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Differentiation of white wines by their aromatic index

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Abstract

Wines from four Galician white varieties (Albariño, Loureira, Treixadura and Dona Branca) with 1992 to 1995 vintages have been analysed, in order to obtain their characterisation by the aromatic index. Monoterpenes, higher alcohols, ethyl esters, fatty acids, acetates, volatile phenols and heavy sulphur compounds were analysed by gas chromatography alone and together with mass spectrometry. Flavour compositions were similar for each wine obtained from grapes harvested in different years. Comparisons between odour unit values (OUV) from each wine variety and from these vintages were similar. However, odour profiles of Galician wines from these years were clearly differentiated. A correct differentiation could be achieved between samples elaborated with different varieties, when principal component and linear discriminant analysis were applied to the OUV data.

Keywords: White wine; Aromatic index; Principal component analysis; Linear discriminant analysis

1. Introduction

The wine aroma depends on many factors, environmental and management practices [1], grape varieties [2,3], wine-making techniques [4], yeast [5,6], etc. Aroma and flavour constituents of different grapes and wines have been extensively studied in the last few years. Among the hundreds of compounds identified in grapes and wines [7], terpene alcohols and their derivatives were considered to be a specific constituent of Muscat aroma [8]. Norisoprenoid compounds contribute to the varietal character of Chardonnay wines [9] and methoxypyrazines contribute to Sauvignon and Cabernet-Sauvignon wine aromas [10]. However, the major fermentation alcohols, esters and fatty acids are quantitatively dominant in wine aroma [11,12].

However, the particular importance of each compound on the final aroma depends on the correlation between chemical composition and perception thresholds, because most of the volatile compounds were present at concentrations near or below their individual sensory thresholds.

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Albariño, Loureira, Treixadura and Dona Branca are the typical white varieties from Galicia (northwest Spain) and northern Portugal. Young white wines, dominated by fruity and floral odours, were elaborated in both regions with these grape varieties. The objective of this study was to determine the free classical aromatic content of Albariño, Loureira, Treixadura and Dona Branca wines obtained over four consecutive vintages and to identify the characteristic aromatic profile. In order to investigate the distinction between these monovarietal wines in function of the grape varieties used, principal component analysis (PCA) and linear discriminant analysis (LDA) were used.

2. Experimental

2.1. Wine samples

The vinification of Albariño wines from 'Rías Baixas' Denominación de Origen (DO) (Certified Brand of Origin) wineries and Loureira, Dona Branca and Treixadura wines from micro-vinification was carried out in the same way. The grapes were crushed and destemmed and the Albariño juices were sometimes subjected to maceration for 6–8 h. The grapes were then pressed and racked. Alcoholic fermentation was carried out at 17°C and afterwards malolactic fermentation at 20°C. After fermentation is finished, the wines are stored at −5°C for 10–15 days and then bottled.

2.2. Isolation of volatile compounds

The extraction of volatile compounds from the wine samples adjusted to pH 7 by the addition of NaOH, was performed three times with liquid–liquid extraction using diethyl ether–pentane (1:1, v/v). For quantification, an internal standard (3-octanol, 10 mg l^{-1}) was added to the wine sample. The organic extract was dried and concentrated to 0.5 ml with a low stream of nitrogen prior to analysis by gas chromatography (GC) and GC-MS.

2.3. Gas chromatographic analysis

Higher alcohols, esters, fatty acids, acetates, free terpenes and volatile phenols were analysed by GC. Each wine sample from each vintage was analysed in triplicate. A Varian (Model 3400) chromatograph equipped with a flame ionisation detector was used. A capillary column Carbowax 20M (50 m × 0.25 mm, 0.25 μm) was employed. The operating conditions were the following: injector and detector temperatures, 230°C; column temperature, programmed from 45 to 230°C at 3°C min^{-1} and final isotherm of 25 min; carrier gas pressure (Helium), 12 psi. A 1 μl sample of the extract was injected in splitless mode (30 s).

Heavy sulphurs were analysed by GC in a Hewlett-Packard HP5890-I chromatograph with flame photometric detector (at $\lambda = 393$ nm) [13], under the same capillary column and chromatographic conditions indicated for the other family of mentioned compounds.

A Hewlett-Packard model 5890 Series II hyphenated with a HP 5970b mass spectrometer was used. Three microlitres of the organic extract were injected in splitless mode (purge time, 30 s; purge rate, 70) on a capillary column and the chromatographic conditions were the same as described above, except the total carrier (helium) flow that was 18 psi. The spectrometric conditions were electronic impact (ionisation energy, 70 eV) and source temperature, 250°C. The acquisition was made in scanning mode (mass range, 30–300 amu, 1.9 spectrum s^{-1}). Identification was performed by comparing their retention times with those of authentic compounds.

2.4. Data processing

To evaluate the contribution of a chemical to the aroma of a wine, an aromatic index (expressed as odour unit values, OUV) was calculated as follows

$$\text{OUV} = [\text{Concentration of compound}]/[\text{threshold}].$$

Statistica [14] was used to carry out the PCA and the LDA of the wine samples in order to differentiate each wine variety by its sensorial properties.

3. Results and discussion

The relative sensorial contribution of each substance to the wine aroma was estimated by means of OUV, calculated as the ratio between the concentration in each wine and the perception threshold found in the literature [13,15,16]. This OUV number permits the valuation of the degree of participation of each compound in the final aroma, because some substances provide the agreeable shades, while others could be contributing negatively. A graph with two factors, positive and negative, can be drawn for a determined wine.

Aromatic compounds such as monoterpenes, described as 'floral' [17]; 2-phenyl ethanol, which is described as 'rose-like', 'sweet' and 'perfume-like' [17]; acetates, which have an aromatic description of 'sweet', 'fruity' and 'banana-like' [17] and ethyl esters, with an aromatic description of 'apple-like', 'fruity' and 'sweet' [17] are considered as compounds capable of exerting a positive strong influence on the wine aroma. On the contrary, the higher alcohols, which have an aromatic description of 'alcoholic', 'sweet' and 'choking' [18]; 1-hexanol, described as 'coconut-like', 'harsh' and 'pungent' [17]; vinyl-phenols, which have a characteristic 'meaty smoky odour' [16] and methionol, described as 'boiling cabbage' [13], can contribute negatively to wine aroma.

3.1. Aromatic profile of each wine variety

Odour unit values average data (mean $\pm$ S.D.) from each Galician white wine and from each vintage are summarised in Tables 1–4.

The major positive OUV for Albariño wines (Table 1) is due to the ethyl esters of fatty acids, which are present at levels between 7.70, for the last vintage, and 9.08 units for the first year analysed. Ethyl hexanoate is the most important compound, since it contributes half of this OUV. Ethyl butyrate and octonoate OUV's were the next most significant compounds, as they accounted principally for the other half of this total OUV.

High amounts of acetates were detected in Albariño wines. Isoamyl acetate strongly affects the positive aromatic profile, being present in amounts of about 4.45 units. Hexyl and 2-phenethyl acetates are other acetates present in small amounts and no large differences were found between different vintages.

The Albariño variety was characterised by a higher intensity of floral descriptors [19,20]. Free monoterpenes were responsible for these floral notes and linalool had the highest aroma value (1.30–1.58), followed by geraniol. Versini et al. [19], using PCA, shows a good separation between the Albariño, Loureira and Godello wines with nine free monoterpenols.

Ethyl acetate and lactate and higher alcohols are the most important compounds situated on the opposite side of the OUV graph. The first generally surpasses the ethyl esters in the OUV amount. Their content is higher in 1992 wines and lower in the following year. The higher content of ethyl lactate in Albariño wines, principally in wines from 1992, is due to the typical high malic acid level and a tendency to malolactic fermentation during the wine-making process. 1-Propanol and isoamyl alcohols seem to be the most interesting higher alcohols among those investigated, because their OUV's are 1.23 and 0.71, respectively.

Butyric and isobutyric acids were not identified in Albariño wines. Hexanoic acid is the compound that contributes most to the final OUV, being present in amounts between 0.84, in the 1993 vintage, and a half in first year wine, followed by octonoate and decanoate acids whose contributions were similar to the principal acid.

The relatively large amount of vinyl-phenols in Albariño wines is particularly interesting. The content of 4-vinyl-phenol OUV's being double. Methionol and 1-hexanol exhibit an OUV of close to 0.1 and again should not be considered important in Albariño wines.

Dona Branca wine is the variety that presents the most variation in aromatic composition for the 4 years studied (Table 2). In these samples, free monoterpenols and ethyl esters are the compounds that contribute most to their positive aroma, principally in the 1992 vintage, with 2-phenyl ethanol in the 1993 wines, and corroborate the 'floral' and 'fruity' contribution.

The most aromatic Dona Branca wine, for 1992, presents the highest amounts in linalool, ethyl hexanoate and isoamyl acetate. While, theoretically, the less aromatic wine (1993) had the maximum OUV values for 2-phenyl ethanol and citronellol. Higher alcohols, ethyl acetate, and ethyl lactate are the compounds that may counteract the positive aromatic fraction.

The 1992 wine presents the maximum values for fatty acids, volatile phenols and higher alcohols, and the minimum for the others. Whilst the 1995 wine shows the contrasting values.

The highest amount in positive OUV in Loureira wines (Table 3) is due to the free monoterpenes, which are present at levels of between 4.69 for 1992 and 1.78 for the following year. Linalool being clearly the most abundant followed by geraniol. Ethyl esters, as in the other wines studied, are the next group of compounds which contribute positively to their aroma, with a very constant level from all the years analysed of approximately 2.80, but the principal contributor to this OUV is the ethyl butyrate. The other substances, 2-phenyl ethanol and the three acetates appear at very similar levels for the four

Table 1
Aromatic index[a] and S.D. for Albariño wines from 1992 to 1995 vintages

Compounds	1992		1993		1994		1995	
	OUV	S.D.	OUV	S.D.	OUV	S.D.	OUV	S.D.
Linalool	1.31	0.93	1.30	0.98	1.58	0.25	1.49	0.18
α-Terpineol	0.00	–	0.00	–	0.00	–	0.00	–
Citronellol	0.01	0.00	0.04	0.69	0.04	0.29	0.06	0.16
Nerol	0.03	0.74	0.02	0.51	0.02	0.65	0.02	0.17
Geraniol	0.37	0.85	0.14	0.53	0.24	0.19	0.38	0.28
2-Phenyl ethanol	1.21	0.60	0.99	0.61	1.19	0.12	1.00	0.10
Phenethyl acetate	0.12	8.60×10^{-2}	0.18	4.14×10^{-2}	0.08	2.70×10^{-2}	0.08	3.60×10^{-2}
C_4C_2	2.45	1.60×10^{-2}	3.02	3.40×10^{-2}	2.29	7.60×10^{-2}	2.15	5.20×10^{-2}
C_6C_2	4.21	1.20×10^{-2}	3.82	6.10×10^{-2}	3.51	7.30×10^{-2}	3.79	8.40×10^{-2}
C_8C_2	1.99	2.20×10^{-2}	1.32	3.00×10^{-2}	1.47	1.30×10^{-2}	1.44	1.60×10^{-2}
$C_{10}C_2$	0.41	0.93×10^{-2}	0.30	3.40×10^{-2}	0.33	2.50×10^{-2}	0.29	0.56×10^{-2}
$C_{12}C_2$	0.01	0.84×10^{-2}	0.02	1.00×10^{-2}	0.03	1.90×10^{-2}	0.02	0.38×10^{-2}
Isoamyl acetate	4.27	2.90×10^{-2}	4.83	2.80×10^{-2}	4.26	2.80×10^{-2}	4.44	2.40×10^{-2}
Hexyl acetate	0.19	6.60×10^{-2}	0.17	3.50×10^{-2}	0.15	2.80×10^{-2}	0.15	5.30×10^{-2}
Butyric acid	0.00	–	0.00	–	0.00	–	0.00	–
Isobutyric acid	0.00	–	0.00	–	0.00	–	0.00	–
Hexanoic acid	0.46	2.80×10^{-2}	0.84	2.60×10^{-2}	0.63	1.34×10^{-2}	0.66	1.40×10^{-2}
Octanoic acid	0.26	4.30×10^{-2}	0.53	3.40×10^{-2}	0.35	1.31×10^{-2}	0.35	0.97×10^{-2}
Decanoic acid	0.23	1.30×10^{-2}	0.29	1.60×10^{-2}	0.18	1.10×10^{-2}	0.20	9.30×10^{-2}
Ethyl acetate	9.23	0.85	7.43	0.39	8.11	0.11	7.84	0.19
Ethyl lactate	8.92	3.12	3.54	2.48	4.60	0.23	4.09	0.27
4-Vinyl-guaiacol	0.63	2.48	0.42	2.75	0.36	0.56	0.37	0.43
4-Vinyl-phenol	1.52	3.12	0.68	1.71	0.85	0.62	0.76	1.30
1-Hexanol	0.14	1.90×10^{-2}	0.17	2.10×10^{-2}	0.13	1.30×10^{-2}	0.13	1.70×10^{-2}
Methionol	0.09	5.00	0.10	4.54	0.11	0.75	0.11	1.12
1-Propanol	1.32	0.61	1.31	0.25	1.24	0.14	1.06	0.14
2-Methyl-1-propanol	0.27	0.65	0.25	0.34	0.28	0.10	0.27	0.21
2-Methyl-1-butanol	0.06	0.55	0.05	0.28	0.05	0.19	0.05	0.17
3-Methyl-1-butanol	0.75	0.86	0.72	0.25	0.71	0.20	0.66	0.15

[a] Aromatic index (expressed as OUV) calculated as a relation between the concentration of the substance in the wine and its perception threshold.

Table 2
Aromatic index[a] and S.D. for Dona Branca wines from 1992 to 1995 vintages

Compounds	1992		1993		1994		1995	
	OUV	S.D.	OUV	S.D.	OUV	S.D.	OUV	S.D.
Linalool	1.13	1.15	0.62	1.00	0.93	0.93	0.72	0.46
α-Terpineol	0.00	–	0.00	–	0.00	–	0.00	–
Citronellol	0.00	–	0.09	0.58	0.00	–	0.00	–
Nerol	0.00	–	0.00	–	0.00	–	0.00	–
Geraniol	0.27	1.15	0.10	0.58	0.27	1.15	0.15	1.01
2-Phenyl ethanol	0.51	0.18	1.76	0.90	0.61	0.29	0.51	0.11
2-Phenethyl acetate	0.02	0.01×10^{-2}	0.01	0.40×10^{-2}	0.01	0.51×10^{-2}	0.02	0.21×10^{-2}
C_4C_2	0.88	1.00×10^{-2}	0.60	0.96×10^{-2}	0.63	1.01×10^{-2}	0.52	0.61×10^{-2}
C_6C_2	2.89	1.55×10^{-2}	0.56	0.89×10^{-2}	0.89	1.55×10^{-2}	0.64	0.42×10^{-2}
C_8C_2	0.35	1.00×10^{-2}	0.21	1.39×10^{-2}	0.14	0.42×10^{-2}	0.12	0.50×10^{-2}
$C_{10}C_2$	0.30	0.15×10^{-2}	0.02	0.40×10^{-2}	0.03	0.30×10^{-2}	0.02	0.21×10^{-2}
$C_{12}C_2$	0.01	0.06×10^{-2}	0.00	–	0.00	–	0.00	–
Isoamyl acetate	0.60	1.80×10^{-2}	0.15	4.90×10^{-2}	0.62	2.52×10^{-2}	0.60	1.25×10^{-2}
Hexyl acetate	0.01	0.05×10^{-2}	0.02	1.16×10^{-2}	0.02	1.51×10^{-2}	0.02	0.26×10^{-2}
Butyric acid	0.00	–	0.00	–	0.00	–	0.00	–
Isobutyric acid	0.00	–	0.22	0.14	0.00	–	0.00	–
Hexanoic acid	0.57	1.53×10^{-2}	0.30	7.02×10^{-2}	0.34	3.51×10^{-2}	0.31	2.64×10^{-2}
Octanoic acid	0.43	7.50×10^{-2}	0.17	0.10	0.10	7.50×10^{-2}	0.09	3.05×10^{-2}
Decanoic acid	0.21	4.00×10^{-2}	0.11	0.23	0.08	1.25×10^{-2}	0.07	0.51×10^{-2}
Ethyl acetate	2.03	0.10	2.29	2.00	1.71	1.00	2.60	0.34
Ethyl lactate	0.68	1.50	2.00	1.73	2.05	2.08	1.90	2.52×10^{-2}
4-Vinyl-guaiacol	0.07	2.65	0.39	3.61	0.46	2.52	0.44	8.89
4-Vinyl-phenol	0.83	4.51	0.27	2.52	0.28	3.05	0.31	3.00
1-Hexanol	0.04	0.25×10^{-2}	0.16	3.50×10^{-2}	0.04	1.10×10^{-2}	0.03	1.10×10^{-2}
Methionol	0.26	4.04	0.63	6.66	0.67	5.51	0.66	6.56
1-Propanol	2.48	0.58	1.07	0.58	2.42	0.70	1.86	0.14
2-Methyl-1-propanol	0.23	0.58	0.70	1.00	0.26	0.39	0.29	0.32
2-Methyl-1-butanol	0.04	0.58	0.08	1.00	0.04	0.13	0.04	0.34
3-Methyl-1-butanol	0.46	0.58	0.95	1.00	0.52	0.34	0.55	0.37

[a] Aromatic index (expressed as OUV) calculated as a relation between the concentration of the substance in the wine and its perception threshold.

vintages. Two groups of compounds contribute strongly in the negative part of the Loureira wine aroma. These are ethyl acetate and the higher alcohols, which are presents in mean values of 12 and 3.10 OUV, respectively. The other substances are not present in important amounts and were very similar in the four vintages.

Treixadura wine is characterised by the higher amounts of ethyl esters, 5.17–5.36 OUV (Table 4). As found in the other wine varieties, all the analysed substances present very constant values in all the vintages studied. On the contrary, ethyl acetate, higher alcohols and ethyl lactate are the major OUV's in the negative fraction for this monovarietal wine, with values of 5.1, 3.0 and 2.2 OUV, respectively. The insignificant terpenic aroma in Treixadura wines is due to the absence of monoterpene alcohols such as linalool, citronellol and geraniol, which had the lower perception thresholds.

3.2. Comparison between different wine varieties

Generally, the OUV of each single varietal wine was very similar with relation to the four vintages studied. In order to compare the different Galician white wines, and for a better appreciation of similarities and differences between samples, the OUV mean values of four analysed vintages for each wine variety were calculated. As can be observed in Fig. 1, the profile for each monovarietal wine is sensibly different.

Ethyl esters of fatty acids are the most important components in the positive part for all samples. The variety Albariño followed by Treixadura is the wines that present the highest content, 8.23 and 5.25, respectively. Only in Loureira wines do the monoterpenes surpass esters in OUV value.

The amount of OUV monoterpenols in Albariño and Dona Branca wines is higher than that of Treixadura wines, but lower than that of Loureira wines.

The isoamyl and hexyl acetates (summarised as acetates) are also considered responsible, with the impact flavour compounds, to account for the Albariño wines. Ethyl acetate was the only ester whose concentration was lower in Dona Branca wines and very much higher in Loureira wines, and this compound could strongly affect their aromatic profile. The higher ethyl acetate concentration in Loureira, Treixadura and Albariño wines could be responsible for a loss in fruitiness due to ethyl ester amounts.

The higher alcohol OUV is similar for all wines,

Table 3
Aromatic index[a] and S.D. for Loureira wines from 1992 to 1995 vintages

Compounds	1992		1993		1994		1995	
	OUV	S.D.	OUV	S.D.	OUV	S.D.	OUV	S.D.
Linalool	4.26	0.31	1.60	0.17	2.02	0.18	3.71	0.18
α-Terpineol	0.01	1.82	0.00	–	0.00	–	0.00	–
Citronellol	0.01	0.58	0.12	0.10	0.07	0.24	0.10	0.25
Nerol	0.00	–	0.00	–	0.00	–	0.00	–
Geraniol	0.41	0.91	0.05	0.17	0.07	7×10^{-2}	0.08	0.17
2-Phenyl ethanol	1.01	0.28	0.97	0.22	1.02	0.15	1.07	0.18
2-Phenethyl acetate	0.08	0.50×10^{-2}	0.07	0.57×10^{-2}	0.08	0.30×10^{-2}	0.08	0.25×10^{-2}
C_4C_2	1.77	0.50×10^{-2}	1.85	1.65×10^{-2}	1.82	0.25×10^{-2}	1.74	0.40×10^{-2}
C_6C_2	0.59	0.50×10^{-2}	0.62	0.81×10^{-2}	0.53	0.21×10^{-2}	0.55	0.30×10^{-2}
C_8C_2	0.40	0.30×10^{-2}	0.38	0.50×10^{-2}	0.39	0.15×10^{-2}	0.40	0.43×10^{-2}
$C_{10}C_2$	0.03	0.40×10^{-2}	0.04	0.57×10^{-2}	0.04	0.20×10^{-2}	0.05	0.21×10^{-2}
$C_{12}C_2$	0.00	–	0.00	–	0.00	–	0.00	–
Isoamyl acetate	0.32	0.47×10^{-2}	0.30	0.71×10^{-2}	0.36	0.37×10^{-2}	0.36	0.35×10^{-2}
Hexyl acetate	0.01	0.30×10^{-2}	0.00	–	0.01	0.20×10^{-2}	0.01	0.21×10^{-2}
Butyric acid	0.00	–	0.00	–	0.00	–	0.00	–
Isobutyric acid	0.00	–	0.00	–	0.00	–	0.00	–
Hexanoic acid	0.40	3.51×10^{-2}	0.36	3.00×10^{-2}	0.37	2.00×10^{-2}	0.38	1.53×10^{-2}
Octanoic acid	0.27	3.51×10^{-2}	0.26	5.03×10^{-2}	0.26	1.53×10^{-2}	0.27	2.08×10^{-2}
Decanoic acid	0.15	2.52×10^{-2}	0.16	3.78×10^{-2}	0.16	1.53×10^{-2}	0.14	2.08×10^{-2}
Ethyl acetate	11.22	0.47	11.53	0.20	14.02	0.11	13.77	0.28
Ethyl lactate	0.57	0.33	0.47	0.38	0.50	0.13	0.47	0.20
4-Vinyl-guaiacol	0.22	0.86	0.05	0.64	0.08	0.30	0.10	0.55
4-Vinyl-phenol	0.32	1.76	0.30	0.55	0.30	0.41	0.33	0.36
1-Hexanol	0.22	3.60×10^{-2}	0.23	4.04×10^{-2}	0.22	3.60×10^{-2}	0.21	2.08×10^{-2}
Methionol	0.16	1.50	0.17	1.54	0.16	0.24	0.16	0.53
1-Propanol	2.07	0.95	1.65	0.25	1.96	0.11	1.87	0.10
2-Methyl-1-propanol	0.71	1.00	0.61	0.15	0.66	0.10	0.66	0.11
2-Methyl-1-butanol	0.06	0.21	0.05	0.17	0.06	0.11	0.06	0.14
3-Methyl-1-butanol	0.52	0.85	0.65	0.16	0.52	0.15	0.53	0.17

[a] Aromatic index (expressed as OUV) calculated as a relation between the concentration of the substance in the wine and its perception threshold.

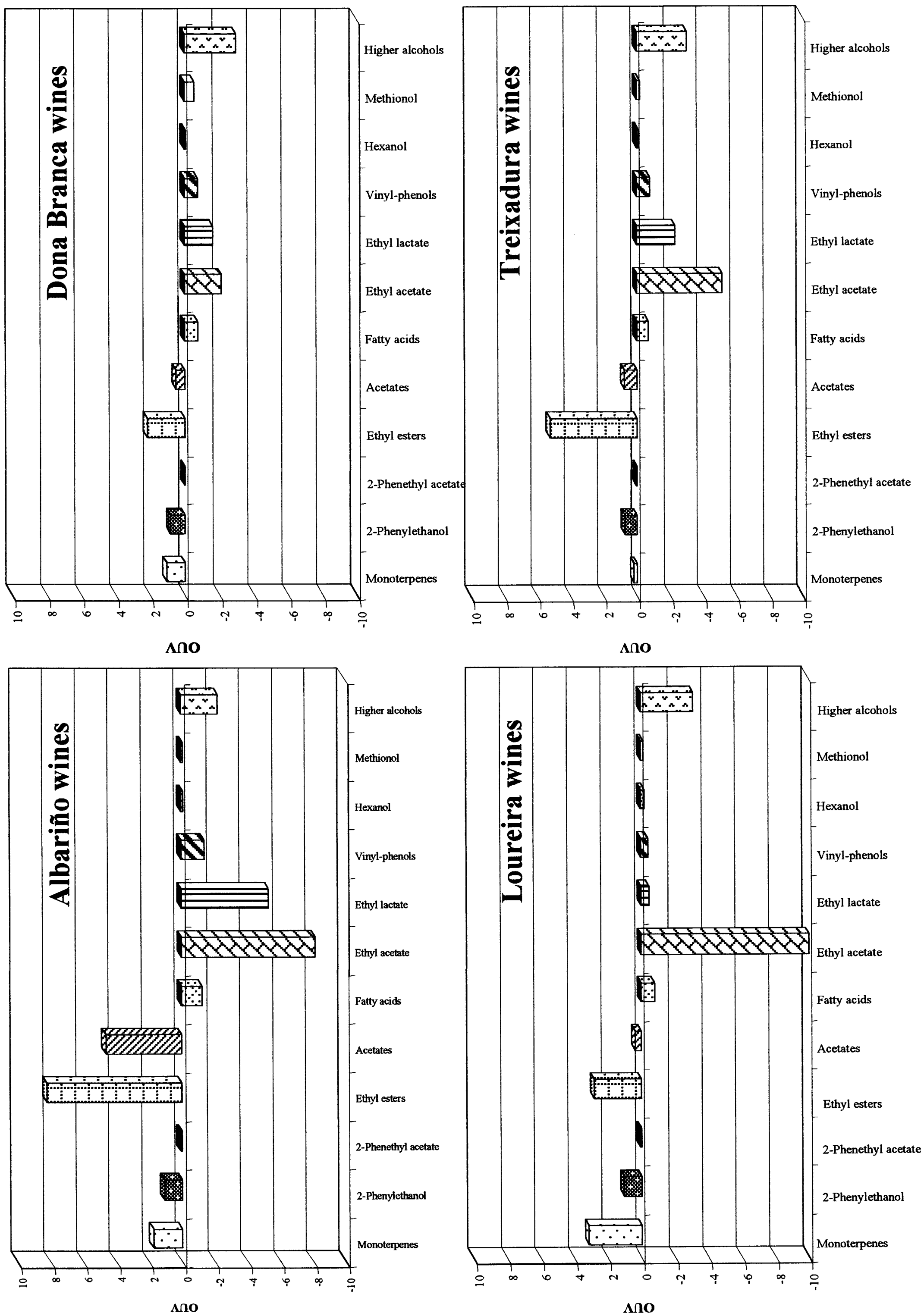

Fig. 1. Mean OUV of Galician wines from 1992 to 1995 vintages.

Table 4
Aromatic index[a] and S.D. for Treixadura wines from 1992 to 1995 vintages

Compounds	1992		1993		1994		1995	
	OUV	S.D.	OUV	S.D.	OUV	S.D.	OUV	S.D.
Linalool	0.10	5.51×10^{-2}	0.10	0.15	0.11	0.49	0.10	0.10
α-Terpineol	0.00	–	0.00	–	0.00	–	0.00	–
Citronellol	0.00	–	0.00	–	0.00	–	0.00	–
Nerol	0.00	–	0.01	0.18	0.01	0.16	0.01	0.10
Geraniol	0.07	0.24	0.10	0.32	0.09	0.27	0.13	0.15
2–Phenyl ethanol	0.82	0.40	0.67	0.10	0.72	0.20	0.75	0.10
2-Phenethyl acetate	0.02	0.50×10^{-2}	0.02	9.20×10^{-2}	0.02	0.25×10^{-2}	0.02	0.38×10^{-2}
C_4C_2	0.84	0.46×10^{-2}	0.88	0.36×10^{-2}	0.81	0.21×10^{-2}	0.76	0.45×10^{-2}
C_6C_2	3.35	0.61×10^{-2}	3.31	0.55×10^{-2}	3.31	0.37×10^{-2}	3.35	0.61×10^{-2}
C_8C_2	1.10	2.52×10^{-2}	1.02	2.14×10^{-2}	0.99	0.26×10^{-2}	1.01	1.22×10^{-2}
$C_{10}C_2$	0.07	0.46×10^{-2}	0.07	0.15×10^{-2}	0.06	0.30×10^{-2}	0.06	0.21×10^{-2}
$C_{12}C_2$	0.00	–	0.00	–	0.00	–	0.00	–
Isoamyl acetate	0.78	0.46×10^{-2}	0.76	0.45×10^{-2}	0.75	0.38×10^{-2}	0.70	0.30×10^{-2}
Hexyl acetate	0.02	0.21×10^{-2}	0.03	0.25×10^{-2}	0.02	0.25×10^{-2}	0.02	0.25×10^{-2}
Butyric acid	0.50	2.52×10^{-2}	0.50	1.53×10^{-2}	0.49	1.53×10^{-2}	0.47	2.64×10^{-2}
Isobutyric acid	0.12	0.30×10^{-2}	0.12	0.30×10^{-2}	0.12	0.68×10^{-2}	0.11	0.35×10^{-2}
Hexanoic acid	0.05	0.10×10^{-2}	0.05	0.25×10^{-2}	0.04	0.35×10^{-2}	0.03	0.43×10^{-2}
Octanoic acid	0.03	0.50×10^{-2}	0.03	0.46×10^{-2}	0.03	0.45×10^{-2}	0.02	0.30×10^{-2}
Decanoic acid	0.01	0.04×10^{-2}	0.01	0.12×10^{-2}	0.01	0.26×10^{-2}	0.01	0.02×10^{-2}
Ethyl acetate	5.08	0.10	5.16	0.11	5.15	0.10	5.16	0.11
Ethyl lactate	2.44	0.74	2.47	0.38	2.14	0.21	2.14	6.66×10^{-2}
4-Vinyl-guaiacol	0.09	0.23	0.10	0.34	0.08	0.12	0.08	0.27
4-Vinyl-phenol	0.66	0.74	0.73	0.45	0.76	0.63	0.80	0.43
1-Hexanol	0.10	1.50×10^{-2}	0.10	2.60×10^{-2}	0.09	2.08×10^{-2}	0.10	1.53×10^{-2}
Methionol	0.17	0.45	0.21	0.35	0.18	0.66	0.19	0.21
1-Propanol	1.98	0.21	2.01	0.16	2.01	0.12	1.92	0.29
2-Methyl-1-propanol	0.29	0.10	0.29	0.24	0.28	0.23	0.29	0.27
2-Methyl-1-butanol	0.06	0.11	0.06	0.15	0.06	0.29	0.07	0.27
3-Methyl-1-butanol	0.70	0.12	0.71	0.23	0.69	0.26	0.66	0.32

[a] Aromatic index (expressed as OUV) calculated as a relation between the concentration of the substance in the wine and its perception threshold.

with the exception of Albariño, which presents lower values. On the contrary, it is the older wines, which show a higher content in vinylphenols.

3.3. Varietal characterisation of wines by means of chemometrical methods

Each sample was assigned a code comprised of one letter, with the exception of Dona Branca wines with two, and two numbers, which indicate respectively the variety name and the vintage year.

The results show that the Galician wines analysed can be well differentiated. PCA confirms this fact. In Fig. 2, the first principal component 'Factor 1' of wine samples is plotted against the second principal component 'Factor 2'. The separations among different categories of wine samples from this 'Factor 1–Factor 2' scatter point plot are obvious. PCA explain 82% of the total variance using the first and second components. Therefore, the simple 'Factor 1–Factor 2' scatter point plot appears to be adequate to distinguish those Galician white wines. The best results are presented with three components. More than 90% of total variance can be explained using the three principal components (PC1, 72%; PC2, 10% and PC3, 9%). The variables that contribute most to the first component are ethyl acetate and ethyl esters. The second factors are ethyl acetate and free monoterpenes. Higher alcohols and 2-phenyl ethanol are the most significant in the third factor. The space defined by the three factors extracted show that a very good separation is obtained between the four different single varietal wines.

In order to find an operative classification role for discriminating the four Galician white wines, supervised-learning pattern recognition techniques must be applied, such as LDA [21–23]. Four categories or classes were predefined: class 1 including Albariño wines, class 2 for Loureira wines, class 3 for Dona Branca wines and class 4 including Treixadura wines. LDA was used again to determine which variables better discriminate between the varieties. Fig. 3 shows the results of the discriminant analysis to which the all OUV values were subjected. The first two discriminant functions (roots), which explains 99.6% of the variability, where can be seen a perfect separation of the four groups involved. The ethyl esters, terpenes, methionol (for root 3), acetates (for roots 1 and 2) and ethyl acetate (for root 3) are the most important variables to characterise the wine samples, according to the variety.

4. Conclusions

Some aromatic compounds were quantified in four types of Galician white wines and their aromatic indexes were calculated based on published data. Data from each type of wine in different vintages had more similarities than differences. Therefore, the aromatic profile (average OUV) varied notably depending on the variety employed.

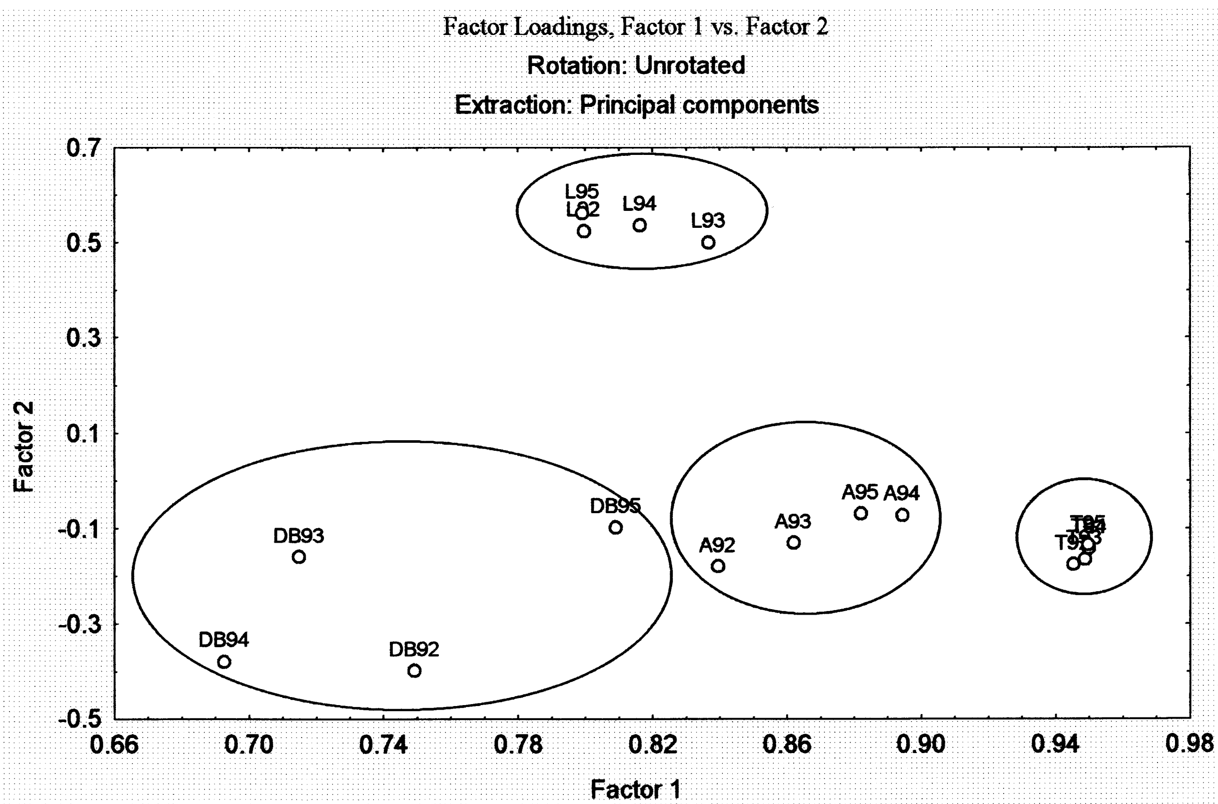

Fig. 2. Plot of the first principal component with respect to the second principal component, using the principal component based on OUV for wine samples. (DB, Dona Branca wines; A, Albariño wines; L, Loureira wines and T, Treixadura wines).

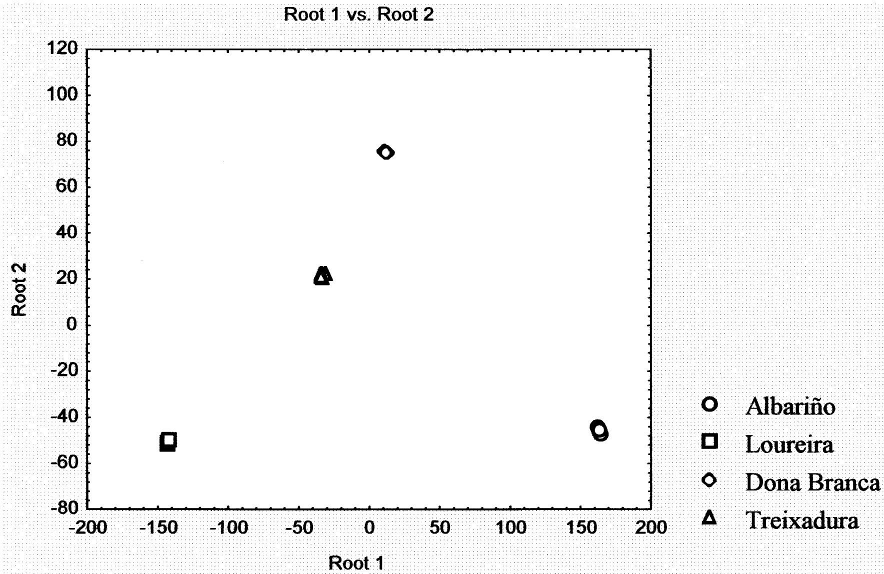

Fig. 3. Discriminant plot for the Albariño, Dona Branca, Loureira and Treixadura wines classification.

Ethyl esters, ethyl acetate and higher alcohols were the most dominant compounds in all of the wines, as they accounted for the largest proportion of the total aroma. Ethyl lactate is another ester present in large amounts that is likely to contribute to the flavour of these Galician white wines.

The high amount of monoterpene OUV in Loureira and Albariño wines could explain the floral aroma and flavour descriptors.

Dona Branca wines are quite different, showing, in general, a minor content of volatile compounds. No large differences in 1-hexanol and methionol were found between these white wines, but higher values of the second are observed in Dona Branca wines.

PCA and LDA corroborate a very clear and good differentiation between the Galician wines analysed. Significant differences in OUV aroma were found among the white wines studied. As shown by chemometrical methods of the OUV ratings, the major differences in aroma among these four varieties could be attributed to the variation in the intensity of fruity and floral attributes, principally due to ethyl esters, acetates, monoterpenes and 2-phenyl ethanol content.

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