Scientific Research
MINERALITY IN WINES

Chemical Basis of Minerality perception in Wines
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Private Research
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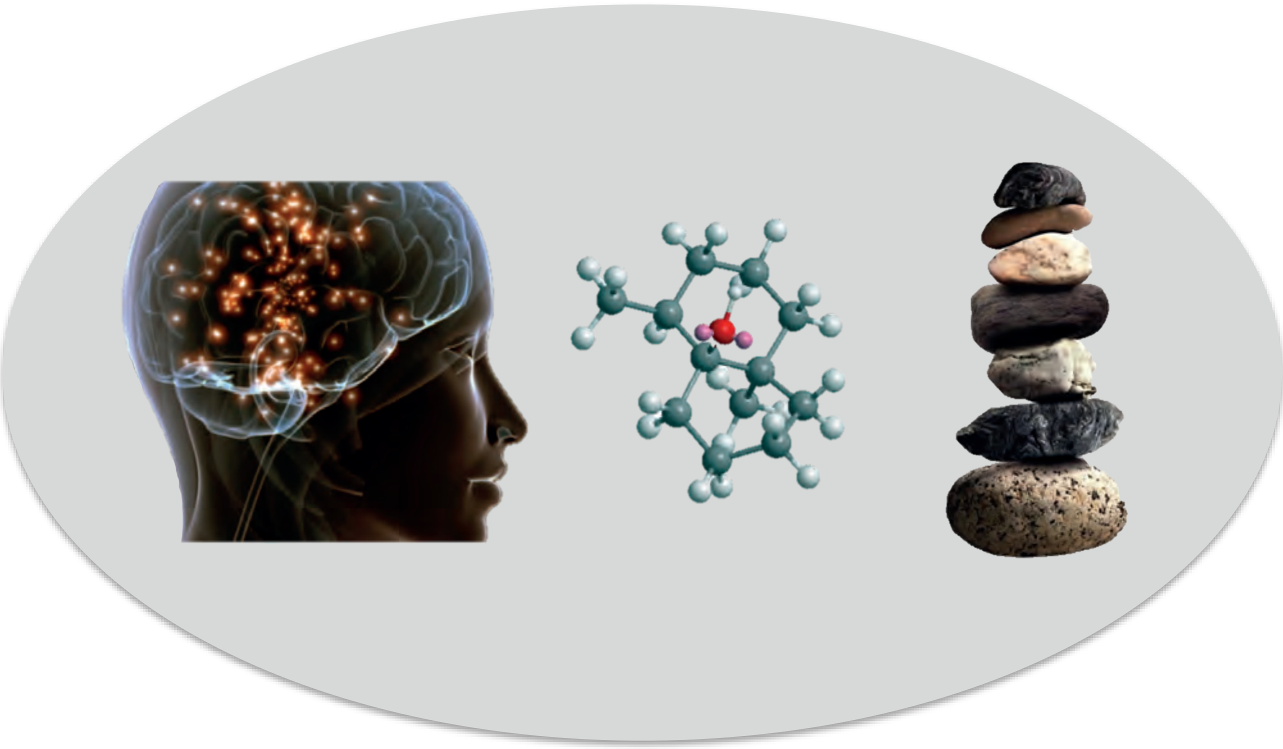
Very special thanks to
Elvira Zaldivar & M.P. Fernández



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MINERALITY PERCEPTION IN WINES

Why the research

"Curiosity leads the human being to ask many questions, sometimes to investigate in depth, spending a long time to reflect upon the results obtained with the aim of trying to find explanations. The importance of science is invaluable for development and progress."

This study on the relationship between the chemical composition of wine and the perception of minerality arises from a passionate decision of two enthusiasts of the world of wine, who share concerns, curiosities and the need to try to find answers to questions unsolved for a long time.

Antonio Palacios García, Director of Laboratorios Excell-Ibérica in Logroño (La Rioja, Spain) and David Molina, Director of Outlook Wine (WSET App in Spain) decided in early 2012 to start a privately funded research study, promoted and financed exclusively by themselves in order to preserve maximum objectivity and necessary rigour. The total cost of the study amounted to €50,000. The bulk of the investment covered the high costs of comprehensive chemical tests, as well as the modification of synthetic wine with compounds that were isolated and identified as potentially responsible for the perception of minerality in wine.

This study could not have been accomplished without the invaluable collaboration of Elvira Zaldívar, head of the Department of Quality Control of Laboratorios Excell-Ibérica, and Purificación Fernández of the University of La Rioja.

After two long years of dedication, Antonio Palacios and David Molina offer generously this valuable information to the wine industry, hoping that professionals, students, and wine lovers, may enjoy it and draw their own conclusions, always with the clear objective of contributing and helping progress.

We are aware that this study has limitations and does not cover the totality of the full spectrum of perception of minerality of wine. We hope that it will serve as a stimulus to push other enthusiasts with new research in the same field.

Finally, our thanks again to all contributors and speakers who participated in the Symposium held in Barcelona (Dr. Josep de Haro, Sarah Jane Evans MW, Dr. Fernando de Toda, and Sam Harrop MW) who contributed to the success of the conference on "Minerality in Wine" celebrated in June 2014. Thank you all!

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Chemical basis of mineral character at olfactory and gustatory level in white and red wines

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1. Summary

The concept that transmits the term mineral in wines is certainly one of the more mysterious attributes from the chemical point of view. Minerality in wines is often associated with the ¨*terroir*" concept, often with clear commercial purposes where the expression is linked to the soil allowing to justify or argue the authenticity of origin of the wine. It would therefore be easy to link the sensory term mineral to the composition and content of minerals present in a wine, even though there are'nt enough data-based studies as to set this direct association. The object of this study is the chemical and sensory characterization of wines listed from a sensory standpoint as mineral. For the present study 17 wines from various wine-producing areas of the world were analyzed on the basis of their chemical composition of metals, aromatic compounds, both positive and negative, acidity, succinic, sulfur and organic acids, among others. They all had a common bond as to have been classified as mineral wines at international level, both by professionals from the wine sector and by prescribers from the wine journals and commercial sector. In order to avoid controversy the names of producers and wine brands were omitted and the only definition of the wines was by regions and grape varieties. A statistical analysis of the set of data concerning the chemical composition studied was subsequently performed. Finally, 11 chemical compounds were found which stood out and were classified in three categories with a direct relationship to the descriptor minerality.

2. Introduction

During the last decade the term minerality has enjoyed a spectacular boom by critics, winemakers, sommeliers and specialists in the marketing of the wine sector. The fruity, floral, spicy and wood aromas are of great importance in the description of the wines classified as great wines, but certainly the term minerality today occupies the first place among the attributes of high quality wines. In the market the use of the term mineral is usually synonymous with a superior level of quality.

However, even having this high status the term mineral has been defined very vaguely to date. There is currently a huge vacuum in the identification of chemical compounds responsible for or associated with the aromatic and gustatory sense defined as mineral.

Often this term is accompanied by descriptors of salty, burnt match, silex or flint that produces gunflint scents which smell like a lighter so to speak. Based on this description a hypothesis could be established that metallic elements and above all the vineyard soil cations are responsible for this smell and mineral taste.

To have a more complete and consistent vision on the meaning of the term mineral it is essential to define it from the perspective offered by geological science. The International Mineralogy Association (IMA) defines a mineral as an element or chemical compound, usually in crystalline form, which has been formed as a result of a geological process and possesses a specific degree of purity.

More than 4,000 minerals are known, of which 100 are those most commonly found in the composition of the soil and another 50 are to be found occasionally[1]. In relation to wine these minerals are classified according to the physiological need of the plant for macronutrients and micronutrients. In the soil minerals are broken down into simpler and smaller molecules through contact with water, the atmosphere, temperature changes, and the action of microorganisms, among other factors[2]. It is important to stress that only the chemicals that are soluble in water can be absorbed by the roots of the plant.

The appearance of the vineyards' soils may be very different at first sight, however these usually present within a margin a similar chemical composition[3]. Notably, the bioelements necessary for the metabolism of the plant (nutrition, survival and development) must be in ionic state to be introduced inside the vine. Thus the plant, through complex reactions of redox type and the use of specific and selective absorption pumps of ionized elements present in its roots, gets these chemical elements flowing inside and distributed to all cell tissues of the vine, including the grapes. To make this happen it is essential that metals or minerals are water-soluble. However, it is fundamental to highlight that the plant absorbs what it needs and not what is found in each soil type fortuitously.

The distribution and proportion of these elements in grape berries is approximately 40% in the skin, 50% in the pulp and 10% in the seeds. Therefore minerals are components that are present naturally in grapes, consequently in the grape juice and finally in wine. However, the origin and the presence of these elements is not only to be found in the chemical nature of the vineyard soil but also in the treatments received from applications of the winegrower (fertilizers, pesticides, herbicides, fungicides, etc.) and the winemaker during the winemaking process (additions, corrections and other possible treatments).

Of all the common elements present in the soil, the most relevant cations in terms of concentration are potassium[4], followed by calcium and magnesium. These elements are normally involved in neutralization of acids in the grapes, in grape juice and finally in wine. It is the potassium, predominantly, which has greater effect on changes in acidity and pH, both in grape juice and wine.

In many tasting notes the gustatory perception of minerality is frequently related to wines characterised by high acidity. In the mouth, acid taste can be linked not only with pH parameter but also with the total acidity of the wine, in which are taken into account all organic acids present (formed by the vine or fermentation). Previous research has also linked the term minerality with the presence of a particular acid such as succinic[5], responsible for producing a saline sensation on the palate at gustatory level. In fact, succinic acid despite being an acid has a more salty taste than an acid taste. The emergence of this acid is due to the biochemical metabolism of fermentative yeasts throughout Krebs[6] cycle, as well as through the decarboxylation of the α−Ketoglutaric acid by means of chemical oxidative reactions[7].

The object of the present study is the identification of the chemical compounds present in wine that are responsible for the interpretation of minerality. Learning about these compounds associated with mineral taste and/or aroma, both in white wines and red wines, will undoubtedly contribute a greater knowledge about this peculiar sensory perception, associating the term with a chemical base responsible for its perception.

A set of 17 wines were selected for this study, among which were white and red wines of different vintages and wine regions chosen by their reputation as being mineral wines. The whole set of wines were methodically studied by means of gas chromatography-mass spectrometry techniques, ICP/mass chromatography and enzyme techniques, in addition to other analyses of routine type frequently used in the enological sector. Additionally, the chosen wines were subjected to a thorough sensory analysis by two qualified tasting panels, one made up of winemakers and other by professionals non-producers of wine. Both panels did not receive any information about the aim of the tasting, thus avoiding influences, suggestions and preferences to achieve maximum objectivity in the tasting sessions. Finally, the resulting data matrix was analyzed through multifactorial statistical tools like the Principal Components Analysis (PCA).

3. Materials and methods

A total of 17 wines sold and available on the market were selected by having been classified as mineral. The list of wines used in this study is described in Table 1.

The determination of the majority of aromatic compounds was performed following the method proposed by Ortega López, Cacho and Ferreira[8] by gas mass chromatography and FID detector:

- **The analysis of minority compounds** was done using the sample preparation method proposed by López, Aznar, Cacho and Ferreira[9] and detection by gas mass chromatography.
- **The volatile compounds from wood** were analyzed by extraction liquid-liquid and subsequent analysis by gas chromatography-mass spectrometry.
- **Aromatic compounds responsible for organoleptic defects** in wine were quantified by gas mass chromatography through solid phase micro extraction (SPME).
- **For the quantification of chemical compounds with sulfur** content in its chemical structure was used the technique of gas chromatography with flame photometric detector, also known by its acronym GC-FPD.
- **The determination of metals** was developed by inductively coupled plasma mass spectometry (ICP/MS).
- **The routine parameters** such as the determination of alcohol content, pH, total acidity, color intensity, total polyphenol index and free and total sulfur dioxide were analyzed following the guidelines of the official methods of wine analysis published in the Spanish Official Bulletin (BOE) number 1988-11256.
- **Organic acids** were analyzed by enzymatic methods using Y-15 scanner and manually by spectrophotometry (succinic acid).

To interpret the chemical data matrix obtained in an objective manner was used a statistical software type ANOVA and Principal Components Analysis (PCA) by discriminating techniques.

The analysis of the validity of one of the two tasting panels participating in the study, composed by the group of winemakers, was studied using the software "Panel Check" developed by the University of Denmark. The data obtained from the tasting sessions were analyzed altogether by ANOVA, Principal Components Analysis (PCA) by discriminant techniques and linear regression.

Nº	Typology	Variety	Year	Wine region/ style of production
1	White wine	Godello	2011	Valdeorras (Spain)
2	White wine	Sauvignon blanc	2008	Loire Valley (France)
3	White wine	Treixadura	2011	Ribeiro (Spain)
4	White wine	Godello	2011	Ribera Sacra (Spain)
5	White wine	Riesling	2008	Niederösterreich (Austria)
6	White wine	Garnacha gris	2011	Empordà (Spain)
7	White wine	Ribolla	2010	Primorska (Slovenia)
8	White wine	Xarel·lo	2011	Penedès (Spain)
9	White wine	Riesling	2010	Mosel (Germany)
10	White wine	Riesling	2009	Mosel Trocken (Germany)
11	White wine	Riesling	2009	Mosel Kabinett (Germany)
12	Red wine	Tinta del país	2007	Vino submarino (Spain)
13	Red wine	Blaufränkisch	2008	Burgerland (Austria)
14	Red wine	Syrah	2008	Rhône North (France)
15	Red wine	Poulsard	2010	Jura (France)
16	Red wine	Garnacha, Syrah	2011	Montsant (Spain)
17	Red wine	Syrah	2007	Aragón (Spain)

Table 1. Description of the wines used in the study.

4. Results and discussion

4.1 Sensory analysis using trained panels of tasters

To carry out the sensory part of the study two different tasting panels were set, one in Rioja and another in Barcelona, formed by 20 sensory judges each and trained in sensory analysis. The first of them formed by winemakers and the second by wine sector professionals non-producers of wine. The objective was to get a picture of the minerality of wine as viewed by winemakers, professionals and consumers at the same time, and check if both groups perceived clearly the differences and the similarities in the use and interpretation of the term minerality.

The two panels of tasters were given to taste the 17 wines selected by their reputation as mineral wines on the international market. Among the questions asked during the two tasting sessions the term minerality was introduced as an adjective, but it did not appear as an attribute of greater relevance with respect to the rest. It was a complete blind wine tasting to avoid prior subjective interpretations and influences. The objective of this phase was to select among all the wines studied a set of 6 wines, white and red, that had been defined by consensus as the most mineral wines in their sensory perception by both tasting panels. In the same way a second objective was aimed to identify 2 wines, one white and one red, whose definition would clearly be far from the term minerality in its perception, to be used as control samples i.e. as a reference opposed to the perception of minerality.

4.1.1 Aromatic phase of tasting

In white wines both tasting panels agreed to identify the wines numbered in the Table as 2 (Sauvignon blanc, 2008 central Loire) and 11 (Riesling, Mosel Kabinett 2009) as the more mineral. One of the panels also noted sample number 10 (Riesling, Mosel Trocken 2009) with this attribute. Young white wines were the farthest from the descriptor "minerality", while those having spent more time in the bottle seemed to be the more mineral.

There was a clear consensus among both tasting panels for the aromatic phase of the red wines studied. On this occasion the wines numbered 12 (Tinta del País, submarine 2007) and 14 (Syrah, Rhône north 2008) were chosen by both panels to categorize them as mineral. However, sample 15 (Poulsard, Jura 2010) moved away in its description of the attribute minerality on the sensory map obtained by both panels.

4.1.2 Gustatory phase of tasting

In the mouth, both panels identified the white wines numbered 2 (Sauvignon blanc, Loire central 2008) and 10 (Riesling, Mosel Trocken 2009) as mineral, while white wine 11 (Riesling, Mosel Kabinett 2009) was defined as low on this attribute by one of the panels. Away from the term mineral was located white wine 7 (Ribolla, Primorska 2010) which was thus identified as control wine for white wines.

The sensory analysis of red wines by both tasting panels showed in the gustative phase a new concordance in choosing wines numbered 12, 14 and 16 (Tinta del País 2007, Syrah 2008, Grenache and Syrah) as the more mineral. Figure 1 shows the display of attributes within the gustative phase of the panel of experts from the wine sector enologists (expert winemakers). Framed in red is the coordinate axis displaying the minerality attribute (left graph) and wines numbered 12 and 16 which are close to this attribute (right graph). Framed in green, sample 15 (Poulsard, Jura 2010) whose responses by the sensory judges placed it away in the provision of statistical variables of minerality, being only nearest to the attribute acidity. Figure 2 shows the arrangement of attributes within the aftertaste phase of the winemakers panel (expert winemakers).

Table 2 shows a summary of the white and red wines that were found by consensus in both tasting panels as close (in red) or far (in green) to the term minerality, according to the variance studied using Principal Components Analysis.

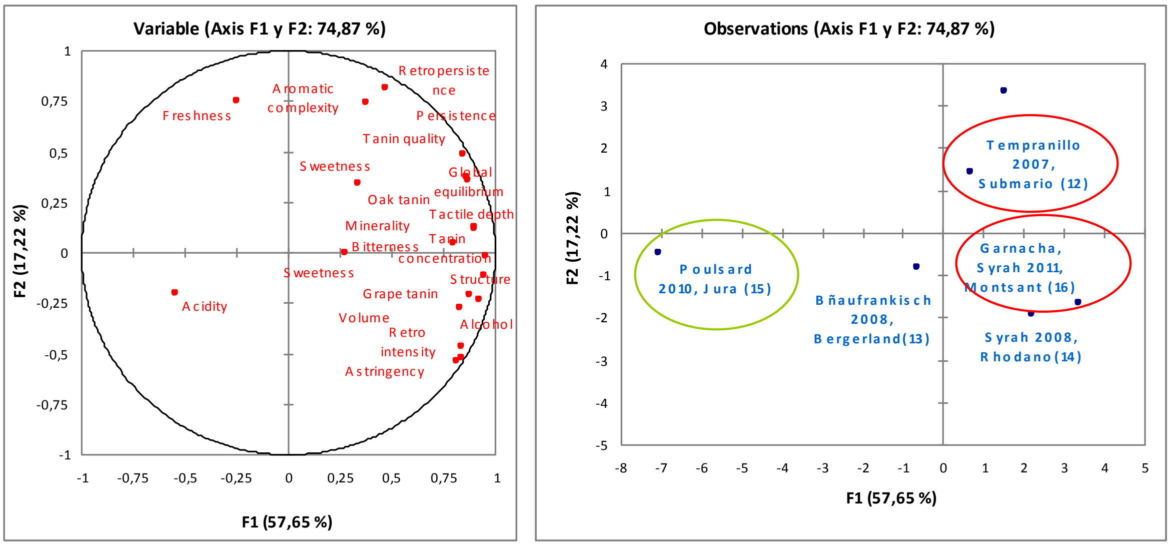


Figure 1- Results of analysis by PCA and coordinates of positions found in the sensory analysis of red wines by the winemakers panel for the gustatory phase. The axis explain 74.87% of the variance. Green indicates wines with less mineral character and red more mineral character.

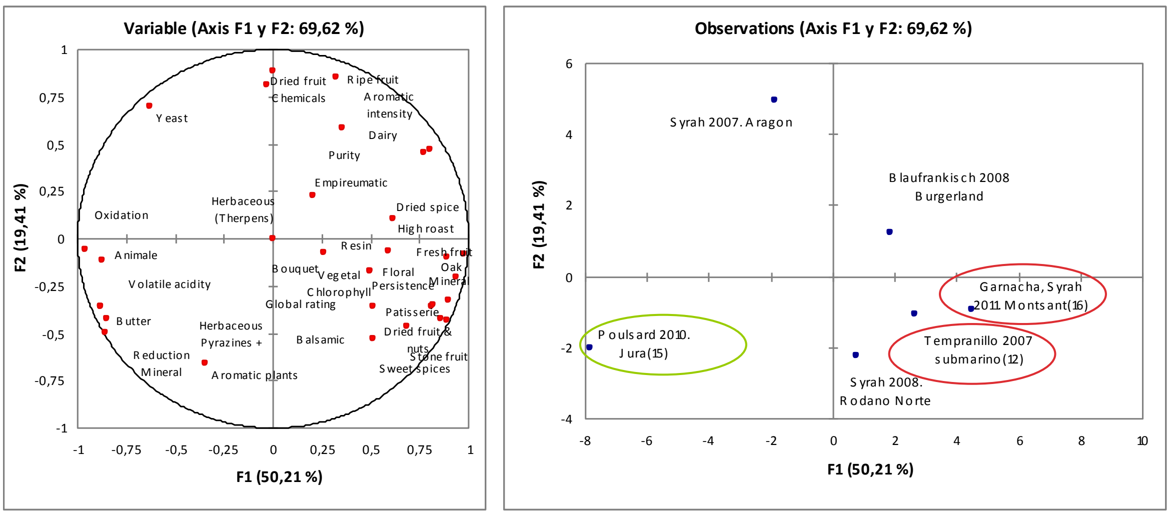
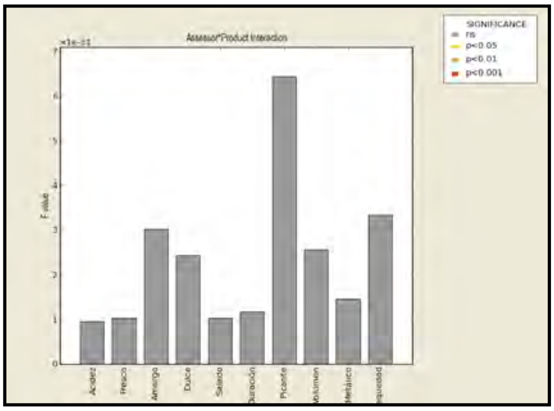


Figure 2- Results of analysis by PCA and coordinates of positions found in the sensory analysis of red wines by the winemakers panel for the aromatic phase. The axis explain 69.62% of the variance. Green indicates wines with less mineral character and red more mineral character.

White wines				Red wines			
Close to attribute minerality		Far from attribute minerality		Close to attribute minerality		Far from attribute minerality	
2	Sauvignon blanc, Loire central, 2008	7	Ribolla 2010, Primorska	12	Tinta del país, 2007, vino submarino	15	Poulsard 2010, Jura
10	Riesling 2009, Mosel Trocken			14	Syrah, 2008, Rhône north		
11	Riesling 2010, Mosel Kabinett			16	Garnacha, Syrah, 2011, Montsant		

Table 2- Summary of results of the sensory study where wines are defined as close or far to the concept minerality according to tasting panels participating in the study.

In order to validate the competence of the tasting panels, the panel of winemakers was validated by computer software Panel Check. Figure 3 shows the study of possible interactions between sensory judges and products. The picture on the left framed in grey indicates that there isn't a significant interaction between these factors and therefore the results obtained can be considered as satisfactory.



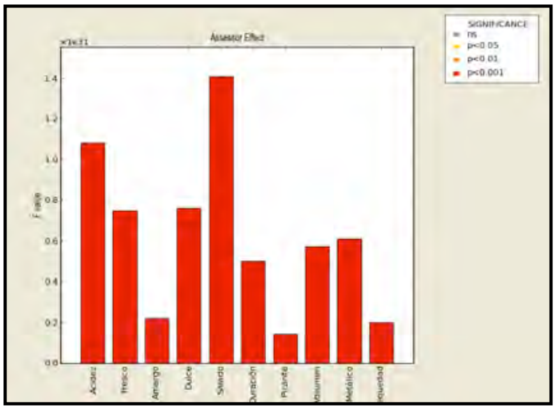


Figure 3- Validation results from the sensory panel by Panel-Check software. Graphs show the results of the University of La Rioja tasting panel. The picture on the left shows the possible interactions between judges and product. The table on the right shows the interactions between judges.

4.2 Analysis of the chemical composition

The set of 17 wines was analyzed in its detailed chemical composition by different analytical techniques aiming to characterize its composition. Based on the results of the sensory analysis, where 6 wines were defined as mineral and 2 wines as remote from that attribute, the chemicals that characterized and differentiated wines from each other and thus define the chemical footprint of minerality were located . Additionally was set the hypothesis that the attribute "minerality" was not the result of the presence of a single chemical compound, but also of the possible synergy established by the presence of several chemical components or families of compounds.

4.2.1 Enological routine analysis

Previous studies point to the possible interaction between the composition of organic acids in wine and the feeling of acidity with the descriptor minerality.

The acidity of wine is due to its composition in organic acids, all of them are synthesized by the plant or come from the microbial metabolism. Occasionally their concentrations are modified by corrections or interventions in the winery.

In the grape there are two main acids, tartaric acid which is the most abundant and malic acid whose content may change videly depending on the variety, climatic conditions, output achieved, grape maturity at harvest and water and heat stress of the vineyard. Malic acid is normally in concentrations much lower than tartaric acid and it may even be absent in those wines that have made the malolactic fermentation wholly or partially. During alcoholic and malolactic fermentation other acids are also generated that are not present initially in the grapes or the grape juice. Among these the most important ones are lactic acid, softer and dairy, acetic acid producing a sharp sour sensation, and succinic acid that has an intense and salty taste. From a sensory point of view, tartaric, lactic and malic induce presumably an increased sensation of astringency, especially the latter.

Routine parameters in wines analyzed by official methods were studied in this section. Organic acids were analyzed using enzymatic techniques.

Figures 4 and 5 below display the Principal Components Analysis (PCA) showing the importance of the presence of succinic acid in wines numbered 10 and 16 as well as the importance of related parameters, such as the total acidity, pH and free sulfur dioxide, particularly in wines numbered 2, 11 and 12. These results are consistent with previous studies that already pointed to the relationship between the term minerality and acidity or saltiness in mouth feel.

Figure 4. PCA of white wines, organic acid composition and routine parameters.

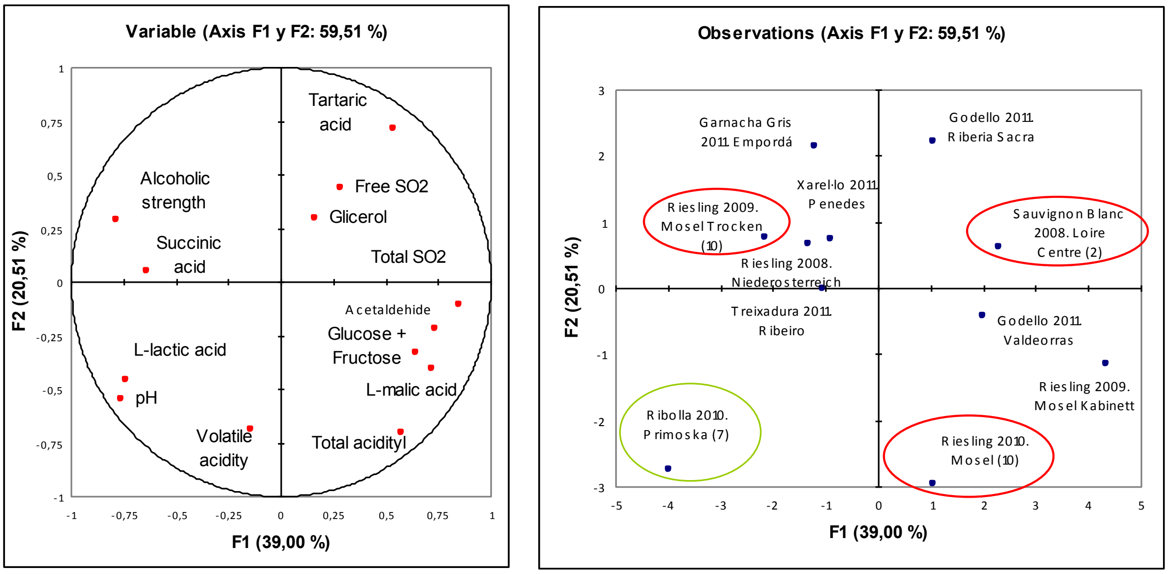
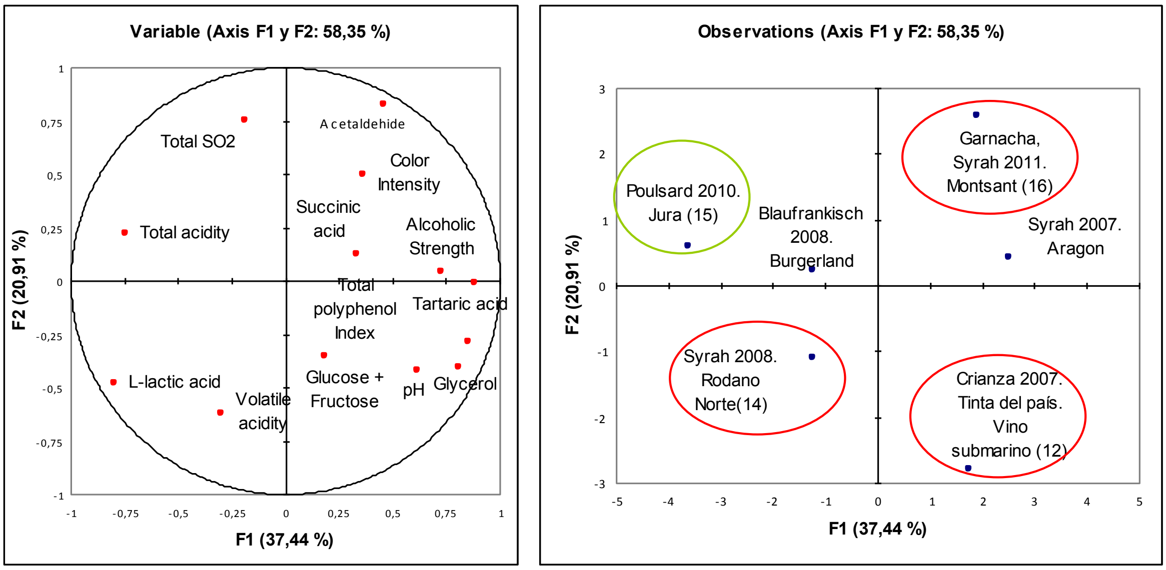


Figure 5. PCA of red wines, organic acid composition and routine parameters.



4.2.2 Analysis of metal content

The term minerality itself suggests easily in the tasting that its perception may be due to the content in minerals of a wine, and therefore that its metal composition may be the origin of such mineral perception, both olfactory and gustatory.

Tables 3 and 4 show the average concentrations of metals more abundant in red and white wines, respectively expressed in ppb (parts per billion) and ppm (parts per million). With this premise, it was decided to analyze the concentration of metals present in the wines studied by inductively coupled plasma mass spectometry (ICP/MS). The results obtained, both in white wines and red wines, represented in Figures 6 and 7 show a scattering of samples defined as mineral, not being grouped in the same quadrant or close to each other. Although in samples 10 and 11 its concentration in copper, potassium, zinc and phosphorus seems relevant, and in sample 14 its zinc concentration seems also relevant.

Element	Red wines	White wines	Element	Red wines	White wines
Co	2.1	2.33	Li	2.35	4.9
Ni	22.1	16.1	Rb	856	479
Cu	66.1	73.2	Cs	2.92	1.97
Zn	444	444	Sr	610	449
As	7.11	5	Ba	193	101
Mo	14.2	6.5	La	0.56	0.66
Ag	0.023	0.023	Ce	0.97	1.37
Cd	0.61	0.51	U	0.37	0.58
Pb	17.8	13.2	Th	0.047	0.096
Bi	0.49	0.34	V	29.1	21

Table 3. Average concentrations (ppb) of metallic elements (30) in red and white wines.

Element	Red wines	White wines
K	1,110.9	344.6
Mg	135.8	96.4
Ca	90.3	75.2
Na	18.2	30.3
Fe	3.98	1.64

Table 4. Average concentrations (ppm) of metallic elements (31) in red and white wines.

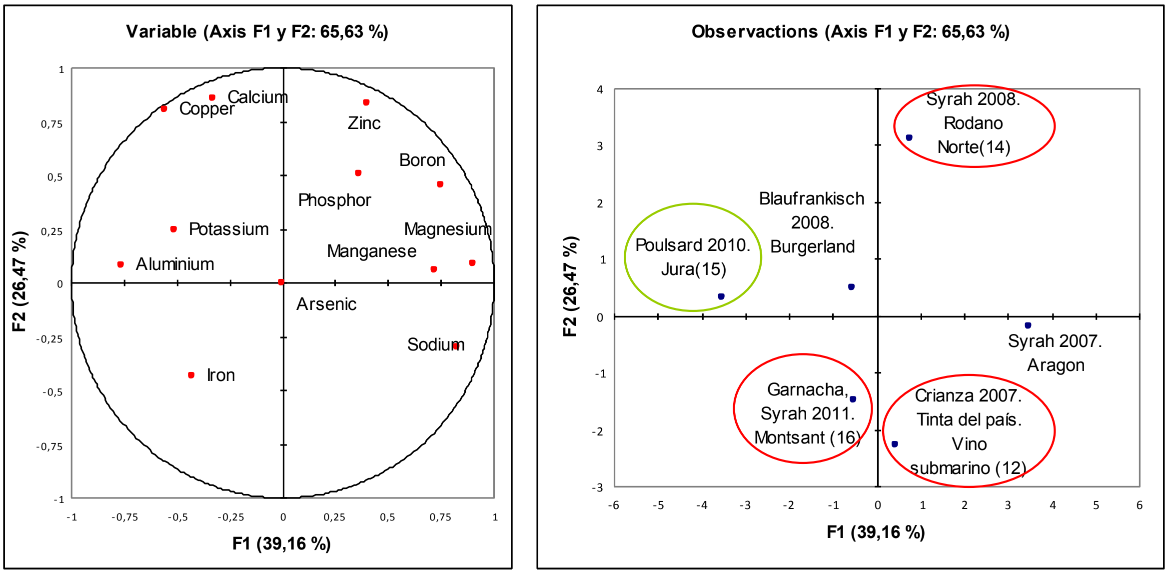


Figure 6. PCA of red wines, composition in metals.

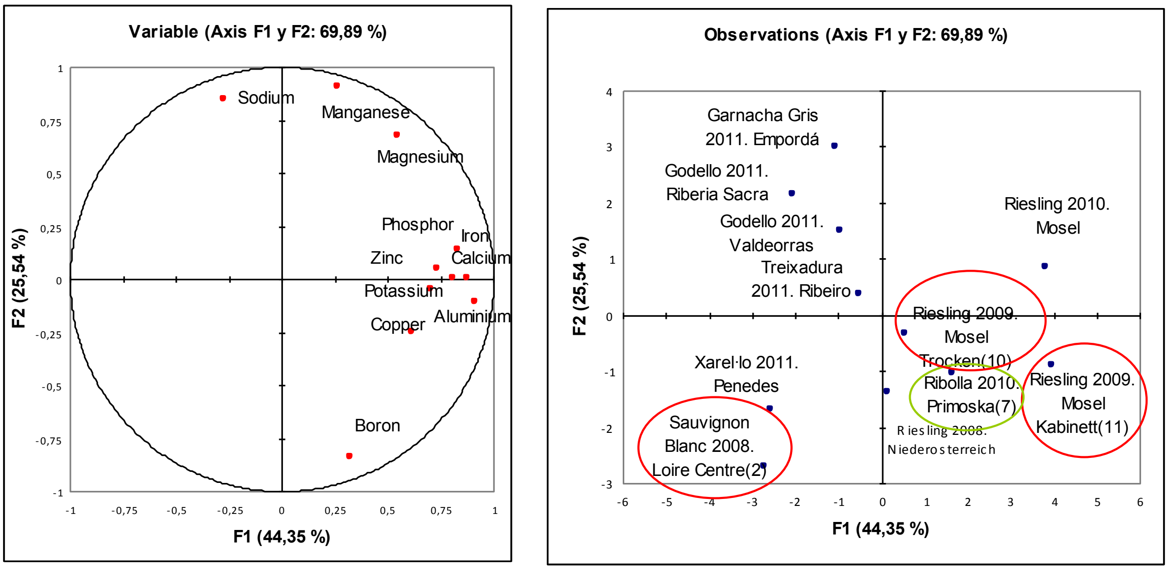


Figura 7. PCA of white wines, composition in metals.

4.2.3 Analysis of aromatic compounds -majority and minority- and thiols of wines

There are many ways in which wines could be classified according to their aromas, although a widespread classification is to treat flavourings according to the phases of the winemaking process in which they appear.

- **Varietal aromas:** This classification would first include the aromas from the variety and the grapes. Compounds included in this section are the linalool smells of rose wood; the nerol smells of rose; α-terpineol that has a camphor odor; limonene or citronellol of dominant citrus note; and, *cis*-rose oxide with aromas that remind of rose. Other important varietal compounds of organoleptic relevance are the C13-norisoprenoids such as β-damascenone, with an odor that varies from blackberry ice cream to apple or prunes, and β-ionone, violet-scented. Also the pyrazines with vegetal aromas of pepper type.

  A separate classification is needed for the so-called varietal thiols whose concentration in wines, although tiny, brings fruity aromas of maracuyá, passion fruit and herbaceous notes from the presence of 4-mercapto-2-methylpenta-2-ona, with scent of boxwood. Statistical analysis for these compounds as well as for varietal compounds does not show a clear relationship of its presence with perceptions in mineral wines, both for the subgroup of white and red wines.

- **Fermentative aromas:** In the family of the fermentation aromas, among the most important are acetate isoamyl, with an aroma of banana; the acetates of isobutyl, hexyl and phenylethyl (all three of fruity and floral character); and, compounds of ethyl isobutyrate and ethyl isovalerate, with aromas of strawberry and pineapple. Also important to be highlighted in this group are compounds as the isobutyric acid (cheese, rancid butter smell) and the isovaleric acid (sweat and aged cheese). Moreover it includes fatty acids whose aromatic notes resemble cheese, butter, fat, such as ethyl lactate, and the ethyl esters of fruity aromas such as the apple-scented ethyl hexanoate, the acetate 3-methyl butyl with smell of banana, and the ethyl octanoate with notes of pineapple.

- **Aromas of ageing and evolution:** Finally, the aromas derived from wood and maturation by oxygen during the ageing of the wine. Aldehydes include the phenylacetaldehyde with aromas of honey and beeswax (common in aged white wines) and eugenol (common in wines aged in oak) clove-scented. Among the best known compounds yielded by the barrel are the Whisky-lactones with coconut, floral and wood aromas. Vanillin aroma of vanilla and caramel and the ethyl vanillate reminiscent of pollen.

Based on this classification all of the 17 wines were analyzed in their varietal aroma fraction, prefermentation, fermentation and ageing. In order to simplify the processing of the data these were analyzed statistically taking separately the majority aromatic compounds, the minority aromatic compounds and the thiols of the white and red wines.

It should be noted that some odorant compounds can dominate in the chemical concentration of a wine or be very intense aroma wise, but what normally perceives a taster is the effect of all the odorant compounds together. To interpret this perception taking separately each of the components does not provide an interpretation adjusted to reality.

Results represented in Figures 8 and 9 display the analytical results of varietal aromas in PCA charts. The representation of the white wines (Figure 9) shows a position away from mineral wines for such compounds. Thus, white wines identified as mineral (2, 10, and 11) are located in the quadrant opposite positions of the varietal compounds such as the linalool or α−terpineol. Something similar is seen in the disposal of varietal aromas for red wines (Figure 8), where wines numbered 12 and 14 are positioned in the quadrant opposite the coordinates found for varietal compounds. This evidence seems to confirm previous studies where minerality is dissociated from the fruit and varietal aromas.

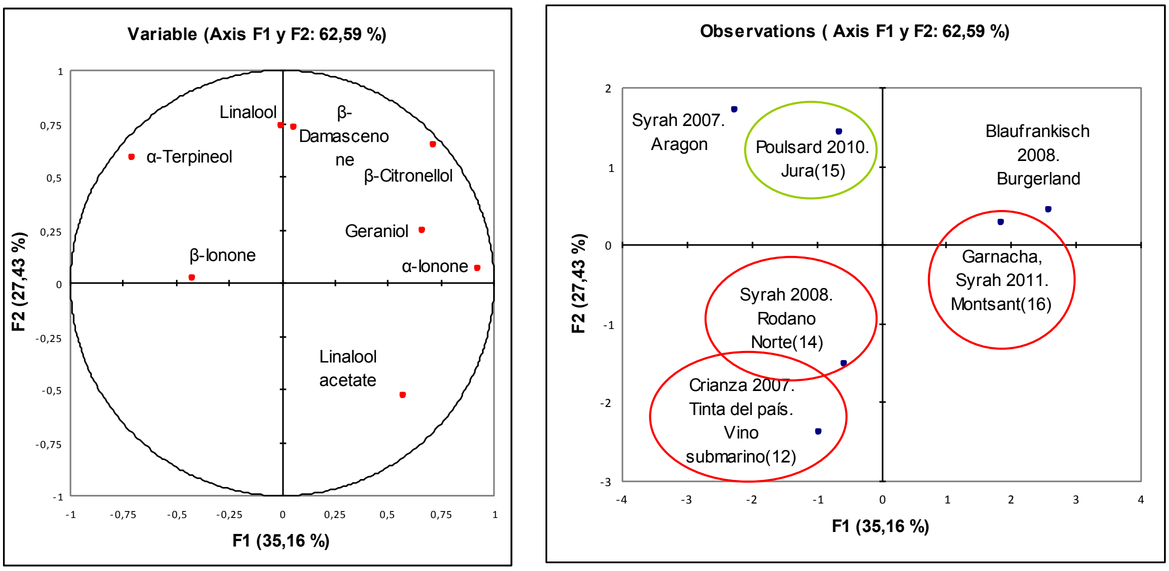


Figure 8. PCA of red wines on varietal aromatics.

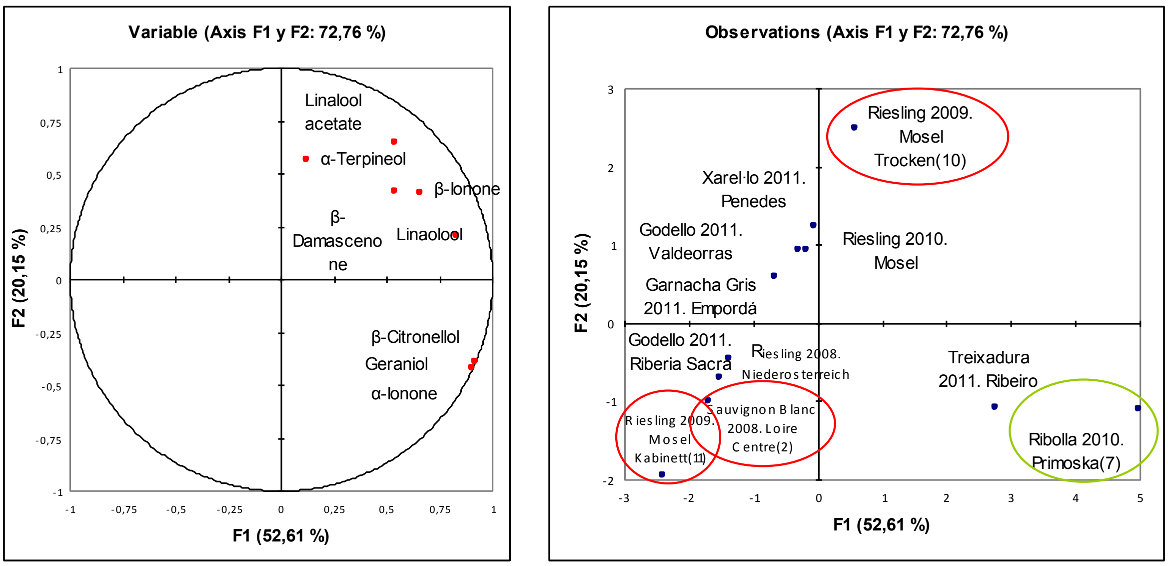


Figure 9. PCA of white wines on varietal aromatics.

The preferment and fermentation aromas of white wines of mineral character indicate compounds such as fatty acids: octanoic acid (soap, sour dairy) and ethyl decanoate (fruit, solvent) as well as ester ethyl succinate and benzoic derivative of the β−phenilethanol, related to the mineral character (Figure 10). The white wine farthest from minerality is situated in a different quadrant and is related to oxidation aromas like acetaldehyde. For red wines (Figure 11) the correlation is established with compounds like m-Cresol (phenolic, smoke), β−phenilethanol (floral: rose, orange blossom) and γ−butyrolactone.

Figures 9 and 10 show the Principal Components Analysis for aromas related to the fermentation process, both for white wines and red wines.

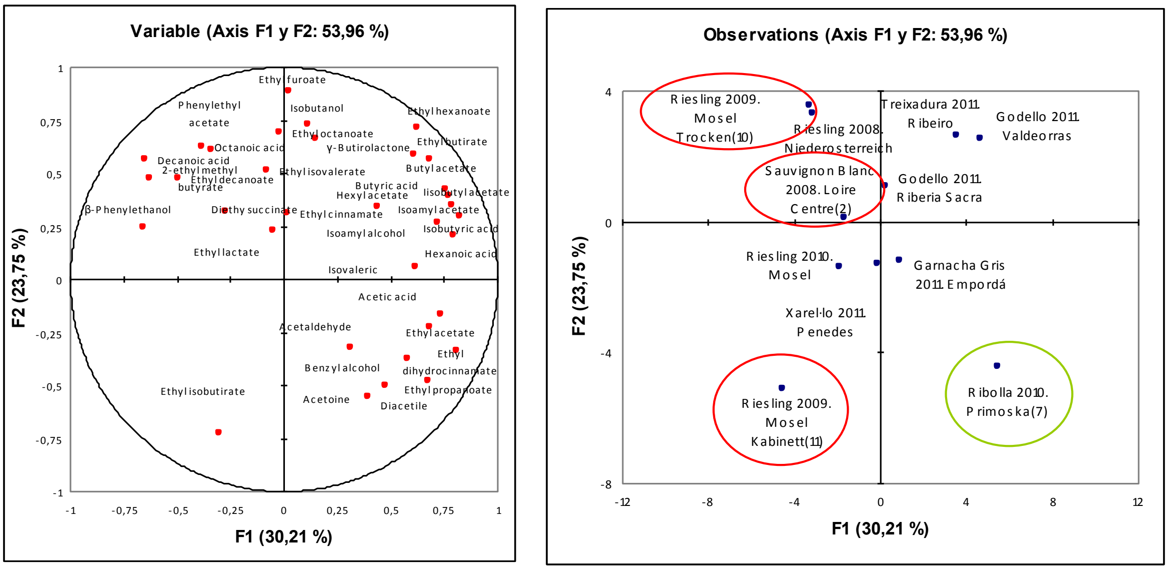


Figure 10. PCA of white wines, fermentative aromatic compounds.

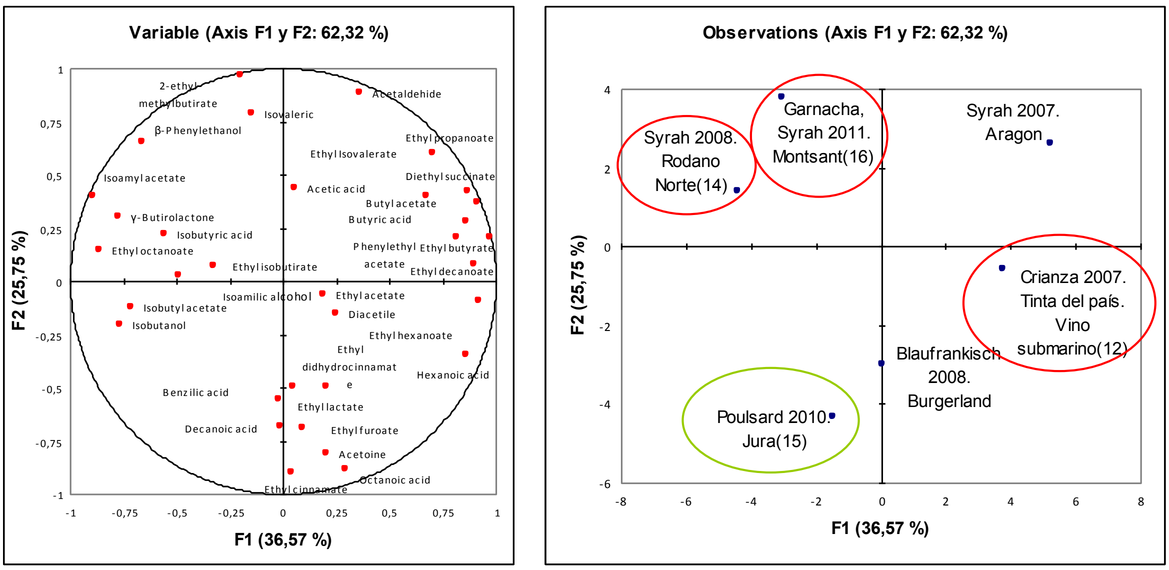


Figure 11. PCA of red wines, fermentative aromatic compounds.

To end the phase of the aromas of wine the volatile compounds from ageing were analyzed, as developed below in point 4.2.4. Both types of white and red wines with mineral perception appear to be related with the presence of γ−decalactone (coconut, fruit) responsible for aromas of coconut, as well as the presence of animal aromas produced by volatile phenols such as 4-ethylphenol (animal) and 4-ethylguaiacol (animal).

4.2.4 Analysis of volatile compounds from the wood

The study of compounds transferred by the ageing of wine in oak was carried out on 7 of the 17 wines studied as those which had been in contact with wood: 5 white wines and 2 red wines. Two samples of white wines classified as mineral (2 and 10) were related to the furfural aldehydes (almonds) and 5-methylfurfural (almonds). The red wine number 16 was positioned close to volatile compounds with animal scents, such as 4-ethylphenol and 4-ethylguaiacol. The statistical results are shown in Figure 12.

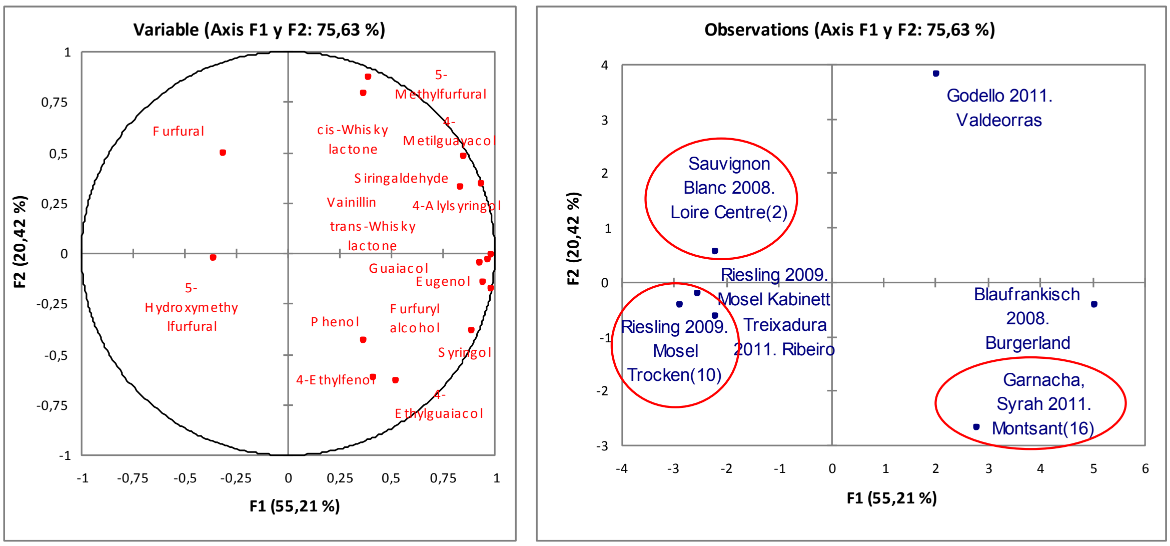


Figure 12. PCA of white and red wines taking into account the volatile compounds from the wood.

4.2.5 Analysis of compounds responsible for organoleptic defects in wine

Another important aspect to consider in the aromatic classification of wines is the presence of certain volatile chemical compounds responsible for the potential appearance of organoleptic defects. In addition, it is well known already that the potential negative effect of these compounds depends on their concentration in wine. In certain cases, at low concentrations they can contribute to the perception of complexity, breaking the balance of qualitative aromatic buffer when its concentration is increased. There are many tasters and consumers who tolerate and even like some presence of ethylphenol produced by *Brettanomyces* in certain wines.

The main negative attributes of the wines can be classified in different families of aromatic groups:

- **Vegetal:** Here are to be found the vegetable families (with aromas of herbaceous, green pepper and ivy) where the main molecules involved are the isobutylmethoxipirazines (IBMP) with vegetable connotations. Some markets like Chile or Argentina tolerate its presence in wine tasting, however Bordeaux penalizes it.
- **Mould-earthy:** The family of musty-earthy scents (wet earth, characteristic cork taste) of this section features geosmin and trichloroanisole molecules (TCA and derivatives haloanisoles). The geosmin is generated by bacteria (*Streptomyces coelicolor*), cyanobacteria and some fungi (*Penicilium expansum*). The soil is a complex structure rich in minerals and organic matter, as well as microbiological organisms (bacteria, yeasts and fungi). The characteristic smell of the soil has been reduced in our case to the component called geosmin. This substance is synthesized by microorganisms in the soil and produces aromas that remind us of newly turned or wet ground and presenting also an extremely low sensory threshold, on the order of 50 ng/L, with a remarkable odorant power.
- **Acetals:** The third family of aromas associated with typical defects is the acetic/acetate, with wines characterised by "chopped" acetic (vinegar) or ascescents smells of glue (ethyl acetate).

- **Sulfur compounds:** Reduction defects were also studied as occurred by the presence of complex sulfur compounds, with scents that are reminiscent of rotten eggs, as the sulfide and mercaptans, and aromas of gas, stew, garlic and cabbage.
- **Animal:** The family of animal aromas with scents of stable, leather, phenolate, and horse sweat, are associated to molecules 4-ethylphenol and 4-ethylguaiacol, commonly the result of microbiological contamination by *Brettanomyces*.
- **Lactics:** The family of the unpleasant lactic aromas (butter and sour milk) are represented by diacetyl in high concentrations, when the malolactic fermentation suffers deviations.

The statistical results obtained for these families of compounds are shown in Figures 13 and 14. It can be seen that both types of wines (white and red) are correlated again with the presence of volatile phenols 4-ethylphenol (animal) and 4-ethylguaiacol (animal). Two of the white wines appear linked to the presence of coconut aromas coming from the compound γ−decalactona (coconut, fruit) in a similar way as shown in the ageing aromas section.

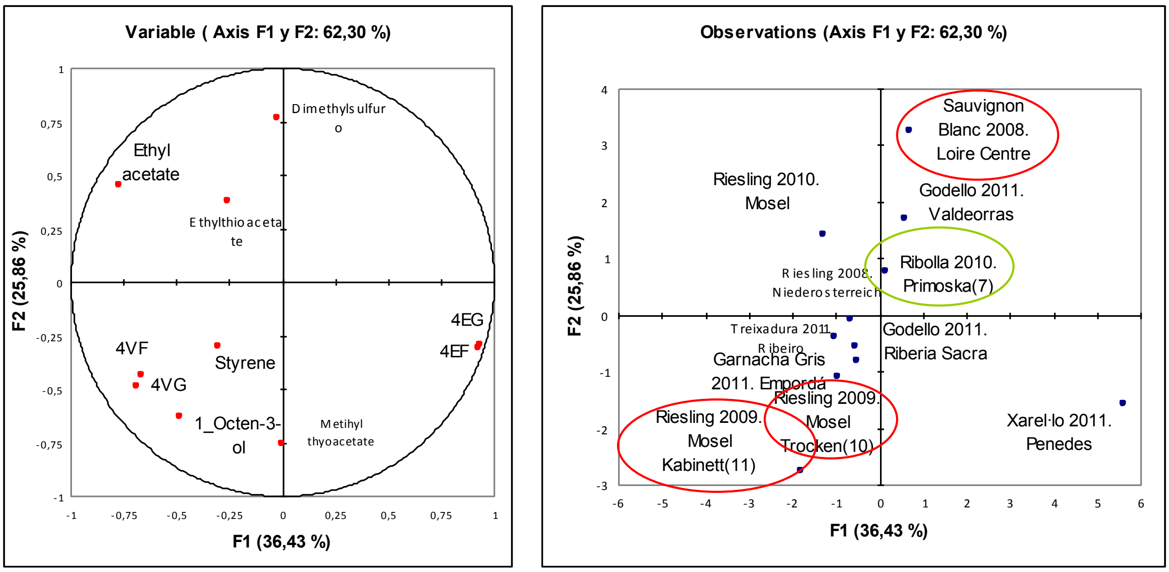


Figure 13. PCA of white wines in relation to the chemical compounds associated with organoleptic defects in wine.

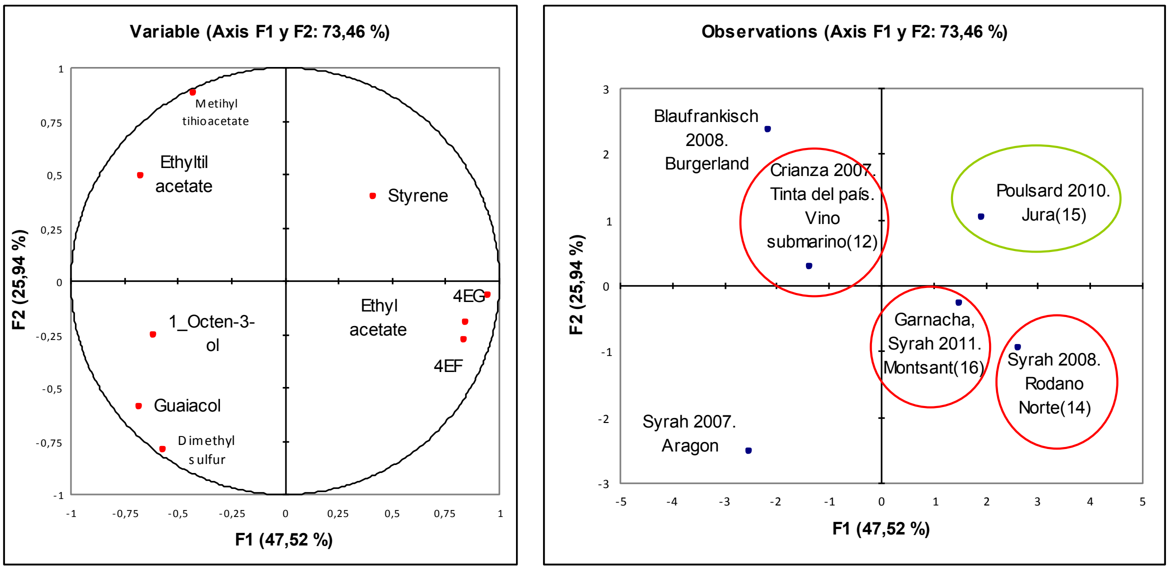


Figure 14. PCA of red wines in relation to the chemical compounds associated with organoleptic defects in wine.

4.2.6 Statistical analysis using linear regression

The statistical analysis of linear regression is used to verify that there is a linear relationship between two variables, allowing to determine the range of dependency between the two. With this premise the statistical analysis was performed for each of the chemical compounds analysed in the 17 wines studied and the average scores obtained from the tasting sessions of both panels. To simplify the processing of the data an associative hypothesis was established between chemical compounds and the descriptor minerality in olfactory and gustatory level. Tables 5 and 6 summarize the results of linear regression on the white and red wines, whose probability to be linked was higher than 80%. The first column represents the analytical group pertaining to each compound, the second specifies with what type of descriptor it is related, and the fourth column represents the probability of linear relationship found between both variables. Highlighted in bold are the matching parameters that show a probability greater than 80% of linear relationship.

ANALYTICAL GROUP	DESCRIPTOR MINERALITY	PARAMETER	% PROBABILITY
Enological	Gustatory	**Ph**	82.88
Enological	Gustatory	Tartaric acid	86.06
Enological	Gustatory	IPT	93.54
Prefermentative aromatics	Aromatic	m-Cresol	82.10
Fermentative aromatics	Aromatic	**Butyric acid**	88.51
Fermentative aromatics	Aromatic	**Hexanoic acid**	90.29
Fermentative aromatics	Aromatic	Ethyl isovalerate	80.33
Fermentative aromatics	Aromatic	Ethyl butyrate	84.67
Fermentative aromatics	Aromatic	Ethyl decanoate	92.94
Fermentative aromatics	Aromatic	Isobutanol	81.00
Fermentative aromatics	Aromatic	**Ethyl hexanoate**	92.84
Ageing aromatics	Aromatic	4-Ethylguaiacol	91.77
Ageing aromatics	Aromatic	***cis*-Whisky-lactone**	96.70
Ageing aromatics	Aromatic	Eugenol	92,03
Ageing aromatics	Aromatic	δ-Octalactone	81.88
Ageing aromatics	Aromatic	2,6-Dimethoxiphenol	89.55
Ageing aromatics	Aromatic	**4-Allyl-2,6-dimethoxiphenol**	88.58
Ageing aromatics	Aromatic	**Methyl vanillate**	94.70
Defects	Aromatic	4-Ethylguaiacol	89.80
Sulfur defects	Aromatic	Ethyl thioacetate	97.59
Thiols	Aromatic	2-Methyl-3-furanthiol*	99.15
Thiols	Aromatic	2-Furfurylthiol	91.07
Thiols	Aromatic	**4-Mercapto-4-4-methyl-2-2-pentanone**	94.62
Thiols	Aromatic	**3-Mercaptohexanol**	95.39
Metals	Gustatory	Boron	80.01

Table 5. Summary of the results obtained in the statistical analysis of linear regression on red wines. Compounds associated with minerality with a 80%.

ANALYTICAL GROUP	DESCRIPTOR MINERALITY	PARAMETER	% PROBABILITY
Enological	Gustatory	Alcoholic strength	80.99
Enological	Gustatory	**pH**	88.36
Enological	Gustatory	Glucose + Fructose	86.44
Enological	Gustatory	Total sulfur dioxide	95.50
Enological	Aromatic	Total sulfur dioxide	80.28
Enological	Gustatory	Acetaldehyde	95.54
Varietal aromatics	Aromatic	β-Citronellol	91.71
Varietal aromatics	Aromatic	α-Ionone	91.64
Varietal aromatics	Aromatic	β-Ionone	85.90
Varietal aromatics	Aromatic	Linalool acetate	89.77
Fermentative aromatics	Aromatic	**Butyric acid**	97.96
Fermentative aromatics	Aromatic	Isobutyric acid	98.81
Fermentative aromatics	Aromatic	**Hexanoic acid**	94.67
Fermentative aromatics	Aromatic	β-Phenylethanol	94.70
Fermentative aromatics	Aromatic	Benzylic alcohol	96.05
Fermentative aromatics	Aromatic	Isoamyl acetate	89.88
Fermentative aromatics	Aromatic	Ethyl butyrate	85.80
Fermentative aromatics	Aromatic	Ethyl acetate	92.37
Fermentative aromatics	Aromatic	Isoamylic alcohol	99.03
Fermentative aromatics	Aromatic	**Ethyl hexanoate**	85.72
Fermentative aromatics	Aromatic	Acetic acid	96.52
Fermentative aromatics	Aromatic	Decanoic acid	91.82
Fermentative aromatics	Aromatic	Iso valerianic	98.44
Fermentative aromatics	Aromatic	Ethyl isobutyrate	94.07
Fermentative aromatics	Aromatic	Isobutyl acetate	95.97
Ageing aromatics	Aromatic	*trans*-Whisky-lactone	86.90
Ageing aromatics	Aromatic	***cis*-Whisky-lactone**	87.98
Ageing aromatics	Aromatic	Eugenol	95.53
Ageing aromatics	Aromatic	o-Cresol	90.94
Ageing aromatics	Aromatic	4-Vinilguaiacol	87.12
Ageing aromatics	Aromatic	**2,6-Dimethoxiphenol**	89.17
Ageing aromatics	Aromatic	**Methyl vanillate**	98.60
Ageing aromatics	Aromatic	Ethyl vanillate	86.32
Defects	Aromatic	4-Vinilguaiacol	94.79
Thiols	Aromatic	4-**Mercapto-4-4-methil-2-2-pentanone**	90.10
Thiols	Aromatic	3-Mercapto hexyl acetate	89.21
Thiols	Aromatic	**3-Mercaptohexanol**	91.62
Thiols	Aromatic	Bencyl mercaptan	97.56
Metals	Gustatory	Magnesium	84.79

Table 6. Summary of the results obtained in the statistical analysis of linear regression on white wines. Compounds associated with minerality with a 80%.

5. Discussion and conclusions

Many factors are involved in the definition of an olfactory and gustative perception: genetics of the individual, his/her anthropological evolution especially as a taster, knowledge and wealth of vocabulary, ability in the tasting, experience, preferences and beliefs, biases, influence that others may have had in his/her education, physical and psychic condition, as well as other external factors that also influence the final definition of the perception of the aroma. This complexity adhered to the system of perception and interpretation of external stimuli captured by human senses can turn the minerality of wine into a "cognitive" irrefutable reality. However, little is known yet about the chemical nature of the wine which acts on chemical receptors, or of the extremely complex system of connection and neuronal interaction of the brain (cortex, amygdala, hypothalamus) and its relationship in the perception and zoning at the level of brain map. There is no doubt that depending on the psychological level in which we find ourselves, it exerts a considerable influence on the brain interpretation of the stimuli received. Variations in sensory interpretations of a taster evaluating a same wine in a short period of time are a known fact.

The problem then focuses on the outcome of the relationship between the chemical composition of wine and its olfactory perception, and in this context it also includes other aspects necessarily related with:

1) **The soil** and its chemical composition.
2) **Treatments in the vineyard** (fertilizers, herbicides, pesticides, fungicides) affecting the physiology and synthesis of organic compounds of the vine such as the norisoprenoids, the pyrazines and thiol precursors.
3) **The grape** and its final chemical composition, also considering maturity which may vary according to the climatic conditions of each vintage year, yield and ripeness of the grape at harvest.

4) **The influence of enology** at the level of treatments (adjuvants, additives, rectifications, bentonites, tartaric stabilization with cation resins, spinning cones, reverse osmosis, etc.) applied in grape juice and wine.

5) **The alcoholic and malolactic fermentation** both produce chemical compounds resulting from microbial metabolism that have great influence and sensory impact on aromatics and flavours in wine.

6) **The chemical evolution** of the wine during its maturation in barrel and bottle, which also possibly has a strong influence on the minerality of wine linked to potential chemical reactions of oxide-reduction.

All this permits to see clearly that the chemical composition of wine is very varied and complex. Science has isolated and identified until now more than 900 different chemical elements in their volatile composition (olfactory), and most are already grouped by families related among themselves. Many of them have been widely studied and characterized since their presence contributes marked aromatic and/or gustative features in wine. However, some descriptors as it is the case of "minerality" remain yet without a clear scientific consensus on the basis on which this term is constructed, although the results suggest that its origin lies in the formation of synthesis chemical compounds by the physiology of the plant, fermentation, the pH and acidity of the wine, as well as complex compounds as sulfur. Even so, we cannot say the minerality is a falsehood or an irrefutable fact, but rather a rewarding aspect within all possible articulated sensory interpretations of wine, which it really is a box of surprises. Here lies precisely the need for this scientific study, to be followed by other studies that may provide even a greater precision on the topic.

However, even if we fall into the temptation of transferring the soil characteristics to the sensory characteristics of the wine, it will be very difficult to explain it in a scientific way in order to justify it. The vine only takes mineral elements in ionic form dissolved in water and it does so selectively; therefore it doesn't absorb anything directly from the stone, sand or clay, but only cations and anions dissolved. It can be thus deduced that vineyards from dry-farming, warm weather and low water availability have limited absorption of these nutrients. The selectivity of the transport of elements according to its physiological needs as a vegetable does not happen in a deprogrammed way depending on the composition of the soil, but according to its particular need as a living being. However there may be imbalances due to excessive abundance or shortcomings that determine differences in plant nutrition, and therefore in its physiological behavior (vegetative growth and production of grape).

The edafoclimatic conditions affecting more strongly a vineyard and the wines obtained from it are: the geological characteristics of the soil, its structure and size of the aggregates that constitute it, capacity of drainage and water retention, aeration, and chemical composition. Also to be considered are the climatic conditions with average temperatures, thermal differences during the vegetative cycle and the annual distribution of rainfall which determines the availability of water during the growing season. But among these aspects it also follows that the chemical composition (minerals and organic matter) may have an effect on the quality and organoleptic profile of the wine obtained from grapes in a given vineyard, although this does not necessarily imply a direct link with the perception of "minerality" in the tasting.

Once the theoretical concept "*terroir*" is associated with a wine it is easy for the prescribers to associate the term "mineral" in them, especially in dry white wines with high acidity and low expression of fruit aroma. As an example, the absence of marked aromatic elements (esters, terpenes, etc.) and high levels of acidity opens the door to the perception of minerality in wines with this profile, which normally come from geographic areas linked to cold weather, early harvest and sometimes stony soils.

The simple fact of linking a wine to visible stones, rocks and boulders or non-visible constituent minerals of a vineyard is not sufficient to argue its mineral sensory perception, if we are to be strict in terms of scientific curiosity. Although it is understandable that these images on the retina favor, by association and the related psychological predisposition of the taster, the descriptions of the "*terroir*" effect in terms of market. This may create doubts and a sense of ambiguity if it lacks precision or if the mineral perception is not obvious in the wine tasting.

It is true that the physico-chemical state that some wines experience during their different stages of maturation and evolution, as well as the enological or specific vinification techniques applied, can influence in showing a profile associated with descriptors that tasters frequently define as "burnt match smoke", "flint or silex", "gun flint smell", etc. The term "mineral" is often used to define and include these descriptors under a same terminology.

In the 21st century the wine sector must progress, to move beyond and verify what are the chemical compounds that may actually be associated with the description of minerality in wine. Today there is no reason for this term to be attached to the type of descriptors associated with stones or rocks very well known in the world of wine tasting, because it is often associated with the reduced status of wine (complex sulfur compounds).

There are enological practices applied in wineries that show a predisposition to praise the minerality of wine, such as: the preferment maceration of the grapes, fermentation of grape juice with high turbidity, the maximum addition of nutrients to what is strictly necessary, the use of certain yeasts, ageing of the wine with low redox potential (Ev), extended fine lees ageing, certain dosage of SO_2, pH, oxygen management and reductive state of wine, ageing in oak or maturation in air-tight inert container. Therefore the minerality is also a matter of winery and wine elaboration linked to art, knowledge and know-how of the winemaker. Examples of winemaking operation in search of minerality can be found in Burgundy with Chardonnays from certain producers, which try to be imitated in other corners of the globe.

Therefore, one would expect that minerality was associated with certain distinctions such as lower pH and higher acidity in whites particularly those from northern latitudes or marginal cold climate regions due to the altitude. Or in case of red wines it was associated with the system of vinification without aeration, where more succinic acid is accumulated, a chemical element that is closely linked to the perception of minerality mainly due to its clearly salty gustatory effect, which by default is usually associated in tasting with salts or minerals.

As a result of the tasting carried out by the two panels, one of winemakers and the other of professionals non-producers of wine, three white wines were selected as mineral both at olfactory and gustative level: two belonging to the variety Riesling from Mosel (Germany) and another from the variety Sauvignon blanc from the Loire Valley (France). Among the red wines those selected were elaborated with Syrah and Garnacha from Montsant (Spain). On the other hand, both panels also selected two wines as being far and almost opposite to the term minerality: a white wine of the variety Ribolla Primorska from Slovenia and a red wine of the variety Poulsard from the Jura (France).

Once the graphic representations of the chemical compounds in Principal Components Analysis (PCA) were obtained and those compounds that were closer to the 6 wines marked as mineral were chosen, the present study concludes that the compounds more related to the minerality of wine, distinguishing between white and red, are as follows:

- **Gustative Minerality:** Within the routine parameters appear among others, succinic acid, as well as the acidity-related analytical measures.
- **Aromatic Minerality:** Within the aromas some aromatics stand out, like alcohol β−phenylethanol (floral: rose, orange blossom), volatile phenols, such as the compound 4-ethylphenol and 4-ethylguaiacol (animal). Wines with low aromatic fruitiness are liable to be interpreted as mineral if they are also reduced, show high free SO_2 and have a low pH and high total acidity (see Table 5).

Chemical classification	White wines	Red wines
Routine parameters	Free sulfur dioxide	Free sulfur dioxide
	Total acidity and pH	Total acidity and pH
	Succinic acid	Succinic acid
Preferment aromatics	β–Phenylethanol	β–Phenylethanol
	Diethyl succinate	m-Cresol
	Ethyl decanoate	γ–Butyrolactone
Ageing aromatics	γ–Decalactone	γ–Decalactone
	4-Ethylphenol	4-Ethylphenol
	4-Ethylguaiacol	4-Ethylguaiacol
	Furfural/ 5-methylfurfural	Furfural/ 5-methylfurfural

Table 7- Overview of chemical compounds selected for their relevance in white and red wines, defined as mineral and selected by Principal Component Analysis (PCA).

On the other hand, the study of linear regression compound to compound, shows those who are strongly related to the term minerality. Thus, red wines showed a robust relationship with the use of the term at olfactory level of volatile compounds: 2-methyl-3-furanthiol and 3-mercaptohexanol and aromatic compound of ageing and aroma of coconut *cis*-Whisky-Lactone. However, in white wines there is a different relationship covering a larger number of compounds which are different to those for red wines. In the case of white wines the family of organic acids appear, such as butyric acid e isobutyric, alcohols such as isoamyl alcohol, thiols such as benzylmercaptoethanol and compounds resulting from ageing in wood such as methyl vanillate and 4-vinilguaiacol.

The study which has been designed by addressing both the chemical structure of the wines analyzed and their organoleptic characteristics opens a door to future research, with the aim to broaden and develop the relationship of the concept of sensory perception of minerality in wine and its relation with the ¨*terroir*¨ of the region or the geological origin where the grapes have been harvested.

Preliminary results seem to point out that the relationship of the ¨*terroir*¨ and the mineral concept in wine are not closely related to the levels of mineral materials present in the chemical composition of the soil, at least as the sole factor. There seem to be also other compounds related to this term and with greater sensory impact (plant synthesis compounds of fermentative origin, complex sulfur compounds, acids and low pH, geosmin, pyrazines, etc). This statement diverges from the popular belief that the characteristics of the soil are bringing a greater concentration of minerals in its metal form or are forming part of other organic compounds, these being responsible for the minerality of wine. Results in concentration of metallic compounds contained in the set of the wines studied show that the concentration of minerals is not a determining factor in its chemical composition in relation to the wines defined with the attribute "wine of mineral character", there being other families of chemicals that may best explain this concept. It is therefore possible that in the volatile chemical composition of wine there are molecules that in one way or another remind, at olfactory or gustative level, of the world of minerals, while soil does not seem to be the source of them.

But all of this is very complex, and besides market final consumers do not seek stones or minerals when buying a wine to drink, so there seems to be no point in directing them towards such a difficult search. The consumer him/herself will walk the road and if he/she finds this perception by chance, current updated information will be available; but it is important not to complicate the life of the consumer with soil science, geology, climatology, or mineral and chemical crystallography lessons. In this case it is advisable that the sector remains cautious and honest with the market and conveys messages with clarity and simplicity. The physiological interpretation of the senses for the time being may be sufficient.

What seems then more logical and obvious in relation to the impact of the *terroir* on the perception of minerality is that rather than the chemical composition of the soil, it is the geological factors of depth, texture, slope, holding capacity of water next to the weather and practical conditions of viticulture as a whole, what really marks the predisposition of the grapes to produce wines with the sensory profile of mineral character.

Given the results obtained in this study sponsored by Outlook Wine and Excell Ibérica, financed without any subsidy and solely with their own resources to maintain the maximum objectivity, it could be then inferred that: the plant that has suffered some degree of stress (sandy or rocky soils, vineyards on slopes, vegetation, soils poor in groundwater and water retention, etc.) produces a grape whose grape juice composition at the level of aromatic precursors (amino acids and assimilable nitrogen among others) will influence the microbial metabolism that will transform it into wine, crucially bridging the occurrence of volatile compounds that are later interpreted as mineral aromas and molecules in solution or colloidal state, and translated into potentially mineral taste.

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Nº	Typology	Alcoholic strength	Total acidity	Volatile acidity (g/L)	pH	L-lactic acid (g/L)	L-malic acid (g/L)	Succinic acid (g/L)	Tartaric acid (g/L)	Glucose+ Fructose (g/L	Free SO_2 mg/L	Total SO_2 mg/L	Acetaldehyde mg/L	Glycerol (g/L)	Color intensity	(TPI) Total polyphenol index
1	White wine	11.9	7.51	0.52	3.12	0.1	1.6	0.33	1.7	3	3	112	76	7.12	-	-
2	White wine	10.0	8.69	0.49	3.11	0.2	3	0.38	2.6	0.7	13	91	45	7.6	-	-
3	White wine	13.3	6.37	0,29	3.38	0.6	1.6	0.44	1.5	0.9	3	64	51	7.4	-	-
4	White wine	12.5	6.3	0.3	3.14	0.1	1,4	0.35	2.9	1.4	14	83	42	6.6	-	-
5	White wine	11.7	6.4	0.3	3.22	1.2	0.8	0.53	2	1.6	3	56	35	8.4	-	-
6	White wine	13.2	5.2	0,17	3.26	0.1	0,8	0.71	2.1	0.5	6	67	38	9.2	-	-
7	White wine	12.8	7.54	1	3.61	1.78	0.1	0.71	0.9	0.19	3	53	33	5.7	-	-
8	White wine	11.9	4	0.22	3.28	1.1	0.2	0.59	2	0.2	3	91	60	6.1	-	-
9	White wine	11.0	10.97	0.38	3.46	1.2	4.4	0.34	0.7	15.5	6	93	51	7.5	-	-
10	White wine	12.3	4.84	0.24	3.44	1.6	0.6	0.59	1.7	4.9	6	70	32	9.8	-	-
11	White wine	7.5	9.58	0.46	3.12	0.1	2.8	0.53	2.7	73.3	3	104	75	8.9	-	-
12	Red wine	13.3	4.25	0.76	3.68	1.3	0.1	0.59	2.7	0.7	3	6	4	11.1	10.3	68.6
13	Red wine	12.4	6.12	0.6	3.67	1.7	0.1	0.53	1.9	1	3	21	16	8.1	8.7	51.9
14	Red wine	13.4	7.01	0.84	3.63	2.1	0.1	0.52	2.3	0.1	3	11	5	8.9	57	57
15	Red wine	10.8	6.18	0.66	3.44	1.8	0.1	0.67	2	0.2	3	13	6	7.7	24.6	24.6
16	Red wine	13.9	5.46	0.62	3.6	0.6	0.1	0.56	2.9	0.1	3	21	24	8.8	62	62
17	Red wine	13.8	4.84	0.51	3.62	1	0.1	0.88	2.3	0.6	3	9	16	11.8	58.5	58.5

Table 8. Detail of the chemical composition of enological parameters of the 17 wines used in the study.

Nº	Typology	Linalool (µg/L)	β-Citronellol (µg/L)	Geraniol (µg/L)	α-Terpineol (µg/L)	α-Ionone (µg/L)	β-Ionone (µg/Le	β-Damascenone (µg/L)	Linalool acetate (µg/L)	δ-Decalactone (µg/L)	1-Hexanol (mg/L)	*cis*-3-hexen-1-ol (mg/L)	1-Butanol (mg/L)	Methionol (mg/L)	m-Cresol (µg/L)
		VARIETAL GROUP									PREFERMENTATIVE GROUP				
1	White wine	5.91	nd	nd	9.32	nd	0.33	5.81	0.54	nd	1.05	0.06	0.99	0.33	0.50
2	White wine	1.37	nd	0.49	11.65	nd	0.27	261.00	0.42	nd	1.24	0.34	0.72	0.44	nd
3	White wine	20.02	3.20	5.78	34.76	0.18	0.31	5.47	0.45	nd	1.77	0.08	0.75	0.59	0.78
4	White wine	5.30	nd	nd	18,27	nd	0.22	3.41	0.46	nd	1.16	0.07	0.61	0.49	0.33
5	White wine	1.07	nd	nd	26.68	nd	0.19	6.15	0.42	nd	1.01	0.03	0.87	0.42	1.33
6	White wine	3.96	nd	nd	13.91	nd	0.32	3.93	0.57	nd	0.54	0.07	0.68	0.53	nd
7	White wine	20.87	5.51	7.19	20.29	0.32	0.32	6.95	0.58	nd	1.70	0.07	0.46	0.48	3.38
8	White wine	4.16	nd	nd	7.22	nd	0.36	5.62	0.58	nd	0.86	0.15	0.36	0.58	nd
9	White wine	6.18	nd	nd	44.14	nd	0.29	6.36	0.50	nd	1.28	0.04	0.45	0.20	0.70
10	White wine	22.88	nd	nd	169.97	nd	0.27	5.92	0.53	nd	1.20	0.03	0.66	0.68	0.82
11	White wine	1.13	nd	nd	25.71	nd	0.21	3.28	0.25	nd	0.94	0.02	0.36	0.12	nd
12	Red wine	2.10	1.64	nd	8.56	nd	0.24	2.08	0.24	nd	1.85	0.18	1.23	0.75	0.67
13	Red wine	11.87	4.61	3.46	12.15	0.15	0.25	2.39	0.27	nd	1.65	0.02	1.09	1.66	1.00
14	Red wine	8.28	2.53	nd	17.68	0.05	0.30	1.66	0.28	nd	1.19	0.18	0.70	1.97	1.51
15	Red wine	7.79	3.84	0.83	21.31	nd	0.23	5.19	0.22	nd	1.05	0.11	0.43	0.95	1.69
16	Red wine	6.59	5.11	nd	5.83	0.18	0.25	4.37	0.25	nd	0.49	0.01	1.13	1.15	0.65
17	Red wine	12.87	3.24	nd	33.40	nd	0.30	3.55	0.22	nd	2.37	0.18	3.98	0.91	0.60

Table 9. Detail of the chemical composition of varietal aromatics and prefermentative compounds of the 17 wines used in the study.

Nº	Typology	Butyric acid (mg/L)	Isobutyric acid (mg/L)	Hexanoic acid (mg/L)	Octanoic acid (mg/L)	Phenylethyl acetate (mg/L)	Hexyl acetate (mg/L)	Diethyl succinate (mg/L)	Ethyl isovalerate (μg/L)	β-Phenylethanol (mg/L)	Benzyl alcohol (mg/L)	Isoamyl acetate (mg/L)	Ethyl butyrate (mg/L)	γ-Butyrolactone (mg/L)	Ethyl decanoate (mg/L)
								FERMENTATIVE GROUP I							
1	White wine	2.07	1.92	5.92	7.21	0.12	0.02	3.48	49.87	14.10	0.02	0.63	0.33	5.42	0.15
2	White wine	0.80	1.06	2.69	4.91	0.28	nd	7.22	50.49	15.01	nd	0.07	0.15	6.01	0.17
3	White wine	2.85	1.05	4.50	5.93	0.10	0.03	3.80	36.10	17.86	0.03	0.60	0.45	9.12	0.14
4	White wine	1.32	0.95	3.92	6.43	0.09	0.01	4.73	53.15	18.88	0.01	0.30	0.24	7.77	0.23
5	White wine	1.15	1.04	3.98	11.44	0.28	nd	8.20	50.48	96.05	nd	0.06	0.22	7.25	0.23
6	White wine	1.72	1.17	4.43	4.71	0.10	nd	6.60	73.00	25.42	0.01	0.22	0.25	5.01	0.09
7	White wine	1.41	1.56	4.26	4.77	0.02	nd	6.10	22.97	24.60	0.08	0.28	0.25	6.21	0.14
8	White wine	0.95	1.05	3.60	5.36	0.05	nd	4.17	52.83	28.84	0.01	0.24	0.18	6.79	0.19
9	White wine	0.77	0.75	3.24	6.41	0.03	0.02	2.80	38.16	28.30	nd	0.19	0.22	5.31	0.23
10	White wine	0.97	1.08	2.55	8.18	0.16	nd	8.18	53.36	125.64	nd	0.11	0.30	8.02	0.43
11	White wine	0.51	0.23	2.93	5.93	0.05	nd	3.73	21.93	73.98	nd	0.05	0.11	4.30	0.15
12	Red wine	1.49	2.21	2.01	1.74	0.25	nd	21.89	71.23	30.44	0.01	0.19	0.23	10.45	0.38
13	Red wine	1.04	2.82	1.85	1.62	0.11	nd	9.88	42.82	29.29	0.04	0.19	0.15	14.71	0.28
14	Red wine	0.84	4.02	1.13	1.15	0.14	nd	14.05	49.53	34.97	nd	0.31	0.11	38.23	0.12
15	Red wine	0.84	2.21	1.35	1.64	0.09	nd	11.32	13.41	27.82	0.01	0.23	0.13	13.86	0.06
16	Red wine	1.09	2.46	1.02	0.81	0.06	nd	8.32	45.12	37.54	0.01	0.31	0.14	20.22	0.09
17	Red wine	1.55	2.49	1.79	1.07	0.36	nd	22.80	84.59	28.08	nd	0.17	0.24	11.10	0.37

Table 10- Detail of the chemical composition in fermentative aromatic compounds of the 17 wines used in the study.

Nº	Typology	Acetaldehyde (mg/L)	Ethyl acetate (mg/L)	Ethyl propanoate (mg/L)	Diacetyl (mg/L)	Isobutanol (mg/L)	Isoamyl alcohol (mg/L)	Ethyl hexanoate (mg/L)	Acetoine (mg/L)	Ethyl lactate (mg/L)	Ethyl octanoate (mg/L)	Acetic acid (mg/L)	Decanoic acid (mg/L)	Isovaleric (mg/L)	Ethyl isobutyrate (µg/L)
FERMENTATION GROUP I I															
1	White wine	16.70	93.76	0.10	nd	23.97	164.95	0.80	2.10	23.25	0.81	312.15	1.13	1.04	29.90
2	White wine	6.05	77.58	0.10	nd	28.41	112.79	0.46	2.18	17.67	0.46	260.62	1.30	0.65	21.37
3	White wine	11.10	59.63	0.09	nd	22.44	160.33	0.74	1.03	91.96	0.57	222.02	1.11	0.85	27.41
4	White wine	4.73	63.78	0.10	nd	21.01	154.34	0.63	1.37	23.35	0.92	239.77	1.43	0.82	30.73
5	White wine	10.04	53.63	0.06	0.52	21.81	105.71	0.60	10.05	177.73	0.94	179.55	2.22	0.44	25.09
6	White wine	15.88	47.11	0.16	nd	19.52	189.70	0.49	1.39	17.63	0.46	125.23	0.73	1.54	29.57
7	White wine	17.79	145.92	0.19	4.34	16.49	155.97	0.52	70.81	189.75	0.54	492.86	0.77	0.83	34.39
8	White wine	36.83	43.45	0.09	1.75	24.16	159.86	0.48	25.24	87.42	0.70	127.44	0.91	1.01	31.13
9	White wine	11.93	60.61	0.09	0.27	16.57	90.92	0.52	5.44	134.60	0.67	127.19	1.53	0.43	42.48
10	White wine	4.92	58.38	0.07	nd	25.78	141.37	0.54	8.65	227.21	0.80	138.35	1.96	0.58	22.15
11	White wine	10.82	44.23	0.07	nd	10.34	68.46	0.31	11.73	5.96	0.38	132.34	1.29	0.29	70.33
12	Red wine	17.96	121.01	0.20	1.67	35.69	214.97	0.27	26.00	211.09	0.14	424.87	0.45	1.38	243.81
13	Red wine	13.04	73.21	0.08	11.15	68.41	302.19	0.22	34.26	198.82	0.13	302.96	0.74	1.51	224.31
14	Red wine	19.56	103.86	0.09	0.85	113.42	282.05	0.15	10.07	268.16	0.16	407.15	0.39	1.44	296.09
15	Red wine	12.79	88.80	0.04	1.83	71.19	213.17	0.15	18.65	212.56	0.15	288.44	0.39	0.42	83.70
16	Red wine	21.33	74.82	0.08	4.20	47.31	245.88	0.13	1.06	53.46	0.16	345.55	0.22	2.57	189.56
17	Red wine	26.76	83.24	0.24	5.90	35.92	246.55	0.25	4.95	180.13	0.12	335.00	0.30	1.49	26.66

Table 11- Detail of the chemical composition in fermentative aromatic compounds of the 17 wines used in the study.

Nº	Typology	Isobutyl acetate (µg/L)	2-ethyl methyl butyrate (µg/L)	Butyl acetate (µg/L)	Ethyl furoate (µg/L)	Ethyl dihydrocinnamate (µg/L)	Ethyl cinnamate (µg/L)
				FERMENTATIVE GROUP III			
1	White wine	34.70	29.68	10.13	30.45	0.53	1.26
2	White wine	26.35	42.04	3.86	28.05	nd	nd
3	White wine	35.09	25.93	5.04	40.73	0.51	1.39
4	White wine	23.47	37.04	4.56	25.76	0.50	nd
5	White wine	18.37	54.06	4.09	33.16	0.68	2.91
6	White wine	14.61	54.11	4.89	12.11	0.73	nd
7	White wine	32.49	15.58	4.48	8.98	1.69	1.61
8	White wine	19.02	36.91	3.63	20.25	nd	nd
9	White wine	21.51	34.70	3.10	14.89	nd	0.62
10	White wine	23.87	55.76	4.50	30.53	nd	1.35
11	White wine	8.97	31.74	nd	13.10	0.53	0.95
12	Red wine	40.28	47.30	nd	11.21	0.88	1.28
13	Red wine	67.07	30.02	nd	7.61	0.55	1.05
14	Red wine	119.17	71.39	nd	11.26	0.66	0.87
15	Red wine	61.98	13.82	nd	20.72	2.04	1.52
16	Red wine	44.40	89.36	nd	4.69	0.56	0.63
17	Red wine	34.92	62.72	10.43	9.81	1.27	0.67

Table 12. Detail of the chemical composition in fermentative aromatic compounds of the 17 wines used in the study.

Nº	Typology	Guaiacol (µg/L)	4-Ethyl guaiacol (µg/L)	*trans*-Whisky lactone (µg/L)	*Cis* -Whisky lactone (µg/L)	Eugenol (µg/L)	4-Ethylphenol (µg/L)	Benzal dehyde (µg/L)	δ-Octa lactone (µg/L)	o-Cresol (µg/L)	γ-Nona lactone (µg/L)	4-propyl guaiacol (µg/L)	γ-deca lactone (mg/L)	4-vinyl guaiacol (µg/L)	2,6-dimethoxi phenol (µg/L)
AGEING GROUP I															
1	White wine	28.78	0.84	90.19	116.72	15.12	0.48	17.29	1.88	1.29	4.22	nd	5.42	66.94	47.48
2	White wine	6.14	nd	25.70	36.28	5.68	0.34	10.24	0.86	nd	1.88	nd	6.01	15.85	10.15
3	White wine	11.92	0.33	1.56	1.33	5.97	1.00	38.67	0.68	1.13	7.03	nd	9.12	85.13	10.29
4	White wine	6.90	nd	2.94	4.12	1.57	0.32	8.43	1.18	0.52	3.08	nd	7.77	39.44	3.80
5	White wine	10.80	0.37	2.34	nd	1.09	1.18	71.19	3.23	0.57	7.21	nd	7.25	88.42	nd
6	White wine	9.28	nd	2.17	nd	0.89	0.82	14.73	0.70	0.65	3.11	nd	5.01	61.41	4.34
7	White wine	32.36	13.57	57.49	97.26	17.46	8.42	44.83	0.59	2.58	6.88	0.01	6.21	48.90	89.47
8	White wine	10.60	119.45	nd	nd	2.02	101.74	10.43	0.61	0.55	1.93	nd	6.79	30.55	5.29
9	White wine	11.29	0.23	nd	nd	0.74	0.53	44.88	0.81	0.44	4.55	nd	5.31	121.31	3.94
10	White wine	15.05	0.25	1.64	nd	0.83	0.59	53.57	3.77	0.44	12.38	nd	8.02	140.55	8.25
11	White wine	11.38	0.28	nd	3.79	1.03	0.63	25.76	nd	0.48	7.80	nd	4.30	75.68	6.09
12	Red wine	30.80	0.69	87.87	224.59	31.83	2.22	12.76	1.13	1.29	10.62	nd	10.45	20.18	84.00
13	Red wine	44.22	15.52	144.58	183.14	37.55	28.06	70.21	1.12	1.74	6.85	0.03	14.71	29.56	87.13
14	Red wine	41.37	91.50	116.81	147.74	24.92	773.76	29.91	1.10	1.92	23.02	0.04	38.23	50.51	67.25
15	Red wine	16.93	105.38	27.95	52.04	7.70	259.62	44.58	0.57	1.31	9.85	0.01	13.86	22.05	21.21
16	Red wine	16.27	74.29	89.25	127.84	19.84	652.64	8.56	0.70	1.42	18.09	0.08	20.22	145.50	50.67
17	Red wine	41.50	14.06	80.80	114.82	20.43	71.46	10.95	1.13	2.02	12.33	0.01	11.10	74.09	72.33

Table 13. Detail of the chemical composition in aromatic compounds from the ageing phase of the 17 wines used in the study.

Nº	Typology	Isoeugenol II (µg/L)	4-Vinylphenol (µg/L)	4-allyl-2,6-dimethoxiphenol (µg/L)	Methyl vanillate (µg/L)	Ethyl vanillate (µg/L)	Acetovanillone (µg/L)
AGEING GROUP I I							
1	White wine	nd	158.93	13.13	8.53	15.67	41.35
2	White wine	nd	51.28	3.24	7.31	1.51	11.92
3	White wine	nd	230.64	15.70	9.06	18.08	57.27
4	White wine	nd	54.85	3.21	10.72	3.69	17.20
5	White wine	nd	162.44	1.46	97.79	5.36	62.80
6	White wine	nd	94.25	1.58	30.13	15.35	76.06
7	White wine	nd	221.36	30.54	28.78	32.02	70.45
8	White wine	nd	73.20	3.06	2.86	2.98	41.19
9	White wine	nd	201.87	nd	99.94	5.99	52.24
10	White wine	1.60	193.12	1.10	146.15	19.84	64.73
11	White wine	nd	114.27	0.77	97.60	6.49	52.74
12	Red wine	nd	154.35	26.95	10.34	163.19	75.24
13	Red wine	nd	44.15	38.92	62.04	950.58	175.16
14	Red wine	nd	150.29	23.29	60.66	451.68	84.45
15	Red wine	nd	53.05	5.21	85.89	106.43	182.51
16	Red wine	nd	127.17	16.22	25.31	243.49	92.18
17	Red wine	nd	121.19	17.87	44.48	343.05	62.27

Table 14. Detail of the chemical composition in aromatic compounds from the ageing phase of the 17 wines used in the study.

Nº	Typology	2-Methyl-3-furanthiol*	2-Furfurylthiol	4-Mercapto-4-4-methyl-2-2-pentanone	3-Mercapto hexyl acetate	3-Mercaptohexanol	Benzyl mercaptan
		AROMATIC THIOLS GROUP					
1	White wine	340.4	16.6	14.4	13.9	113.5	5.0
2	White wine	154.9	3.8	28.3	12.6	81.1	5.4
3	White wine	465.7	4.1	34.1	10.7	312.8	4.5
4	White wine	148.2	3.8	8.4	2.9	43.5	2.7
5	White wine	587.4	5.8	92.5	4.0	341.4	8.1
6	White wine	370.1	1.2	12.3	3.4	67.6	4.3
7	White wine	427.5	3.4	18.7	5.0	73.4	3.8
8	White wine	241.8	2.0	15.7	4.5	140.8	5.1
9	White wine	257.5	2.2	18.7	2.1	217.3	10.6
10	White wine	432.0	3.0	110.1	2.6	863.7	15.6
11	White wine	199.9	0.9	69.5	3.7	371.0	8.0
12	Red wine	843.5	19.5	75.4	7.4	1,406.8	4.3
13	Red wine	341.5	12.2	20.9	14.1	109.6	11.5
14	Red wine	89.7	5.2	20.7	13.1	76.8	6.7
15	Red wine	88	8.0	17.9	6.9	109.9	5.7
16	Red wine	97.7	2.5	11.4	1.5	102.7	1.7
17	Red wine	234.5	4.1	20.3	4.5	393.4	5.2

Table 15. Detail of the chemical composition in aromatic thiol compounds of the 17 wines used in the study.

Nº	Typology	Guaiacol	4-Methylguaiacol	Phenol	Eugenol	Isoeugenol	4-Alylsyringol	Maltol	Syringol	Furfural	Furfuryl alcohol
GROUP OF VOLATILE COMPOUNDS FROM THE WOOD I											
3	White wine	3.1	nd	nd	4.5	nd	nd	nd	17.5	91.2	69.6
1	White wine	7.9	5.7	nd	11.3	nd	9.7	nd	21.3	959	663
2	White wine	2.3	nd	4.1	nd	nd	nd	nd	7.2	1,871	nd
10	White wine	nd	nd	nd	nd	nd	nd	nd	nd	170	nd
11	White wine	1.9	nd	7.4	nd	nd	nd	nd	nd	1,144	67.5
13	Red wine	nd	16.6	4.1	36.8	nd	32	nd	53.9	294	1,557
16	Red wine	nd	9.1	2.5	17.8	nd	11.2	nd	61.6	78	1,170

Nº	Typology	5-Methylfurfural	5-Hydroxymethylfurfural	Siringaldehyde	*cis*-Whisky lactone	*trans*-Whisky lactone	Vanillin	4-Etihyguaiacol	4-Ethylphenol
GROUP OF VOLATILE COMPOUNDS FROM THE WOOD II									
3	White wine	3	167	13.2	nd	nd	11.9	nd	nd
1	White wine	150	866	194	558	84.6	115	nd	nd
2	White wine	37.6	2,012	22.1	3.8	6.7	68.6	nd	nd
10	White wine	4,5	506	4.6	nd	nd	4.7	nd	nd
11	White wine	23.2	27,802	6	nd	nd	64.4	nd	nd
13	Red wine	38	393	186	26	182	147	16.8	30
16	Red wine	17.7	597	118	77.7	95.5	73	84.9	791

Tables 16 and 17. Detail of the chemical composition in volatile compounds from the wood in 7 of the 17 wines used in the study.

Nº	Typology	Ethyl acetate mg/L	1-Octen3ol µg/L	(+) Fenchona µg/L	(+) Fenchol µg/L	Guaiacol µg/L	2MIB ng/L	Geosmin ng/L	2M35DP ng/L	IPMP ng/L	IBMP ng/L	TCA ng/L	TeCA ng/L	TBA ng/L	PCA ng/L
				GROUP OF COMPOUNDS RESPONSIBLE FOR ORGANOLEPTIC DEFECTS I											
1	White wine	112	2.6	nd	nd	6.7	nd	nd	nd	nd	nd	nd	nd	nd	nd
2	White wine	114	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
3	White wine	94	10	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
4	White wine	108	4.9	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
5	White wine	78	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
6	White wine	99	6.9	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
7	White wine	128	8.5	nd	nd	20	nd	nd	nd	nd	nd	nd	nd	nd	nd
8	White wine	52	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
9	White wine	111	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
10	White wine	88	9.8	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
11	White wine	104	17.4	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
12	Red wine	110	nd	nd	nd	37.1	nd	nd	nd	nd	nd	nd	nd	nd	nd
13	Red wine	98	8,5	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
14	Red wine	118	nd	nd	nd	20	nd	nd	nd	nd	nd	nd	nd	nd	nd
15	Red wine	113	7.2	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
16	Red wine	108	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
17	Red wine	102	16.6	nd	nd	47.6	nd	nd	nd	nd	nd	nd	nd	nd	nd

Table 18. Detail of the chemical composition in compounds associated with organoleptic defects of the 17 wines used in the study.

Nº	Typology	4EF µg/L	4EG µg/L	4VF µg/L	4VG µg/L	Diacetyl mg/L	2-amine acetophenone µg/L	Dimethyl sulfur µg/L	2-ethoxi-3,5-hexadiene µg/L	Styrene µg/L	Indole µg/L
GROUP OF COMPOUNDS RESPONSIBLE FOR ORGANOLEPTIC DEFECTS I I											
1	White wine	nd	7	8	nd	nd	nd	nd	nd	0.3	nd
2	White wine	nd	nd	nd	nd	nd	nd	nd	nd	0.2	nd
3	White wine	nd	nd	217	42	nd	nd	nd	nd	0.3	nd
4	White wine	nd	nd	112	46	nd	nd	nd	nd	0.2	nd
5	White wine	nd	nd	144	58	nd	nd	nd	nd	1.5	nd
6	White wine	nd	nd	97	56	nd	nd	nd	nd	0.2	nd
7	White wine	nd	16	nd	nd	nd	nd	nd	nd	0.3	nd
8	White wine	102	139	nd	nd	nd	nd	nd	nd	0.2	nd
9	White wine	nd	nd	150	71	nd	nd	nd	nd	0.3	nd
10	White wine	nd	nd	150	71	nd	nd	nd	nd	0.2	nd
11	White wine	nd	nd	143	70	nd	nd	nd	nd	1.1	nd
12	Red wine	nd	0	nd	nd	nd	nd	nd	nd	0.3	nd
13	Red wine	26	21	nd	nd	nd	nd	nd	nd	0.3	nd
14	Red wine	997	117	nd	nd	nd	nd	nd	nd	0.3	nd
15	Red wine	254	106	nd	nd	nd	nd	nd	nd	1	nd
16	Red wine	762	90	nd	nd	nd	nd	nd	nd	0.2	nd
17	Red wine	74	23	nd	nd	nd	nd	nd	nd	0.2	nd

Table 19. Detail of the chemical composition in compounds associated with organoleptic defects of the 17 wines used in the study.

Nº	Typology	Methanethiol (µg/L)	Ethanethiol (µg/L)	Dimethyl sulfur (µg/L)	Diethyl sulfur (µg/L)	Methyl thioacetate (µg/L)	Ethyl thioacetate (µg/L)	Dimethyl disulfur (µg/L)	Diethyl disulfur (µg/L)	Dimethyl trisulfur (µg/L)	Benzothyazol (µg/L)
GROUP OF SULFUR COMPOUNDS RESPONSIBLE FOR ORGANOLEPTIC DEFECTS											
1	White wine	nd	nd	26.1	nd	nd	4.1	nd	nd	nd	nd
2	White wine	nd	nd	84.4	nd	nd	4	nd	nd	nd	nd
3	White wine	nd	nd	18.8	nd	nd	3.6	nd	nd	nd	nd
4	White wine	nd	nd	11.1	nd	6.3	5.2	nd	nd	nd	nd
5	White wine	nd	nd	27.4	nd	0	3.4	nd	nd	nd	nd
6	White wine	nd	nd	2.5	nd	4.4	3.8	nd	nd	nd	nd
7	White wine	nd	nd	17	nd	4.1	8.4	nd	nd	nd	nd
8	White wine	nd	nd	7.1	nd	4.8	2.6	nd	nd	nd	nd
9	White wine	nd	nd	27.6	nd	nd	17.9	nd	nd	nd	nd
10	White wine	nd	nd	11.9	nd	3.6	4.2	nd	nd	nd	nd
11	White wine	nd	nd	17.1	nd	10	2.9	nd	nd	nd	nd
12	Red wine	nd	nd	36.5	nd	4.5	5.4	nd	nd	nd	nd
13	Red wine	nd	nd	27.6	nd	9.8	6.3	nd	nd	nd	nd
14	Red wine	nd	nd	37.5	nd	nd	4.1	nd	nd	nd	nd
15	Red wine	nd	nd	14.1	nd	4.4	3.4	nd	nd	nd	nd
16	Red wine	nd	nd	24.5	nd	nd	4.4	nd	nd	nd	nd
17	Red wine	nd	nd	77.9	nd	nd	4.3	nd	nd	nd	nd

Table 20. Detail of the chemical composition in compounds associated with organoleptic defects caused by sulfur compounds of the 17 wines used in the study.

Nº	Typology	Aluminium (mg/L)	Arsenic (mg/L)	Boron (mg/L)	Cadmium (mg/L)	Copper (mg/L)	Iron (mg/L)	Manganese (mg/L)	Nickel (mg/L)	Lead (mg/L)	Zinc (mg/L)
					GRUPO DE METALES I						
1	White wine	0.78	< 0.1	1.88	< 0.01	0.09	0.69	2.24	< 0.1	< 0.05	0.65
2	White wine	0.82	< 0.1	4.23	< 0.01	0.09	0.49	0.37	< 0.1	< 0.05	0.50
3	White wine	1.16	< 0.1	2.61	< 0.01	0.09	1.34	2.10	< 0.1	< 0.05	0.40
4	White wine	0.67	< 0.1	1.59	< 0.01	0.09	0.49	2.13	< 0.1	< 0.05	0.65
5	White wine	1.33	< 0.1	4.45	< 0.01	0.14	0.83	0.67	< 0.1	< 0.05	0.95
6	White wine	0.93	< 0.1	2.35	< 0.01	0.09	0.86	2.86	< 0.1	< 0.05	0.59
7	White wine	1.44	< 0.1	4.58	< 0.01	0.14	1.68	1.42	< 0.1	< 0.05	0.94
8	White wine	0.49	< 0.1	4.30	< 0.01	0.09	0.58	0.48	< 0.1	< 0.05	0.30
9	White wine	2.28	< 0.1	3.70	< 0.01	0.09	1.92	2.53	< 0.1	< 0.05	1.06
10	White wine	0.82	< 0.1	4.50	< 0.01	0.09	0.66	2.03	< 0.1	< 0.05	0.81
11	White wine	3.05	< 0.1	4.04	< 0.01	0.40	1.64	1.34	< 0.1	< 0.05	0.75
12	Red wine	0.49	0.09	3.84	< 0.01	0.09	0.89	1.67	< 0.1	< 0.05	0.27
13	Red wine	0.49	0.09	7.02	< 0.01	0.13	1.32	0.93	< 0.1	< 0.05	0.55
14	Red wine	0.49	0.09	7.34	< 0.01	0.15	0.62	1.58	< 0.1	< 0.05	1.05
15	Red wine	0.76	0.09	4.29	< 0.01	0.15	1.90	0.57	< 0.1	< 0.05	0.61
16	Red wine	0.49	0.09	4.94	< 0.01	0.09	3.12	0.86	< 0.1	< 0.05	0.25
17	Red wine	0.49	0.09	9.92	< 0.01	0.09	1.11	1.36	< 0.1	< 0.05	0.93

Table 21. Detail of the chemical composition in metals of the 17 wines used in the study.

Nº	Typology	Mercury (mg/L)	Calcium (mg/L)	Phosphor (mg/L)	Magnesium (mg/L)	Potassium (mg/L)	Sodium (mg/L)
			GROUP OF METALS II				
1	White wine	< 0.01	74.2	189	88.0	338	22.7
2	White wine	< 0.01	59.3	55.3	54.5	558	12.6
3	White wine	< 0.01	65.9	153	72.4	811	24.5
4	White wine	< 0.01	66.3	107	84.7	419	47.7
5	White wine	< 0.01	96.4	125	84.0	418	14.5
6	White wine	< 0.01	61.6	116	93.8	625	59.5
7	White wine	< 0.01	55.7	214	78.8	893	14.9
8	White wine	< 0.01	61.3	77.0	75.7	487	16.8
9	White wine	< 0.01	141	181	93.9	1,033	21.1
10	White wine	< 0.01	94.1	193	84.1	761	13.7
11	White wine	< 0.01	119	235	89.6	736	16.5
12	Red wine	< 0.01	42.2	130	98.4	893	21.6
13	Red wine	< 0.01	53.8	215	89.6	1,232	9.99
14	Red wine	< 0.01	80.6	226	114	1,181	12.6
15	Red wine	< 0.01	69.9	140	60.3	792	9.99
16	Red wine	< 0.01	57.0	219	106	1,060	17.2
17	Red wine	< 0.01	51.6	197	118	118	42.7

Table 22. Detail of the chemical composition in metals of the 17 wines used in the study.