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Discrimination and sensory description of beers through data fusion

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ABSTRACT

Beer samples of the same brand and commercialized as a same product, but brewed in four different factories were analyzed with three techniques, an MS e-nose, a mid-IR optical-tongue and a UV–visible, to see if the factories show differences and to find out if the differences found could be attributed to different sensory properties. The data from the three instruments were fused to improve the ability of classification with respect to the individual use of the techniques. Two levels of data fusion were studied: low and mid level fusion, and the classification was performed by linear discriminant analysis (LDA). Mid-level fusion provided better classification results (above 95% correct classification) than those of low-level fusion and also than those obtained when using the individual techniques. Moreover, by means of the score and loading plots obtained by Fisher-LDA, it was possible to interpret the chemical information provided by the three techniques, and we were able to relate the variables associated to each sensor to the main compounds responsible of the sensory perception.

1. Introduction

The great advance of the so-called chemical sensors and their growing applications in food analysis has attracted a considerable research interest in developing alternative techniques or new applications in the field of food sensory analysis. So, mass spectrometry (MS) and spectroscopic techniques, also known as optical sensors, such as near and mid infrared (NIR, MIR), Raman and ultra violet–visible spectroscopy, have been adapted to be used as alternative instruments in food analysis.

The analysis carried out by each instrument provides data from the samples, which can be related to the sensory attributes that allow their characterization if the suitable chemometric techniques are applied. However, the complete characterization of the samples requires the simultaneous use of several techniques that can describe the gustative, olfactive and visual aspects. The compilation of data coming from different sources provides complementary interpretations and facilitates a full product description. The combination of information provided by several analytical instruments is what is called *data fusion*. Data fusion involves treating a large number of multivariate signals of a different nature, and implies the use of chemometric strategies.

One of the first works related to data fusion in food analysis involved the combination of auditive, tactile and olfactive data from a microphone, a force sensor and an electronic nose, respectively, to mimic the human appreciation of potato chips [1]. The authors of this work also proposed to include vision and taste sensors in further studies. Thereafter, some studies have been carried out fusing the data obtained from electronic tongues and noses [2–7]. The first attempt to develop a sensory system to mimic a taste panel was carried out by Rodríguez-Méndez et al. [8]. In this study, the combination of three sensory modalities: an array of gas sensors (e-nose), an array of electrochemical liquid sensors (e-tongue), and an optical system to measure colour by means of CIElab coordinates was successfully used for the discrimination of wines. Similar studies in wines [9–11] and olive oils [12,13] can be found in the literature.

There is a distinction between the levels at which the sensor data can be fused [14]. The most basic, the so-called low-level fusion, consists on building a single data vector with the fused signals from different sensors to form a sort of supra-sensor system [3]. The medium-level fusion consists of extracting features from the signal of each sensor and then fusing them [15]. A basic application is to fuse the first principal components (the ones explaining the maximum variance of the data) of the signals collected from each sensor. Finally, in the high-level fusion [16], multivariate models (e.g. classification models) are built separately for each instrumental technique and, then, the individual classification results are combined to produce the final classification.

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The application of data fusion techniques in sensory studies appears as an important tool for quality control (including authenticity studies) in the food and beverage industries. Many industries are making efforts to obtain a unique product with sensory properties that give the product a mark of identity. Depending on the geographical areas where the raw material is obtained, the production volume and/or the commercial strategies, some brands produce their products in several factories located in different areas. Thus, to maintain the authenticity of their products they have to standardize the mechanisms of production in all factories. However, in practice this is difficult and there is a risk of influencing consumer acceptability.

The quality and authenticity assessment of food products are usually carried out by expert taste panels, who evaluate if the products have the properties that characterize them. However, this sensory analysis is difficult because the taste panels present disadvantages such as sensory saturation and subjectivity, mainly.

For this reason, in this study we applied low- and mid-level data fusion to the data obtained by an MS e-nose, a mid-IR optical-tongue and a UV–visible. The objective was two-fold: to see if the beer samples, of the same brand but brewed in four different factories, showed differences due to their origin, and find the way to interpret these differences based on the instrumental data obtained. Finding differences between beers of the same brand can be important, for instance, to develop strategies for process standardization and fraud control. Although the sensory interpretation of the differences between factories would require the use of a trained sensory panel, the study of the instrumental variables producing the differences may provide useful preliminary chemical information.

The techniques chosen have two advantages: they are faster and cheaper than other analytical techniques, such as gas chromatography or liquid chromatography. The use of data fusion strategies was motivated by the belief that the data coming from three instrumental techniques would improve the performance of the methodology with respect to the data obtained by a single technique. This was already pointed out by [13], who showed that the joint use of an MS e-nose and a near infrared (NIR) and a UV–visible spectrometer provide good classification results in the analysis of olive oils. For data processing, LDA was used to classify the beers and to find relationships between samples and variables. Additionally, the most discriminant variables were selected and a chemical interpretation for that discrimination was discussed.

2. Materials and methods

2.1. Samples

67 different lager beer samples of a same trademark were obtained from four different factories: 11 from factory A, 15 from factory B, 21 from factory C and 20 from factory D. To ensure the representativeness of the samples, the sampling was conducted over six months and, for each of the 67 samples, we took, randomly, 3 bottles of freshly bottled beer.

Prior the analyses of volatiles, the beer samples were degassed by ultrasonication for 15 min. Then, aliquots of 5.0 ml of beer were placed in 10 ml vials with NaCl (2 M). The addition of NaCl is to increase the ionic strength in the beers and thus achieve a reduction in the solubility of dissolved organic volatile compounds. The vials were hermetically capped with PFTE/silicone septum under N_2 atmosphere. All the samples were prepared and analyzed in triplicate (3 bottles of each of the beer samples). For the mid-IR and UV–visible analyses, the beer samples were also degassed by ultrasonication for 15 min to avoid the interference of the high contents of CO_2 of the beers in the spectra. For mid-IR, aliquots of 10.0 ml of beer were analyzed in triplicate. The final data obtained for each sample by the MS e-nose and mid-IR was the average of the triplicates.

2.2. Chemicals and reagents

The standards of the different sugars and acids studied were of analytical grade. D(−)-fructose, D(+)-glucose anhydrous, sucrose and maltose were supplied by Panreac (Barcelona, Spain). 2-Methyl butanoic and butanoic acid were supplied by Aldrich (Madrid, Spain); propanoic, 2-methyl propanoic and 3-methyl butanoic by Fluka (Madrid, Spain) and acetic acid by Sharlab (Barcelona, Spain). Finally the iso-α-acids were supplied by Barth Haas Group (Nuremberg, Germany).

2.3. Instruments

The volatile composition of beers was analyzed with an HS–MS from Hewlett–Packard (Waldbronn, Germany), composed of an HP 7694 static headspace sampler, an HP 6890 gas chromatograph and an HP 5973 quadrupole mass spectrometer with a diffusion pump. The samples were kept at 65 °C for 1 h and under constant stirring in the autosampler. The headspace generated was transferred to the injection port at 90 °C. The injection was made at 250 °C using an inlet of 1.5 mm i.d. An HP-5MS column (30 m × 0.25 mm × 0.25 μm) was used. The oven temperature program was as follows: 70 °C (1 min), 70 °C min^{-1}, and 180 °C (2.5 min). The carrier gas was helium with a flow-rate of 1.6 ml min^{-1}. All these conditions allow the transference of all the compounds to the detector in only 5 min. The mass spectra were recorded by electronic impact (EI) ionization at 70 eV with a temperature of 230 °C in the ion source and 150 °C in the mass quadrupole.

The analyses of the liquid composition were performed in transmission mode with a mid-IR Nexus (Thermo Nicolet, USA) spectrometer, with a DTGS (deuterate triglycine sulfate) detector. The software package OMNIC version 6.2 from Thermo Nicolet was used for spectra acquisition. The spectra, obtained as the average of 32 scans for each sample, were recorded at 4 cm^{-1} resolution, from 400 to 4000 cm^{-1}. Prior to the analysis of the samples, a background scan with distilled water was made.

Finally, the analysis of the colour was carried out with an UV–vis spectrophotometer Thermo Spectronic, Helios γ model (Thermo Electron Corporation, Cambridge, UK). The spectra were recorded at 0.5 nm intervals from 320 to 800 nm. For all measurements, rectangular quartz cells of 1 mm path length were used. The radiation source was a tungsten lamp (visible wavelength range).

All the data analyses were made using the chemometric package PARVUS [17].

2.4. Multivariate analysis

Principal component analysis (*PCA*) was applied to the data obtained by each instrument for a preliminary visualization after low and mid-level fusion strategies were applied. PCA allows visualizing most of the information contained in a data matrix in a few dimensions (called principal components, PCs), which are orthogonal to each other, thus describing complementary information.

Bayesian linear discriminant analysis (*Bayesian-LDA*) was used to discriminate the beer samples according to their factories. It is based on the hypothesis that the data in the classes follow a normal distribution, being their dispersion described by the same covariance matrix and differing only in the position of their centroid. The classification rule is based on linear discriminant scores, which are directly derived from plugging the density of the multivariate normal distribution into the equation for the *a posteriori* probabilities [17]. A sample (object) is classified in the class for which it has

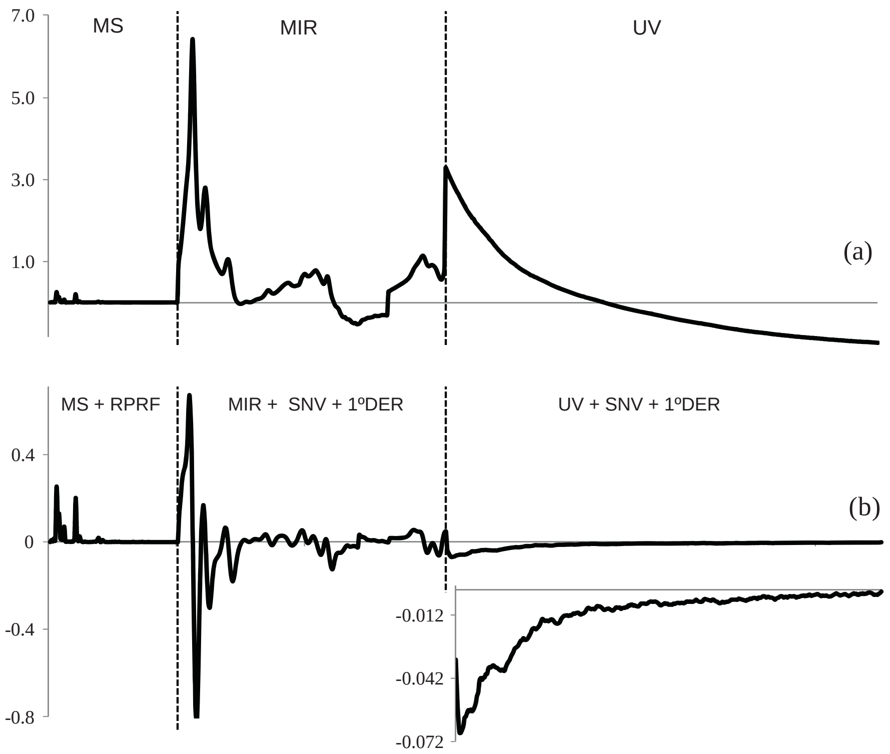

Fig. 1. Representative spectrum of a beer sample, showing the process used to fuse the individual matrices: (a) whole original spectra of the three techniques and (b) final spectra obtained with the pre-processed and transformed signals.

the highest probability. LDA cannot be applied if the number of variables is greater than the number of samples. In such cases, an alternative is to perform a preliminary PCA to the data matrix and then run LDA on the scores of the selected PCs.

Fisher linear discriminant analysis (*Fisher-LDA*) was used to discriminate the beer samples according to their factories and to obtain a visual representation of the data by overlapping the scores and loading plots (bi-plot). Fisher-LDA calculates the canonical variables, that is, the directions with the maximum discriminant power between classes, which are obtained by maximizing the ratio between the between-class variance and the within-class variance, w/p :

$$w = \frac{C}{C-1}\,\frac{\sum_{c=1}^{C} I_c(\overline{d_c}-\overline{d})^2}{I} \tag{1a}$$

$$p = \frac{\sum_{c=1}^{C}\sum_{i=1}^{I_c}(d_{ic}-\overline{d_c})^2}{(I-C)} \tag{1b}$$

$$\overline{d}_c = \sum_{i=1}^{I_c}\frac{d_{ic}}{I_c} \qquad \overline{d} = \sum_{c=1}^{C}\sum_{i=1}^{I_c}\frac{d_{ic}}{I}$$

where C is the number of classes, I is the total number of objects, I_c is the number of objects of class c and d_{ic} is a coordinate where the points are projected.

This means that the distances among centroides of each class must be the longest possible compared to the within-class spread. So, the first canonical variable will be the direction with the maximal w/p ratio.

Additionally, the *Stepwise-LDA* (*SLDA*) [18] algorithm was applied to find the variables (m/z ions, wavenumbers and wavelengths) that best discriminate the factories and to study their chemical origin, which may help in explaining sensory characteristics if these are derived from "sensory compounds". SLDA was applied using the Wilks lambda criterion, which computes the ratio between the determinants of the within-class variance matrix and of the variance matrix for the whole set of samples. The selected variable is the one that produces the largest decrease of this ratio.

The 67 samples analyzed were splitted into a training and a test set. The test set was composed of the 30% of the samples in each factory. So, the training set was formed by 48 samples (8 from factory A, 11 from B, 15 from C and 14 from D) and the test set by 19 (3 from factory A, 4 from B, 6 from C and 6 from D). Moreover, all models were cross-validated, with five cancellation groups. In this process the original set is split in five subsets (or cancellation groups), where a given subset is left out to be used as an evaluation set while the remaining four subsets are used to compute the classification or variable selection rule. The process is executed until each cancellation group is used as an evaluation set (5 times).

2.5. Data pre-treatment

MS e-nose. For the analysis of volatiles the range of m/z used was restricted from 50 to 150 to avoid the ethanol influence ($m/z = 45$ and 46) and because the main compounds that contribute to the beer aroma are fragmented in m/z less than 150. This information was collected in a data matrix of 48×101 (samples (rows) by m/z ratios (columns)) for the training set and 19×101 for the test set. Both training and test sets were normalized with row profile (RPR) to avoid possible signal shifts between injections. This algorithm divides, for a given sample, each m/z abundance by the sum of all m/z abundances for that sample.

mid-IR optical-tongue. The data matrices were initially pre-treated with standard normal variate (SNV) and first-derivative to correct for baseline shifts [19]. The first-derivative of the spectra was taken using the Savitzky and Golay method [20] with second-order smoothing polynomials through seven points. The MIR spectra were collected in a matrix of 48×210 (samples by wavenumbers) for the training set and 19×210 for the test

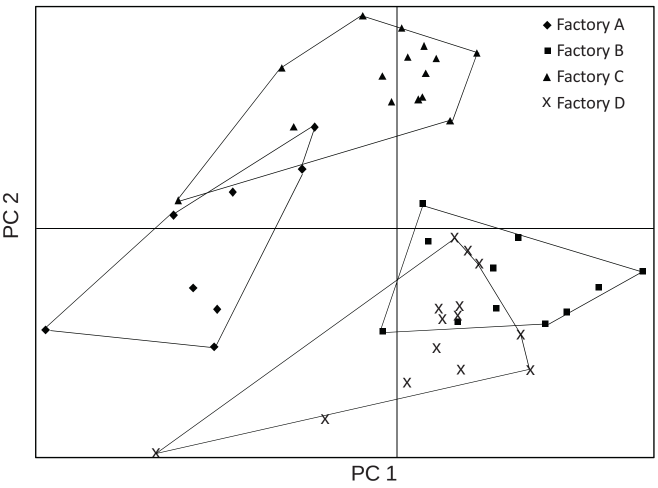

Fig. 2. PCA performed with the fused matrix using the low-level fusion strategy (PC1: 19% and PC2: 15%).

set, in the ranges 1002–1542, 1720–1808 and 2800–2966 cm^{-1}. The region between 1546 and 1716 cm^{-1} contains strong water absorption bands and the one between 1812 and 2796 cm^{-1} is a non-informative absorption region. These regions were deleted before pre-processing.

UV–vis e-eye. The spectral region considered for the colour analysis was 380–550 nm. The matrix obtained had dimensions 48 × 341 (samples by wavelengths) for the training set and 19 × 341 for the test set. Both training and test sets were initially pre-treated with standard normal variate (SNV) and, as in mid-IR, the first derivative was performed to the spectra.

3. Results and discussion

3.1. Low-level fusion

In the low-level fusion approach, the individual spectra obtained from the three techniques were fused in a single matrix of 48 samples (training set) by 652 variables (see Fig. 1). After that, data were autoscaled to compensate for the scale differences and a PCA was carried out on the whole dataset.

The PCA score plot (Fig. 2) shows a different trend of the samples of factory A along the first PC compared to the others factories. The second PC shows a difference between the samples of factories B and D and the ones of factory C. As it can be seen, the samples of each factory, although not totally separated, are located in different regions of the plot, with the exception of B and D that partially overlap.

To check if the beers of the four factories could be discriminated and to analyze the contribution of each technique to this discrimination, Fisher-LDA was applied. As Fisher-LDA cannot work with a large number of variables, PCA was applied to the data and Fisher-LDA was computed with the first seven PCs (65% of explained variance). Seven PCs were enough in this particular case to discriminate between factories using Bayesian LDA. Other LDA models were built with 10 and 15 PCs (73 and 82% of explained variance respectively); however, the classification results were not better than with 7 PCs.

Fig. 3 shows the projections of the sample beers (training and test sets) on the two first canonical variables (CVs), computed by Fisher-LDA and using the seven PCs of the fused matrix. All factories are well discriminated: factories A and B by the first CV and factories C and D by the second CV.

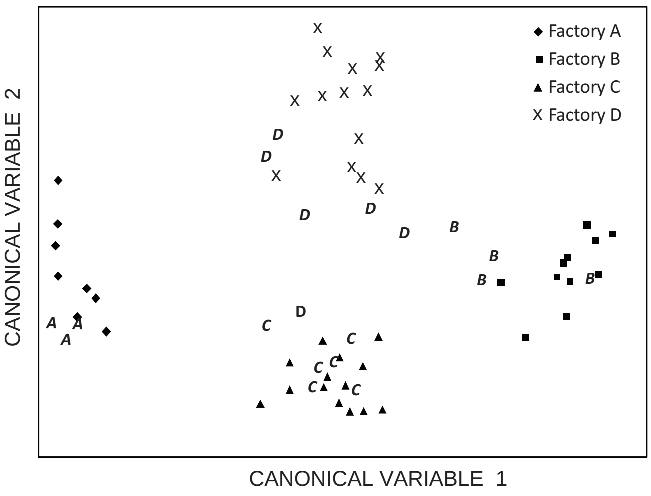

Fig. 3. Score plot of the Fisher-LDA, where the discrimination between the samples of the different factories can be observed. The test set samples are represented by the letters A–D.

Fig. 3 does not show what variables are responsible for the discrimination, what would facilitate a sensory interpretation. In order to get this information, SLDA using the Wilks lambda criterion [18] was applied for variable selection. To ensure robust selection of the most discriminative variables, different cross validation sets were tested when SLDA was applied. Finally, only six variables were found to be the most discriminant according to the Wilks lambda decrease order. The variables considered to perform the Fisher-LDA were: m/z 55 (e-nose); 1068, 1134, 1176 and 1538 cm^{-1} (optical-tongue); and 391 nm (e-eye). The first selected variable the 1538 cm^{-1} wavenumber, was obtained by maximizing the ratio between the total sum of squares and the within-class sum of squares.

Fig. 4 shows the biplot (samples and variables) of the Fisher-LDA using the selected variables. The explained variance is 51% for CV1 and 13% for CV2. It can be seen that the four factories are also discriminated.

Once we obtained the selected variables, the next step was trying to relate them to the absorptions and/or fragmentations of important components in beers in order to extract chemical information related to the differences between samples. All the relations spectral variable – sensory characteristic presented in this study are

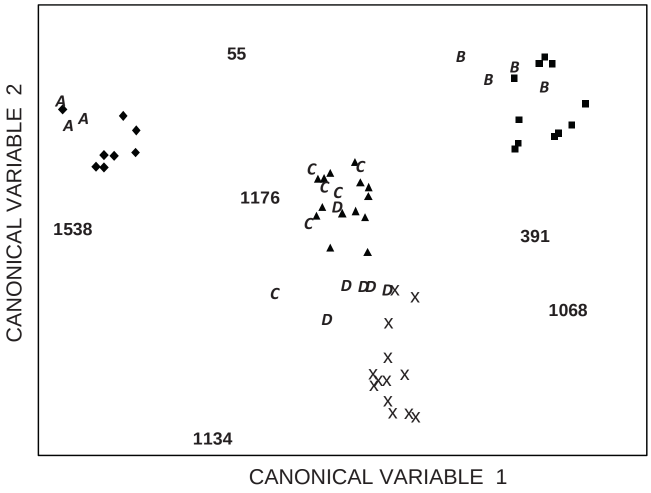

Fig. 4. Fisher-LDA biplot showing the 6 selected variables and the distribution of the beers.

Table 1

Main responsible compounds of taste in beers and their absorption peaks in the infrared region. The spectral regions with the highest absorption for each compound (main absorption range) were obtained from mid-IR measurements. The absorbance of octanoic, lactic, pyruvic and succinic acids and the concentrations of all compounds were obtained from Ref. [23].

Taste	Compound	mg L^{-1}	Main absorption range	Main peaks
Sweetness	Glucose	40–1100	1026–1041; 1068–1110	1033; 1080; 1106
	Maltose	700–3000	1026–1068; 1137–1157	1033; 1056; 1110
	Fructose	0–190	1056–1072	1064; 1149
	Sucrose	0–3300	995–1010; 1049–1068; 1130–1145	1002; 1056; 1137
Sourness	Propanoic	1–5	1211–1242; 1704–1735	1230; 1724
	2-Methyl butanoic	0.1–0.5	1211–1242; 1693–1728	1230; 1708
	Acetic	30–200	1249–1311; 1689–1731	1280; 1708
	Butanoic	0.5–1.5	1199–1222; 1701–1728	1211; 1712
	2-Methyl propanoic	0.1–2	1203–1242; 1697–1728	1222; 1708
	3-Methyl butanoic	0.1–2	1207–1230; 1697–1724	1218; 1708
	Octanoic	2–12	1200–1310; 1675–1750	1711
	Lactic	20–80	1000–1500; 1650–1770	1128; 1220; 1732
	Pyruvic	15–150	1340–1360; 1710–1800	1348; 1726; 1790
	Succinic	16–140	1180–1220; 1650–1750	1204; 1696
Bitterness	Iso-α-acids	10–100	1400–1473; 1510–1608	1431; 1542

only interpretations based on typical absorptions of compounds involved in the sensory activity of the beers, and not a definitive affirmation. For a more complete characterization the evaluation performed by a taste panel would be needed.

The important m/z ions considered by the individual use of MS e-nose related to the main olfactive volatile compounds were presented in a previous study [21]. This study clearly showed a relationship between the samples from factories A and D with alcohols (m/z 55 and 56) and esters (m/z 71, 74, 87, 99, 102 and 104) respectively.

To determine and associate the absorption wavenumbers in mid-IR to the taste substances, we prepared 1 g L^{-1} of four sugars (glucose, maltose, fructose and sucrose), 0.1 g L^{-1} of six acids (propanoic, 2-methyl butanoic, acetic, butanoic, 2-methyl propanoic and 3-methyl butanoic) and 0.1 g L^{-1} of a mixture of six iso-α-acids (related to bitterness) in aqueous solutions with 5% of ethanol. Then, these solutions were analyzed by mid-IR under the same conditions as the beer samples. The absorption wavelength ranges of each compound, together with the wavelength corresponding to the main peaks, are shown in Table 1.

The first selected variable (1538 cm^{-1} in the MIR spectrum), is an absorption in the region of the iso-α-acids, compounds directly related to the bitterness sensation. This variable is close to the cluster of samples of factory A (Fig. 4). Another variable close to samples of factory A is the 55 m/z ion, which is characteristic of volatile alcohols such as 3-methyl 1-butanol and 1-pentanol, among others [21]. Close to factory C, the variable 1176 cm^{-1} lies in the absorption region of fructose [22], which provides sweetness to beers. The MIR variable 1134 cm^{-1} has a high value of Wilks lambda decrease, which means that it is a key variable to discriminate the factories. This is important in factory C in the second CV. This absorption is typical of sucrose, an important carbohydrate related to the sweetness of beers [23].

Finally, as it can also be seen in Fig. 4, there are two variables very related to factory B in the first PC: the MIR wavenumber 1068 cm^{-1} and the UV–vis wavelength 391 nm. The first coincides with an important absorption of fructose, but also of sucrose, glucose and maltose, so it may be related to the sweetness of the samples. The 390 nm wavelength is an absorption of the violet colour whose sensory perception is the yellow-green colour [24] and this belongs to the typical range of absorbance of flavonols [25], a common type of phenols in beers [26], which are yellow pigments [27].

Taking into account that the information contained in the fused spectra comes from analytical tools that register absorptions or abundances of specific compounds related to sensory attributes, the variables selected could be preliminarily interpreted as somewhat related to those attributes that highlight the differences between the samples. However, as stated above, to corroborate these interpretations and execute a complete validation, a further study, involving a sensory panel, is needed.

3.2. Mid-level fusion

This second fusion strategy consists on fusing the principal components obtained individually for each original data matrix (instrumental technique). Unlike low-level fusion, feature reduction is performed here on the principal components. However, these principal components contain relevant information from all the original variables. Different pre-treatment were performed to the matrices prior to PCA. The MS matrix was centred, and SNV and first-derivative were applied to the MIR and UV–visible spectra. The final training fused matrix was built with those PCs obtained from the data of each technique that produced the highest discrimination between factories (based on Fisher weight values). PC1 and PC2 (97% of explained variance) were used in the MS matrix, the first four PCs (96% of explained variance) in the MIR matrix and the first PC (62% explained variance) in the UV–visible matrix, to obtain a final fused matrix of scores of 48 samples by 7 variables (PCs). The test set matrix was also pre-processed like the training set. However, the final score matrix was calculated by projecting the (pre-processed) test set matrix on the loading matrix obtained from the training set, according to Eqs. (2a) and (2b):

$$\mathbf{X}_{TR} = \mathbf{T}_{TR} \cdot \mathbf{P}'_{TR} \tag{2a}$$

$$\mathbf{T}_{TEST} = \mathbf{X}_{TEST} \cdot \mathbf{P}_{TR} \tag{2b}$$

where $\mathbf{X}$ is the original matrix (training or test), $\mathbf{T}$ is the score matrix (training or test) and $\mathbf{P}_{\mathrm{TR}}$ is the loading matrix obtained from the PCA on the training set.

Fig. 5 shows the PCA score plot of the training set data. As it can be seen, the samples from factories C and D overlap in both first and second PC (this overlaping is not observed in Fig. 2) and the samples from factories A and B are well separated by the second PC.

Fig. 6 shows the Fisher-LDA model obtained with the fused matrix of scores of the training set (48 × 7), and where the samples of the test set (19 × 7) have also been projected. This figure is similar to Fig. 3, especially in the first canonical variable, where factories A and B are discriminated. Factories C and D are also discriminated in the second CV. The first PCs of the MS and MIR matrices (MSPC1 and MIRPC2), which explain a 93% and a 62% of variance respectively, are highly related in the first canonical variable to factory B, and seem to indicate the important influence of the aroma (volatile compounds) and the taste in the differentiation of this factory from

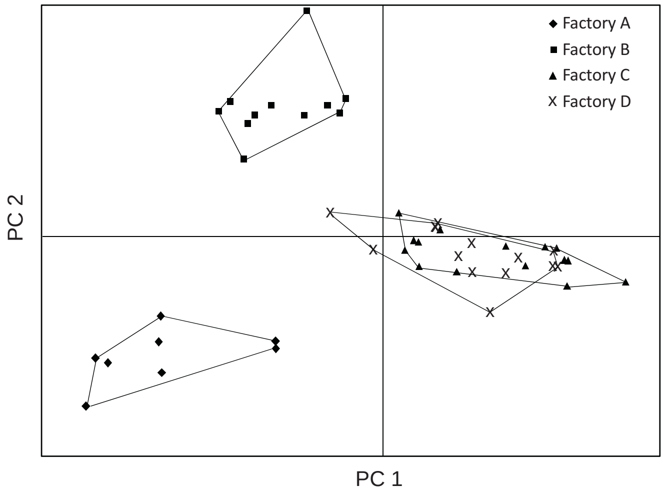

Fig. 5. Score plot of the PCA obtained from the fused matrix using the mid-level fusion strategy (PC1: 21% and PC2: 20%).

the rest. On the other hand, the information of the colour, contained in UVPC1, is highly related to factory C and it is an indication of the importance of the colour in the characterization of these samples.

The discussion above, based on Fig. 6, refers only to the importance of the information provided by each technique in the discrimination of the beers analyzed, and not to a quantitative interpretation of the olfactive, gustative and visual information. This would mean knowing, *a priori*, what sensory properties (olfactory, gustatory, or visual) are the ones that allow a better description and characterization of the beers grouped according to its factory of origin.

3.3. *Data fusion vs individual sensors*

In the last part of this study, we tried to determine what strategy (individual sensors, low-level fusion or mid-level fusion) provides the highest ability of classification of the beer samples into their brewery of origin. For this purpose, we applied PCA-LDA to each data matrix using all variables. Table 2 shows the results, in percentage of classification, after using the MS e-nose, the mid-IR optical-tongue or the UV–vis e-eye individually, and also after applying the two levels of data fusion.

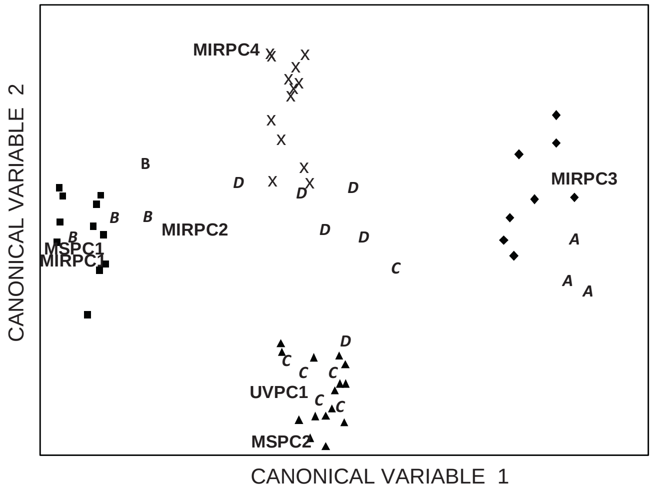

Fig. 6. Fisher-LDA biplot of the first two canonical variables. The legend refers to the spectral nature of the variable (MS, MIR and UV) and the PC number.

Table 2
Results of PCA-LDA applied to the data obtained by the single instruments and also to the fused data. The percentage values of correct classification (% class) correspond to the values of the test sets.

Class	Assigned to class				% class
	A	B	C	D	
Single instruments					
MS e-nose					
A	3	0	0	0	100
B	0	4	0	0	100
C	0	0	4	2	66.7
D	1	0	1	4	66.7
Mid-IR optical-tongue					
A	3	0	0	0	100
B	0	4	0	0	100
C	0	0	5	1	83.3
D	0	0	0	6	100
UV–vis e-eye					
A	2	0	1	0	66.67
B	0	3	0	1	75.0
C	0	0	6	0	100
D	3	2	0	1	16.7

Class	Assigned to class				% class
	A	B	C	D	
Data fusion					
Low-level fusion					
A	3	0	0	0	100
B	0	4	0	0	100
C	0	0	6	0	100
D	0	0	1	5	83.3
Mid-level fusion					
A	3	0	0	0	100
B	0	4	0	0	100
C	0	0	6	0	100
D	0	0	2	4	66.7

Fusing the data allows, in many cases, improving the classification results. The percentage of correct classification in low and mid level fusion is higher compared to the results obtained by each individual technique, with the exception of factory D.

Although the results from each single instrument, mainly from the MS e-nose or from the mid-IR optical-tongue, show a good classification of the samples, it has to be said that data fusion seems to improve the classification results, providing a more complete information on a single super-score matrix.

Low level fusion classifies correctly factories A, B and C (Table 2). In the factory D there is a sample that is missclassified as belonging to factory C. This can be caused by the influence of the UV–visible spectra, which show a poor classification for factory D.

In the case of mid-level fusion it is more evident the possible influence of UV–visible spectra in factories C and D. When using the single matrix of UV–visible spectra all the samples from factory C are correctly classified, whereas most of samples from factory D are misclassified. This tendency can also be seen for mid-level fusion (Table 2 and Fig. 6), where both factories are correlated to UVPC1 in the first canonical variable.

Data fusion allows obtaining additional information with respect to the one obtained from the single techniques. This information enables the interpretation of gustative, olfactive and/or visual trends of a given factory, which is done by associating the absorption/fragmentation patterns of molecules related to the flavour (low-level) or the most representative PCs of each individual technique (mid-level) to a class of beers.

4. Conclusions

Two levels of data fusion have been applied to spectral measurements obtained when analysing beers of the same brand and type but produced in different factories, by using an MS e-nose, a mid-IR optical-tongue and a UV–visible spectrophotometer. Bayesian and Fisher-LDA were used to classify the samples according to the factory of origin and to provide chemical information about those more discriminant variables in the classification of the factories. With the low-level fusion strategy, it was possible to obtain direct chemical interpretation of the differences between factories by comparing the selected variables with the responses given by important chemical compound related to the sensory perception. With the mid-level fusion, the importance of the information provided by each technique in the discrimination of the samples could be established.

The influence of using individual or fused matrices in the classification was discussed. Data fusion (low and mid level fusion) provided a better classification.

This work intends to be a preliminary study of the potential of the data fusion methodology and represents a starting point for future research that involves studies aimed at developing an electronic taster. However, to perform a complete study and validate the sensory interpretations, is necessary the information provided by a tasting panel or by consumers.

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