 °C with stirring at 300 rpm (20.14 g). The pre-conditioned SPME fiber was then placed inside the vial in contact with the headspace (HS) of the sample for 30 min. After retraction, the samples were injected into the gas chromatograph injector placed at 250 °C in splitless mode; the injection time was 6 min. The two-dimensional separations were performed on a polar/non-polar gas chromatography column system consisting of a MEGA-WAX column (polyethylene glycol phase, 40 m length, 0.18 mm thickness, 0.30 μm internal film width, purchased from MEGA Srl (Legnano, Milano, Italy) in the first dimension and a MEGA-1 MS (1.2 m × 0.10 mm x 0.10 μm, MEGA Srl) as the second dimension. The helium flow rate was 1 mL min^{-1}. The separation was carried at a constant flow. The following gradient temperature program was used: initial isotherm for 6 min at 40 °C; then a ramp at 3 °C min^{-1} to 180 °C, followed by a purging ramp at 10 °C min^{-1}, up to 240 °C. The GC × GC interface was a flow modulator (Flux from Leco), with a modulation period of 2.5 s and an injection time of 80 ms. The mass spectrometer was a time-of-flight (ToF) with an acquisition rate of 150 spectra per second, a detector working frequency of 32 kHz, and an acquisition mass range from m/z 35 to 530.

2.8. Statistical analysis

Principal component analysis (PCA) was conducted with GNU R 4.3.1 [43] using the 'PCA' function of the 'FactoMineR' [44] and 'factoextra' [45] packages under Microsoft Windows 10. PCA is a commonly used unsupervised multivariate statistical method that allows datasets with larger numbers of variables to be easily interpreted.

MFA was conducted with GNU R 4.3.1 using the 'MFA' function of the 'FactoMineR' and 'factoextra' packages under Microsoft Windows 10. Soil data, GC × GC-MS, Targeted LC-MS, and sensory analysis were all included in the MFA. MFA is a commonly used unsupervised multivariate statistical method that is similar to PCA but allows for the use of multiple disparate data sources. The squared cosine of a component shows its importance for a given observation [46]. Variables for the final overall MFA analysis were selected based on an initial exploratory MFA and variables with a $\cos^2$ of 0.7 or higher were selected for use. In addition, some graphs were filtered using $\cos^2$ to keep the number of variables to a visually useful and useable number. The initial exploratory MFA was also used to compare GC × GC data with sensory analysis data.

Analysis of variance (ANOVA) was conducted using GNU R and XLSTAT (Lumivero, Denver, CO, USA). Pearson's correlation coefficients (and associated p values) were determined using the 'rcorr' function of the 'Hmisc' package [47] under GNU R.

3. Results and discussion

3.1. Vineyard soils and geology

The soil characteristics of the seven vineyards were analyzed by principal component analysis (PCA) to identify similarities and differences in the soil profiles. The score plot based on the first two principal components (Fig. 2) showed that Vineyards 1, 3, and 7 formed one cluster (Group A), whereas Vineyards 4, 5, and 6 formed another cluster (Group B). Vineyard 2, initially clustered with Group B, was excluded from further analysis due to early harvesting, which likely influenced the chemical and sensory properties of this wine.

The groups defined by PCA along with relevant soil mineralogy and agronomy data are detailed in Supplementary Table 3. These groupings were validated using ANOVA. Group A resulted distinct from Groups B and C ($p \leq 0.05$ for dolomite, quartz, mica, and kaolinite). PCA groupings were primarily defined by PC1, accounting for 34.6 % of the variability. Group A showed a negative correlation with PC1 and quartz, kaolinite, mica, potassium feldspar, hematite, calcite, and mixed-layer clays. Group B correlated positively with PC1 and cation exchange capacity (CEC), plagioclase, chlorite, and dolomite. Both Group A and C exhibited a negative correlation with hematite and calcite.

The vineyards considered in this study exhibited significant heterogeneity in geology and soil characteristics. Although some vineyards shared similar soil types or geological domains, only vineyards 5 and 6 were identical in terms of both aspects. Despite this heterogeneity, PCA and ANOVA identified two distinct clusters. Soil mineral data, soil type, and soil composition were the most important variables responsible for distinguishing the two groups, underscoring the value of combining these data sources for classification.

The extent to which soil and geology differences influence the chemical and sensory properties of wine remains debated [48]. However, relationships exist between terroir-induced abiotic stress and subsequent plant ecophysiological responses. Van Leeuwen and Seguin suggested that geology may influence the typicity but not the quality of wine [10,49]. Croser concluded that these differences may arise in part from variations in plant vigor between soils, cation exchanges between vine roots, and the way different rocks reflect, absorb, and re-radiate heat and light [50]. Van Leeuwen noted that a range of soils worldwide are responsible for producing great wines, with pebble content ranging from 0 % to over 50 %, and clay content ranging from a few percent to 60 % [10]. Such differences are illustrated in this study at a small spatial scale. As van Leeuwen said, 'No other agricultural product has as strong a relationship with the soil as does wine' [10]. The authors suggest that any links between soil and wine sensory characteristics are likely to be very specific to a particular region and cultivar.

The PCA results suggested that Group A was characterized by soils low in dolomite and high in most clay minerals, with low levels of organic matter (OM) and cation exchange capacity (CEC). In contrast, Group B soils were high in dolomite and low in most clay minerals, with high levels of OM and CEC. Group C also had high dolomite levels and low clay mineral levels but lower OM and CEC levels than Group A. Overall, Group A was defined by clay soils, Group B by dolomitic soils, and Group C shared the characteristics of both soils but differed in OM and CEC levels.

3.2. Sensory analysis

3.2.1. PCA of sensory analysis

The sensory analysis of the wines confirmed the classification provided by the soil PCA, with Groups A and B showing separation, although some overlap was observed (Fig. 3 a). Sensory analysis variables were selected based on boxplot graphs (not shown) to exclude those with little variability or significant outliers. This finding is noteworthy, considering the proximity of the vineyards, where distinct sensory differences may not typically be expected. As noted in section

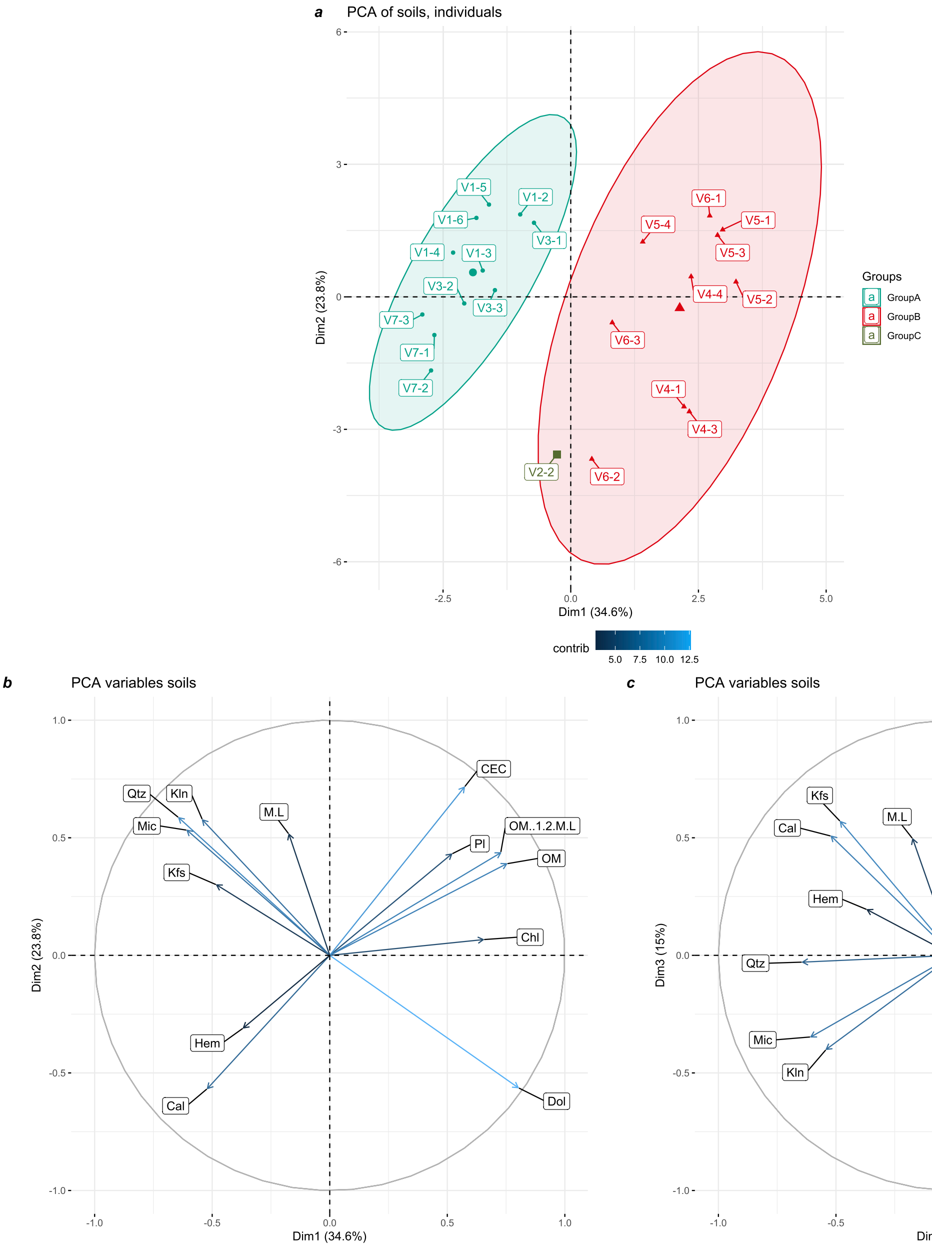

Fig. 2. PCA of vineyard soil data, a. Individuals (soil samples) were grouped based on a multivariate normal distribution with a 95 % confidence level, b. Variables for dimensions 1 & 2, c. Variables for dimensions 1 & 3; Cal: calcite, Qtz: quartz, Kfs: potassium feldspar, Pl: plagioclase, Hem: hematite, Mic: mica, Kln: kaolinite, Chl: chlorite, *M*–L: mixed-layer clay, OM: organic matter, OM.12. ML: Organic matter + ½ mixed layer clay (as per Ferretti and Cruciani [8]), CEC: cation exchange capacity; samples are labeled in the format V-[vineyard number]-[soil sample replicate number]. Note that, due to within-vineyard soil variability, different vineyards have different numbers of replicate measurements.

3.1, Group C (vineyard 2) was excluded from the analysis due to early harvesting, which influenced the chemical and sensory properties of this wine.

In the PCA plot, PC1 explained 29.6 % of the total variance, PC2 explained 20.5 %, and PC3 explained 13.9 %. The primary contributors to PC1 were grass, leather, green apple, sulfur, and rose. For PC2, the main contributors were spicy, moldy, peach, floral, and dried apricot. Sensory analysis indicated that vineyard 3 was the most distinctive, characterized by leather, tropical, sulfur, green apple, and grass notes. Vineyards 4, 5, and 6 were somewhat defined by pineapple and cloves (Fig. 3 b & c).

3.2.2. *Correlations between sensory and wine volatile aroma compounds*

‘Gewürztraminer’ wines are dominated by aromatic compounds, particularly terpenes. Typical examples include linalool, rose oxide, α-terpineol, 1,8-cineole, nerol, and geraniol, with β-damascenone and *p*-cymene also present, albeit often at lower levels [51,52]. These compounds, which are highly volatile, are biogenetically derived from the metabolism of terpenes, fatty acids, and phenylpropanoids [52]. Intriguingly, many of the compounds contributing to the distinct aroma profile of ‘Gewürztraminer’ wines are also identified in lychees (*Litchi chinensis* Sonn.), which are native to the Guangdong and Hainan provinces in southeast China [53]. The presence of similar aromatic compounds in both the wine and the fruit not only suggests a shared sensory experience but also highlights the role of these compounds in shaping flavor and aroma perceptions across different botanical and geographical origins.

Typical ‘Gewürztraminer’ compounds such as linalool and α-terpineol [51] contribute to the characteristic aromas of lavender and citrus. However, at high concentrations, these compounds can mask the

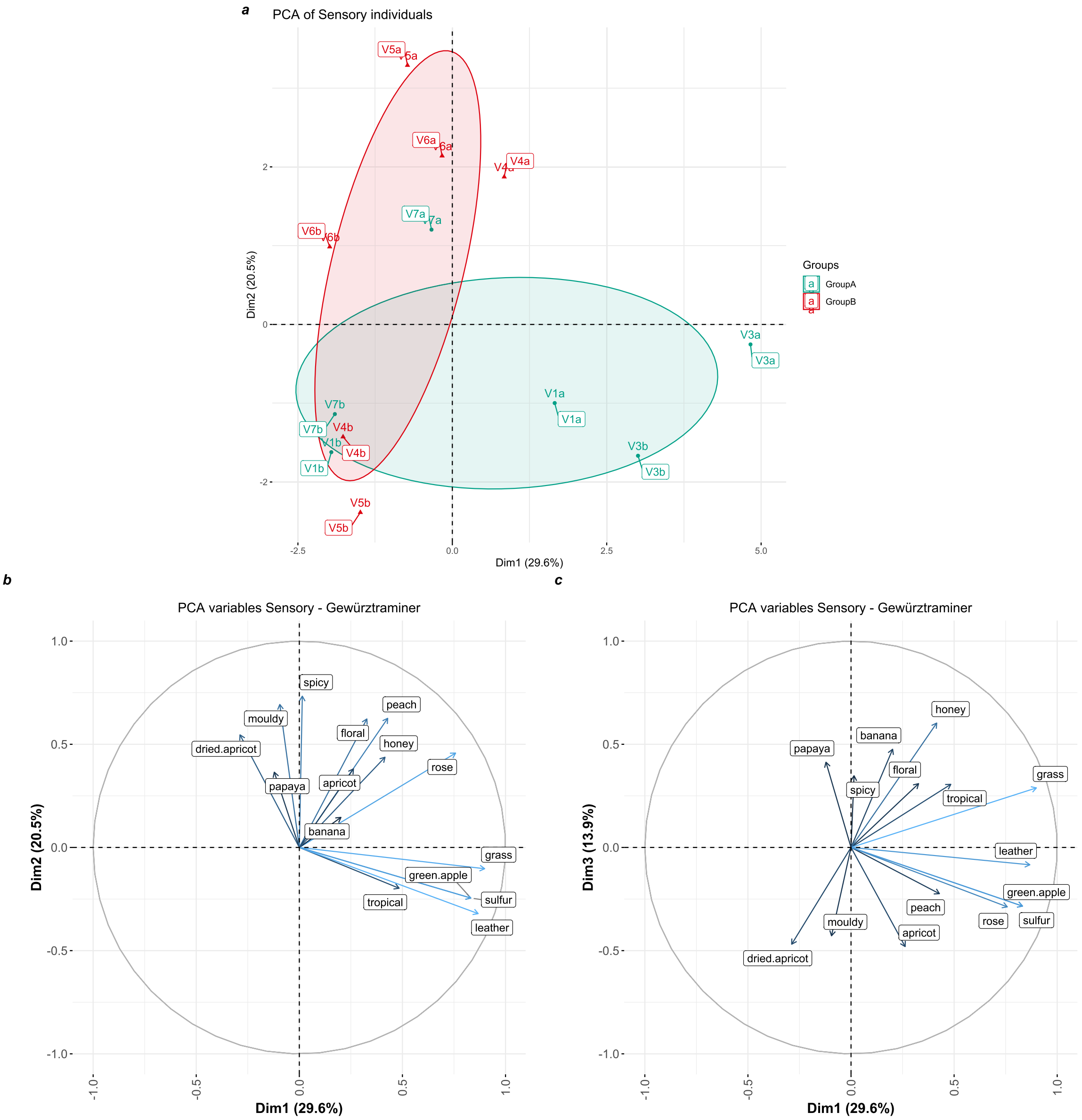

Fig. 3. PCA of sensory data; a. Individuals (wine replicates), b. Variables for dimensions 1 & 2, c. Variables for dimensions 1 & 3; samples are labeled in the format V-[vineyard number]-[replicate], ellipses represent 99 % confidence intervals.

subtle contribution of rose oxide, which is essential for the delicate floral notes of the wine [51]. Furthermore, citronellol and β-damascenone are known to enhance the rose aroma, whereas phenethyl acetate adds a honey note. Notably, nerol oxide, which is structurally similar to *cis*-rose oxide, has also been detected, aligning our findings with previous studies [52].

Vinyl-4-guaiacol and vinyl-4-phenol are important precursors of key aroma compounds in ‘Gewürztraminer’, with their content varying among musts from different vineyards [23]. Fermentation-derived compounds, which are influenced by the initial must composition and terroir, are also of significant interest [23].

Correlations between the sensory characteristics and the GC × GC-MS dataset were examined using Pearson’s correlation coefficients. These correlations indicate associations between the presence of particular volatile compounds and sensory properties, though they do not imply causation. Sensory attributes such as tangerine (Pearsons 0.674, $p = 0.016$) and caramel (Pearsons 0.674, $p = 0.016$) were found to correlate with Group A.2, along with GC × GC compounds ethyl-9-decenoate (Pearsons 0.844, $p = 5.5 \times 10^{-4}$), and ethyl-hexadecanoate (Pearsons 0.687, $p = 0.014$). Attributes like leather (Pearsons 0.816, $p = 0.0012$) and green apple (Pearsons 0.632, $p = 0.027$) correlated with Group A.1, along with ethyl benzeneacetate (Pearsons 0.579, $p = 0.048$), and 2-phenethyl acetate (Pearsons 0.661, $p = 0.019$). Compounds such as linalool (Pearsons 0.719, $p = 0.0084$), β-damascenone (Pearsons 0.676, $p = 0.016$), *p*-tert butylphenol (Pearsons 0.728, $p = 0.0073$), 2-methoxy-4-vinylphenol (Pearsons 0.825, $p = 9.5 \times 10^{-4}$), and citronellol (Pearsons 0.653, $p = 0.021$) correlated with Group B, although no sensory characteristics were correlated with Group B.

The compounds detected along with the calculated retention index, library retention index, and base massic presented in Supplementary Table 6. Supplementary Table 8 details the sensory attributes of selected GC × GC-MS compounds, illustrating how volatile compounds influence the sensory profile of the wines. Key compounds such as β-damascenone, citronellol, linalool, geraniol, benzaldehyde, benzyl alcohol, and 2-methoxy-4-vinylphenol are critical due to their influence on many wine aromas. Only compounds that best defined the groups (based on their cos2 scores) were selected for classification (section 3.4.3) because compounds common across all groups were less useful for distinguishing between them.

These correlations suggest underlying mechanisms linking soil and vineyard characteristics with chemical and sensory properties. Such effects may be site-specific, necessitating further work to determine the precise mechanisms and their impact on wine quality.

3.3. *Antioxidant capacity and chemical profile*

Coulometric analysis was used to quantify the charge transferred during the electrochemical oxidation of wine samples, which was used to express their antioxidant capacity. This capacity is expressed as the total charge measured within a specific potential window (from +50 to +650 mV vs Ag/AgCl). The anodic charge measured by the 16 porous electrodes placed in series with an applied potential from +50 to +650 mV can be used to express the antioxidant capacity because these electrodes facilitate the oxidation of various antioxidant compounds present in the wine. As these compounds oxidize, they transfer electrons to the electrodes, generating a measurable current. The total charge accumulated during this process reflects the overall antioxidant capacity of the sample, as it quantifies the ability of the wine to donate electrons and counteract oxidative processes.

ANOVA showed that Group B wines had significantly higher antioxidant capacity (total charge of 17.5 ± 0.3 μC) compared to Group A (16.2 ± 0.6 μC) ($p < 0.05$). This higher antioxidant capacity was further analyzed in relation to basic oenological parameters, including total phenolic content and sulfur dioxide levels, key oxidative aromatic compounds [54,55], and polyphenolic profile (Fig. 4).

Multifactorial analysis (MFA) handled the multifaceted data and multiple variables simultaneously. This analysis explained 46.2 % of the total variance by the first dimension, 20.6 % by the second dimension, and 10.5 % by the third dimension. In Dimension 1, antioxidant capacity contributed 29.4 %, pH 10.0 %, total phenolics 5.44 %, and ethyl

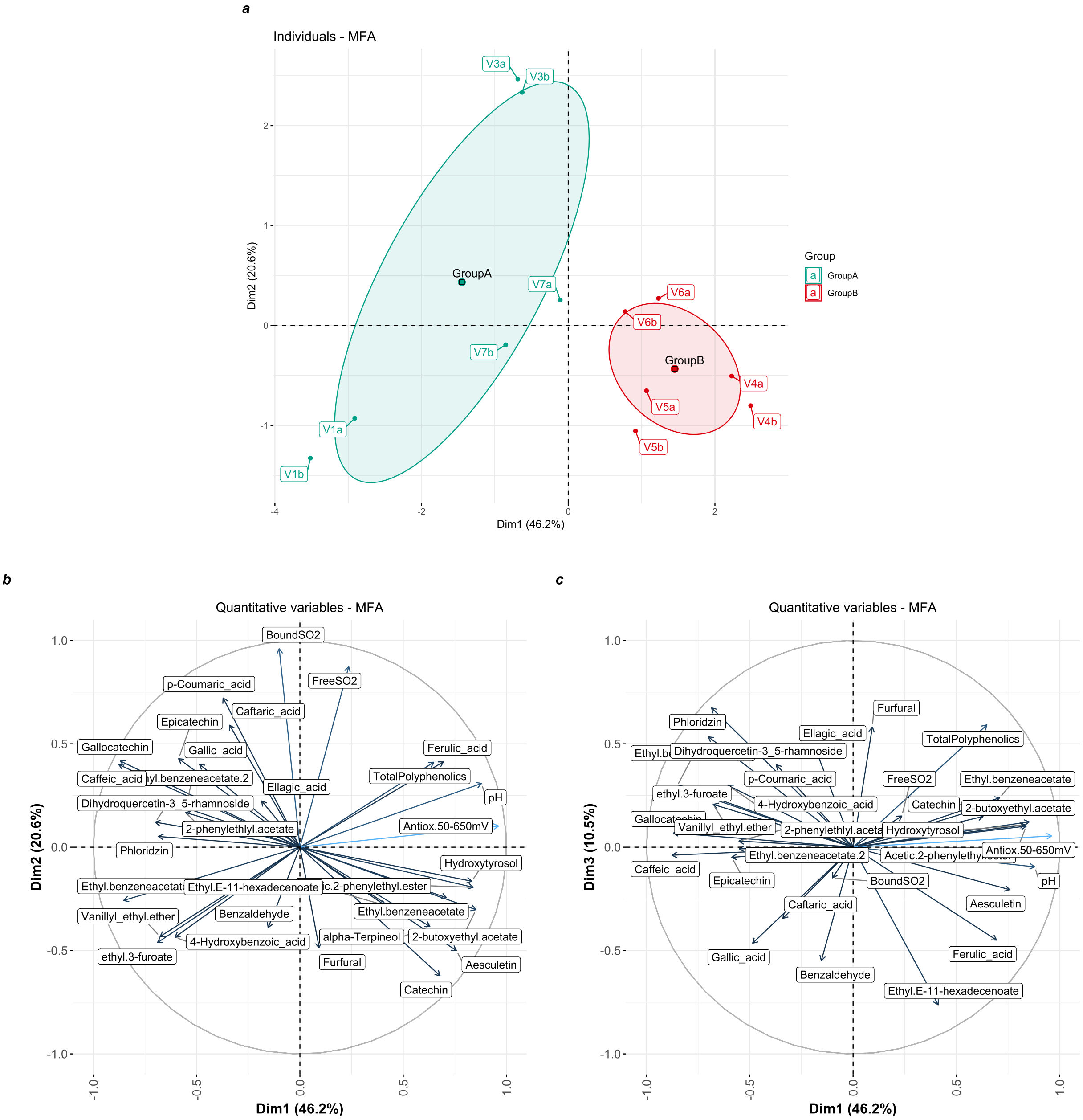

Fig. 4. Correlations between antioxidant capacity and oenological parameters (including key oxidative aromatic compounds and polyphenolic profile); a. Individuals, b. Dimensions 1 & 2, c. Dimensions 1 & 3; samples are labeled in the format V-[vineyard number]-[replicate].

benzeneacetate 4.76 %. In Dimension 2, bound SO_2 contributed 26.8 %, free SO_2 22.2 %, and total phenolics 4.91 % (Supplementary Table 4).

The MFA score plot (Fig. 4 a) showed a similar grouping to that observed in the soil-PCA (section 3.1) and sensory analysis (section 3.2) confirming that these patterns are reflected in wine chemistry. Specifically, antioxidant capacity strongly correlated with hydroxytyrosol (Pearson's correlation 0.827, $p = 0.00091$), pH (Pearson's correlation 0.802, $p = 0.002$), and total polyphenol content (Pearson's correlation 0.701, $p = 0.01$). However, its correlation with free sulfur dioxide was weak and non-significant (Pearson's correlation 0.388, $p = 0.21$) on Dimensions 1 and 2 (Fig. 4 b). These results suggest that antioxidant capacity reflects intrinsic wine properties, with sulfur dioxide levels during winemaking having a limited impact.

The strong correlation between phenolic compounds like hydroxytyrosol and antioxidant capacity highlights the protective effect of these compounds against oxidation. Our findings are consistent with those of Landrault et al. [56] and Paixao et al. [57], who also reported that wine oxidative capacity is influenced by phenolic compounds. This is expected given the well-known antioxidative activity of many phenolic compounds found in wine [56–58].

3.4. Vineyard data exploration and classification using multifactorial analysis of GC × GC-MS, LC-MS, soil, and sensory data

3.4.1. Exploratory analysis

A further exploratory MFA was performed on data from wine analyses (main phenolic compounds by HPLC-PDA-HRMS, antioxidant capacity by LC-CAD, volatile compounds by GC × GC-MS, and sensory analyses), which agreed with the classification from the soil PCA (section 3.1). A unique feature of MFA is that it allows the combination of disparate data sources into a single analysis. In this analysis, Group A was further separated into Group A.1 and Group A.2 based on soil calcite mineral content and altitude. Group A.1 (vineyards 1 and 3) had lower calcite content than Group A.2 (vineyard 7) ($p = 1.70 \times 10^{-5}$, ANOVA) and was also higher in altitude ($p = 4.62 \times 10^{-7}$, ANOVA).

The MFA explained 28.6 % of variance with the first principal component (PC1), 18.6 % with the second (PC2), and 13.5 % by the third (PC3). Contributions from different data sources were as follows: soil type contributed 14.8 % to PC1 and 16.2 % to PC2; soil mineralogy 14.7 % to PC1 and 9.71 % to PC2; soil composition 14.3 % to PC1 and 2.52 % to PC2; antioxidant capacity 13.0 % to PC1 and 1.22×10^{-4} % to PC2; LC-MS 12.9 % to PC1 and 11.1 % to PC2; and GC × GC-MS 12.9 % to PC1 and 4.61 % to PC2. The significant contribution of soil datasets to the MFA underscores their importance.

Compounds identified with LC-MS are listed in Supplementary Table 5, and those identified with GC × GC-MS are in Supplementary Table 6.

This MFA was used to calculate the $\cos^2$ (square cosine) of each variable, reflecting the quality of representation of variables on a factor map, based on squared coordinates [59]. Variables with a $\cos^2$ of 0.7 or higher in Dimensions 1, 2, or 3 were selected for further analysis. Some of these variables are shown in Table 2. No variables met the threshold for inclusion in Dimension 4. Using $\cos^2$ to filter variables allowed for the reduction of the dataset based on how well they represent the overall dataset.

The filtered dataset was used for comprehensive analysis, including all study datasets, which is discussed in section 3.4.3. Additionally, the exploratory analysis explored the connections among the volatile compounds (GC × GC) and the sensory data, discussed in section 3.4.2.

3.4.2. Correlations between vineyard groups, soils, sensory properties, and chemical properties

Correlations between vineyard groups and wine chemistry were analyzed using Pearson's correlation coefficients for soil, sensory, and wine analytical data. Although these correlations do not prove causation, they suggest possible associations between vineyard site and sensory properties for this specific combination of cultivar and vineyards. Significant correlations are presented in Supplementary Table 7.

For instance, there was a notable correlation between the percentage of clay in the soil and apricot flavors (Pearson 0.749, $p = 0.005$). Additionally, the sum of non-clay minerals correlated with pineapple (Pearson 0.642, $p = 0.024$) and spicy (Pearson 0.638, $p = 0.026$) flavors, visible in Dimension 1 and 2 of the MFA (section 3.4.3).

Similar correlations were observed between soil data and wine analytical data. For example, quartz percentage correlated with gallocatechin (Pearsons 0.837, $p = 0.0007$) and caffeic acid (Pearsons 0.908, $p = 0.002$) and anticorrelated with 2-methoxy-4-vinylphenol (Pearsons −0.808, $p = 0.001$), linalool (Pearsons −0.613, $p = 0.03$), and antioxidant capacity (Pearsons −0.802, $p = 0.002$).

Dolomite percentage correlated with 2-methoxy-4-vinylphenol (Pearsons 0.835, $p = 0.0007$), linalool (Pearsons 0.751, $p = 0.005$), and antioxidant capacity (Pearsons 0.877, $p = 0.0002$), and anticorrelated with gallocatechin (Pearsons −0.935, $p = 8.1 \times 10^{-6}$) and caffeic acid (Pearsons −0.973, $p = 1.0 \times 10^{-7}$).

Calcite showed no particular trend for these compounds, but was correlated with ethyl-9-decenoate (Pearsons 0.641, $p = 0.02$), citronellol pentosyl hexoside (Pearsons 0.67, $p = 0.05$), and *p*-coumaric acid (Pearsons 0.744, $p = 0.006$). It was also anti-correlated with monoterpenol pentosyl-hexoside (Pearsons −0.714, $p = 0.009$) and 7-hydroxygeraniol/7-hydroxynerol pentosyl-hexoside (Pearsons −0.67, $p = 0.05$). Calcite, found in lower altitude vineyards, anticorrelated with altitude (Pearsons −0.965, $p = 2.6 \times 10^{-5}$).

Altitude was also correlated with wine analytical data (GC × GC-MS and LCMS) and with aroma precursors such as monoterpenols pentosyl hexoside (Pearsons 0.83, $p = 0.01$) and 7-hydroxygeraniol/7-hydroxynerol pentosyl-hexoside (Pearsons 0.75, $p = 0.02$). This suggests higher production of aroma precursors at higher altitudes, independent of calcite levels. However, altitude strongly anticorrelated with catechin (Pearsons −0.98, $p = 5.3 \times 10^{-6}$), *p*-coumaric acid (Pearsons −0.88, $p = 0.002$), and ethyl hexadecanoate (Pearsons −0.71, $p = 0.03$). Previous studies have also noted the impact of altitude on the chemical properties of wine, as reviewed by Mansour et al. [60]. Higher levels of phenolic compounds at higher altitudes are often attributed to UV protection [60, 61].

Correlations between vineyard groups and wine chemical properties were also examined. Group A.1 showed a negative correlation with several key aromatic compounds, whereas Group B showed a clear positive correlation. For example, linalool had Pearson's coefficient for Group A.1 of −0.743 ($p = 0.006$), for Group A.2 of −0.101 ($p = 0.75$), and for Group B 0.776 ($p = 0.003$), with Groups A.1 and A.2 overlapping. For citronellol, Group A.2 was closer to Group B (Group A.1 Pearson −0.807 $p = 0.001$, Group B.1 Pearson 0.145 $p = 0.65$, Group B

Table 2
Top 5 cos2 values for dimensions 1–4 from the exploratory MFA.

Dim1	Dim1 score	Dim2	Dim2 score	Dim3	Dim3 score	Dim4	Dim4 score
caffeic acid	0.949	monoterpenols pentosyl hexoside	0.834	syringic acid	0.817	green apple	0.651
gravel percent	0.939	asl (height above sea level, in meters)	0.771	homovanillic acid 2	0.665	sulfur	0.651
dolomite percent	0.913	calcite percent	0.709	phloretin	0.559	catechin	0.629
sinapinaldehyde	0.883	monoterpenols pentosyl hexoside 2	0.646	benzenesulfonyl	0.512	acetovanillone	0.591
gallocatechin	0.861	coutaric acid	0.620	ethyl succinate	0.498	beta damascenone	0.579

Pearson 0.653 $p = 0.02$). Conversely, for phenolic compounds such as epicatechin and gallocatechin, the trend is reversed. Gallocatechin had Pearson's coefficient of 0.757 ($p = 0.004$) for Group A.1, 0.272 ($p = 0.27$) for Group A.2, and 0.917 ($p = 2.7 \times 10^{-5}$) for Group B. Epicatechin had Pearson's coefficients of 0.706 ($p = 0.01$) for Group A.1, 0.272 ($p = 0.39$) for Group A.2, and 0.871 ($p = 0.0002$) for Group B.

These trends align with observations from the Cantina Tramin winemaker, who noted that wines from Group B are more aromatic and ready to drink when young, while those from Group A develop aromatic character during ageing due to acid hydrolysis. Such findings are suggestive, but further work is needed to confirm these observations conclusively.

3.4.3. Vineyard classification based on an overall analysis of the filtered dataset

An overall MFA was conducted using the variables selected in the exploratory MFA. This analysis explained 28.6 % of the variance by the first dimension, 18.6 % by the second, and 13.5 % by the third. The contributions of the different data sources were: soil mineralogy (13.4 % to the first dimension and 16.8 % to the second), soil composition (13.2 % to the first dimension and 0.130 % to the second), soil type (13.1 % to the first dimension and 37.4 % to the second), GC × GC-MS (12.5 % to the first dimension and 19.4 % to the second), LC-MS (12.5 % to the first dimension and 17.8 % to the second), sensory data (12.0 % to the first dimension and 0.572 % to the second), and antioxidant capacity (11.6 % to the first dimension and 0.667 % to the second). Soil gravel percentage had the highest individual contribution to the first dimension, at 13.2 %.

The MFA (Fig. 5 a) separates Group A (vineyards 1, 3, and 7, clay soils) and Group B (vineyards 4, 5, and 6, dolomitic soils) based on Dimension 1. Group A is further divided into Group A.1 (lower calcite levels) and Group A.2 (higher calcite levels).

Fig. 5 b and c show the quantitative variables contributing to the classification. Group A is defined by negative contributions from mica, kaolinite, clay percent, caffeic acid, and gallocatechin to Dimension 1,

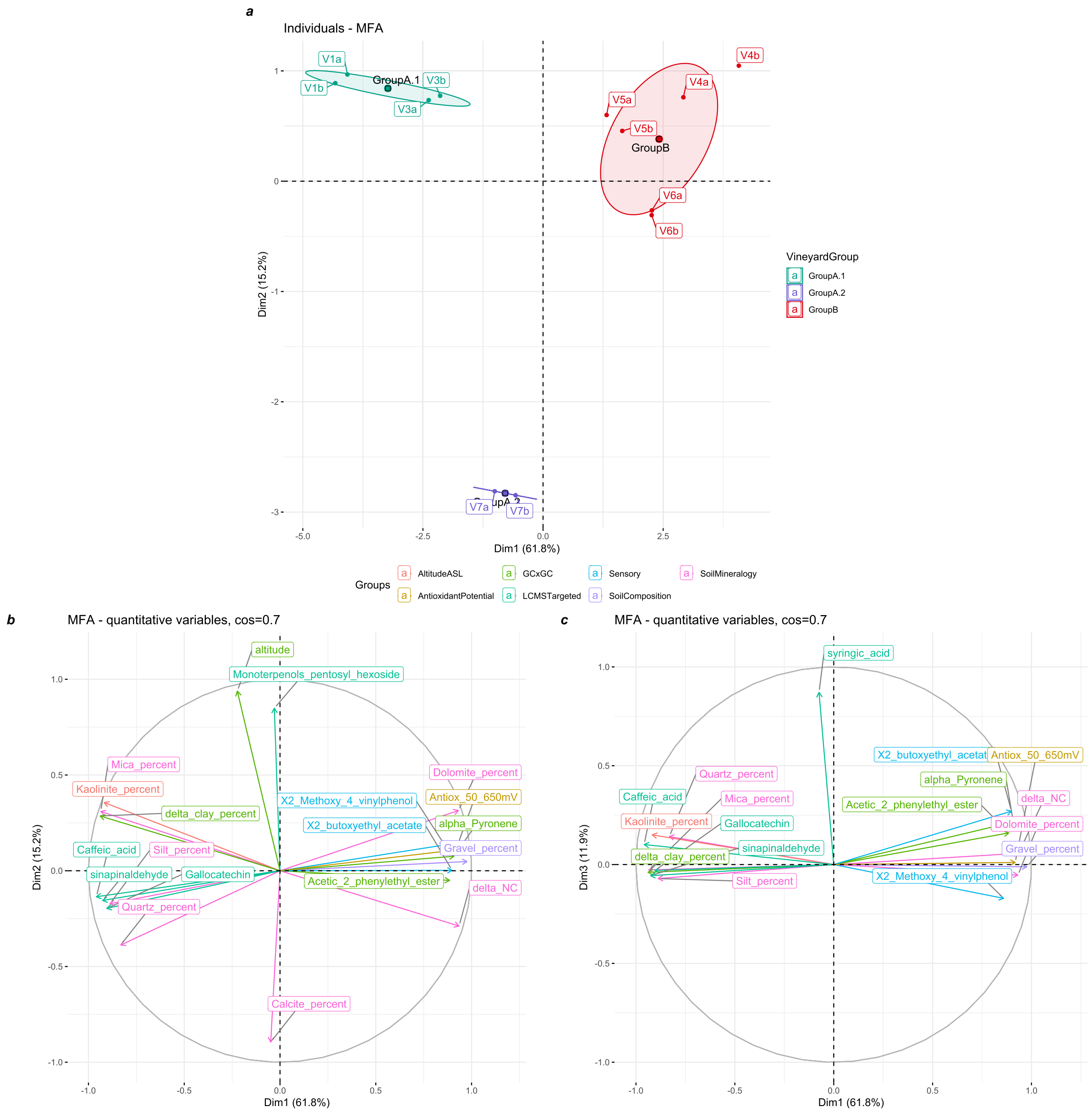

Fig. 5. MFA of filtered data; a. MFA of selected data, colored by group, b. Contribution of quantitative variables to the MFA, dim.1 & dim.2, c. Contribution of quantitative variables to the MFA, dim.1 & dim.3. Delta_NC: sum of non-clay minerals, altitude: altitude above sea level (m); samples are labeled in the format V-[vineyard number]-[replicate], ellipses represent 99 % confidence intervals.

whereas Group B is defined by negative contributions from non-clay minerals, dolomite, 4-vinylguiacol, linalool, and 2-methoxy-4-vinylphenol to Dimension 1. The MFA partial axes can be seen in Supplementary Fig. 2.

The alignment between the soil PCA (section 3.1) and the overall MFA highlights the significant role that soil plays in determining the chemical and sensory properties of wine. Despite their proximity, the two vineyard groups are distinctly separated by Dimension 1. The subgroups within Group A are also distinct.

Group A is characterized by clay soils. Mixed layer clays possess intricate biostimulant catalytic functions due to their nano-structures and the geo-chemical and geo-mineral phenomena occurring in soils. These clays can enhance soil fertility and positively influence vine health and productivity. Subgroup A.1 is low in soil calcite and influenced by kaolinite and mica, key phyllosilicate minerals. Subgroup A.2 is primarily defined by high calcite content. Group A.1 soil, on a siliciclastic geological domain, differ from Group A.2 soils, which are on a terrigenous geological domain. Additionally, Group A.1 is at a higher altitude than Group A.2.

Clay soils without calcite, as in Group A.1, have high water retention capacity, fertility, and cation exchange capacity (CEC), with well-regulated water and nutrient uptake, but may suffer from poor aeration and drainage. It should be considered that from a mineralogical point of view, clays are formed from several minerals of phyllosilicate families, each of which relates in its way to soil fertility [62]. Some of the best clay soils, such as Pomerol (Bordeaux) in France, are noted for their swelling clay smectite content. In Bordeaux, many notable wines are produced on this soil type including Château Pétrus, Château Cheval Blanc, Château Latour, Château Léoville Las Cases, Château Margaux, and Château d'Yquem [63]. Such clay soils are most beneficial when located in higher positions, as in the cases of the examples cited previously [64].

Calcareous clay soils found in regions such as Barolo (Piedmont, Italy), Chianti (Tuscany, Italy), Saint-Émilion (Bordeaux, France), Burgundy (France), and Jerez-Xérèz-Sherry (Spain), among others [49, 65–69], have high calcium content, providing good structure and drainage but can lead to lime-induced iron chlorosis in susceptible rootstocks.

Soils formed on calcareous rocks such as limestone and chalk tend to be shallow and well-structured due to their high Ca content. They are also generally free-draining and alkaline in pH [65], typically between pH 8.0 and 8.5 [64]. More negatively, in other regions lime-induced Fe chlorosis can be a problem on soils that are particularly high in calcite (e.g., chalk or limestone soils), and American rootstocks (except those derived from *Vitis berlandieri* Planch.) are particularly susceptible [64, 66].

Group B, in contrast, was characterized by dolomite, glacial gravel, non-clay minerals, and low clay content. Dolomite-rich soils, common in South Tyrol and regions like Castelli di Jesi in Italy [69,70], have moderate water deficits and high organic material [69]. As an example, Verdicchio dei Castelli di Jesi DOC, which is defined by dolomite, has been shown to be distinct from Verdicchio di Matelica DOC, which is defined by calcareous clay [69].

Dolomite rock (sometimes called dolostone) is defined as a sedimentary rock that is composed mainly of the mineral dolomite. Dolomite is a mineral similar to calcite, but more than half of the sites in the carbonate lattice are filled with magnesium rather than calcium. Therefore, dolomite is a magnesium-rich limestone [70]. Dolomite is chemically more stable than calcite. It supports soil structure and stability, aeration, and a higher pH range. The significance of dolomite soils in the region has been noted previously because dolomite rock is common in the Dolomites, the region in which it was first identified [4,30]. In addition, gravel soils, which are often favored for viticulture due to their excellent drainage properties, can be found in regions such as Grave de Friuli (Friuli) in Italy, the left bank of Bordeaux (including Graves and the Médoc district) and Châteauneuf-du-Pape (Rhône) in France, Gimblett Gravels (Hawke's Bay) and Marlborough in New Zealand, and Ningxia in China. Many of the best sites in the Médoc have gravel soils, which contribute to optimal vine health and grape quality by ensuring well-drained conditions [71].

4. Conclusions

This study used a data-driven approach to identify terroir factors and describe the interactions between the multivariate concept of terroir and wine chemical and sensory properties at the intra-vineyard scale. The seven South Tyrol 'Gewürztraminer' vineyards studied are distinctive in terms of their chemical and sensory characteristics. A PCA of soil data proposed a classification in macro-groups, which was confirmed via analyses of wine data, suggesting that small changes in terroir between the vineyards in Tramin are observable in terms of chemical and sensory properties.

Two macro-groups were identified based on soil composition: one with more dolomitic minerals and another with more clay-silicate minerals. Vineyards 1, 3, and 7 formed one cluster (Group A), and vineyards 4, 5, and 6 formed another cluster (Group B). These groups exhibit distinct physical and mineral features associated with wine groupings. A soil classification based on soil properties (quartz and silicate, phyllosilicates, dolomite, and calcite) correlates with vineyard groups and wine styles. Specific soil features were correlated with wine chemical and sensory properties, particularly phyllosilicates (i.e.clays) in soil.

Soil PCA groupings were confirmed using unsupervised analyses of wine data, which revealed that differences in terroir had measurable impacts on wine properties. An unsupervised analysis also suggested that Group A could be subdivided based on soil calcite levels, with Group A.1 being low in calcite and Group A.2 being high in calcite, likely due to physicochemical differences in clay soils [64,66,69].

These groupings have oenological significance: Group A wines are less aromatic when young but age better, whereas Group B wines are more aromatic when young but less age-worthy. Group A had lower aroma compounds, like linalool, and higher phenolic compounds, like gallocatechin, compared to Group B. Finding definitive links between vineyard groups, soil types, and wine sensory properties remains elusive [48], indicating that more research is needed.

The results confirmed that 'Gewürztraminer' reflects the terroir in which it is grown, which is influenced by various vineyard biophysical factors. Sensory analysis somewhat separated the vineyards, and chemical analysis confirmed our hypothesis that small changes in terroir result in observable differences in wine properties.

Future work could explore other analytical methods, such as nuclear magnetic resonance (NMR) spectroscopy [15,72,73], which is useful for metabolomic analysis and detecting unauthorized production methods [73]. In addition, machine learning techniques can provide further insights into the wine metabolome and its links to terroir [74,75].

In-depth multidisciplinary research, extended to wines from various vintages and additional vineyards, can help better distinguish the origin of stylistic differences attributable to specific terroir sub-factors, enhancing our understanding of the influence of terroir on wine quality.

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CRediT authorship contribution statement

Gavin Duley: Writing – review & editing, Writing – original draft, Visualization, Formal analysis, Data curation. **Carlo G. Ferretti:** Resources, Methodology, Investigation, Funding acquisition, Conceptualization. **Ksenia Morozova:** Writing – review & editing, Visualization, Project administration, Methodology, Investigation, Formal analysis, Data curation. **Edoardo Longo:** Writing – review & editing, Supervision, Methodology, Investigation, Data curation. **Sebastian Imperiale:** Methodology, Investigation, Data curation. **Yubin Ding:** Methodology, Investigation, Data curation. **Simone Poggesi:** Methodology, Investigation, Data curation. **Matteo Scampicchio:** Writing – review & editing, Supervision, Conceptualization. **Emanuele Boselli:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jafr.2024.101298.

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