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Multivariate Analysis of NMR and FTIR Data as a Potential Tool for the Quality Control of Beer

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In this work, principal component analysis (PCA) is applied to the FTIR-ATR and the ^{1}H NMR spectra of 50 beers differing in label and type (ale, lager, alcohol-free), to identify the spectral parameters that may provide rapid information about factors affecting beer production. PCA of FTIR data resulted in the separation of beers mainly according to their alcoholic content, providing little information on components other than ethanol contributing to the variability within the samples. PCA of ^{1}H NMR spectra, performed on the region where major beer components resonate (3.0−6.0 ppm), resulted in the separation of samples into four groups: two groups characterized by the predominance of dextrins, one group of alcohol-free beers characterized by the predominance of maltose, and one group where glucose was found to predominate. By performing PCA on aliphatic and aromatic regions, the contribution of minor components was highlighted. In particular, most ales, lagers, and alcohol-free samples could be distinguished based on their aromatic composition, thus reflecting the high sensitivity of the low-field NMR region toward different types of beer fermentation.

KEYWORDS: Beer; spectroscopy; NMR; FTIR; chemometrics; PCA

INTRODUCTION

The detailed study of beer composition and quality attributes is of paramount importance to accomplish efficient quality control and improved properties such as extended shelf life. High-resolution NMR and hyphenated NMR methods may give a valuable contribution to that study, as shown by recent work (*1*−*3*). In addition, it is important to develop methods which can provide rapid information about factors such as beer geographical origin, processing conditions, and reproducibility within different brewing sites. To accomplish this task, multivariate analysis of spectroscopic data is a possible strategy. Spectroscopic NMR methods provide information on a wide range of compounds present in the food matrix in a single experiment, offering advantages in terms of simplicity of sample preparation and rapidity of analysis. The speed with which NMR spectra can be obtained, often under automation, enables examination of many samples. Because the richness of information often results in high spectral complexity, it calls for the use of multivariate analysis to study large numbers of spectra and extract meaningful information. The application of chemometrics to high-resolution NMR data has been applied in some instances to address different issues of food authenticity and origin. For example, promising results have been obtained concerning the classification of apple juices according to variety (*4*), the detection of adulterations in orange juice (*5*, *6*), the discrimination of coffee samples differing in their manufacturing process (*7*), the differentiation of olive oil according to cultivar, botanical and geographical origin (*8*−*11*), and the characterization of wine geographical origin (*12*−*14*). Compared to NMR, FTIR-ATR spectroscopy represents a cheaper, simpler, and faster way of obtaining compositional information on food samples, and indeed, the usefulness of this technique in tandem with chemometrics has also been demonstrated for several foods, namely fruit products (*15*−*18*), coffee (*19*, *20*), wine (*21*), and meat (*22*), to tackle authentication and adulteration problems.

In this work, principal component analysis (PCA) is applied for the first time to our knowledge to the FTIR-ATR spectra and to the high resolution ^{1}H NMR spectra of a set of fifty beers, to find out if the spectral profile of beer may be consistently correlated with specific compositional properties and/or sample type/origin. These beers have been produced in different countries and belong to different types (ale, lager, and alcohol-free), which basically differ on the corresponding fermentation conditions. Ales are brewed with top-fermenting yeasts at close to room temperatures over some days, whereas lagers undergo longer and cooler fermentation and tend to be less alcoholic than ales. The alcohol-free beers constitute a special type, and may be produced in different ways, such as throttling of fermentation and use of special yeasts, reduction of the stemwort content, and elimination of the alcohol formed (distillation, ultracentrifugation) (*23*).

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Table 1. Some Characteristics of the Beers Analyzed

sample no.	origin	type	% alcohol	pH
1	Portugal	lager	5.2	4.38
2	Portugal	lager	5.1	3.92
3	Portugal	lager	5.2	4.42
4	Ireland	ale	4.2	4.15
5	Portugal	lager	5.1	3.95
6	Portugal	alcohol-free	< 0.5	4.28
7	Portugal	alcohol-free	< 0.5	4.58
8	Portugal	lager	5.8	4.32
9	Portugal	lager	5.1	4.06
10	Belgium	lager	4.9	4.01
11	Portugal	lager	4.3	4.01
12	Portugal	lager	5.0	4.28
13	Portugal	lager	4.2	4.40
14	Spain	lager	5.0	4.00
15	Portugal	lager	5.4	4.52
16	Belgium	lager	4.6	4.14
17	Belgium	ale	6.5	4.32
18	Portugal	lager	5.1	4.00
19	unknown	lager	4.8	4.12
20	Germany	lager	4.8	4.12
21	Germany	unknown	4.8	4.49
22	Belgium	ale	8.5	4.23
23	Belgium	ale	9.0	4.33
24	Belgium	ale	8.0	4.28
25	England	unknown	5.0	3.86
26	England	lager	4.7	4.02
27	England	lager	5.0	4.11
28	Scotland	ale	6.0	3.91
29	Germany	unknown	4.8	4.35
30	Germany	ale	5.0	4.24
31	Germany	ale	5.0	3.97
32	Germany	ale	5.0	4.08
33	Belgium	ale	9.0	4.24
34	Belgium	ale	8.1	4.15
35	Belgium	ale	6.6	4.14
36	Belgium	ale	6.5	4.02
37	Belgium	lager	5.2	4.14
38	Germany	lager	5.0	4.14
39	Holland	lager	5.0	4.24
40	Holland	alcohol-free	< 0.5	4.05
41	Spain	lager	5.4	4.16
42[a]	Holland	alcohol-free	< 0.5	4.22
43	Holland	lager	5.0	4.01
44	Holland	lager	5.4	4.27
45	Portugal	ale	7.2	4.52
46	England	ale	4.7	3.96
47	Germany	ale	4.9	4.01
48	U.S.A.	lager	4.2	3.76
49	England	ale	4.0	4.07
50[b]	Germany	lager	unknown	unknown

[a] Analyzed by FTIR only. [b] Analyzed by NMR only.

MATERIALS AND METHODS

Samples. A set of 50 beers, either produced in Portugal or imported from different countries, was obtained commercially. Some of their characteristics are given in **Table 1**, namely country of origin, type (ale, lager, alcohol-free), alcohol content, and pH. For FTIR measurements, sample preparation consisted simply of degassing the beers in an ultrasonic bath for 10 min. For NMR measurements, beer samples were degassed in the same way and prepared to contain 10% D_2O (internal lock) and 0.02% sodium 3-(trimethylsilyl) tetradeuteropropionate (TSP-d_4) as chemical shift reference.

Spectroscopic Measurements. FTIR spectra were collected on a Bruker IFS55 FTIR spectrometer. A single reflectance horizontal ATR cell (Golden Gate, equipped with a diamond crystal) was used. The data were recorded at 20 ± 1 °C, in the spectral range of 4000−700 cm^{-1}, by accumulating 256 scans with a resolution of 4 cm^{-1}. For each sample, a total of five spectra (replica) were recorded. Between determinations, the crystal was carefully cleaned with water, and to avoid memory effects, the replica spectra were recorded randomly (i.e., intermingled with the spectra of other samples). The spectra were converted into JCAMP format and transferred to a PC workstation for statistical analysis.

The ^{1}H 1D NMR spectra were recorded at 27 °C on a Bruker Avance DRX-600 spectrometer, operating at 599.87 MHz for proton, using the NOESYPR1DSP pulse sequence: RD-90°−t_1−90°−t_m−90°−acquire FID (Bruker library), where RD is the relaxation delay (8.0 s), t_1 represents the first increment in a NOESY experiment (3 μs), and t_m is the mixing period (100 ms). Suppression of the water and ethanol signals was achieved by applying a modulated shaped pulse for 1.6 s of the relaxation delay and the mixing time. Transients ($n = 128$) were collected into 32 768 data points with a spectral width of 8389.26 Hz and an acquisition time of 1.95 s. The spectrometer was equipped with an auto sampler, and the data were acquired under an automation procedure that included temperature stabilization (5 min), automatic tuning and shimming, calculation of the shaped pulse for triple suppression, and acquisition, requiring approximately 30 min per sample. The FIDs were Fourier transformed (with 0.3 Hz line-broadening unless otherwise stated) and the spectra phased, baseline corrected, and calibrated by the TSP signal at 0.0 ppm. The resulting spectra were converted into JCAMP format and transferred to a PC workstation for statistical analysis.

Multivariate Analysis. For PCA of FTIR spectra, the region between 1200 and 800 cm^{-1} was selected, and each spectrum was autoscaled (mean centered and standardized). For PCA of NMR spectra, data matrixes corresponding to different spectral regions were built, excluding the segments containing water and ethanol resonances (at 4.77 ppm and at 1.17 and 3.65 ppm, respectively) to eliminate the variation in these signals suppression. The spectral regions considered were (a) aliphatic region (0.5−3.0 ppm), (b) sugar region (3.0−6.0 ppm), and (c) aromatic region (6.0−10.0 ppm). Each spectral region was normalized by adjusting the total area to unity. The calculations were performed using the program co-developed in the University of Aveiro and the Institut National Agronomique Paris-Grignon (*24*).

RESULTS AND DISCUSSION

PCA of FTIR-ATR Spectra. Figure 1A shows the FTIR spectra of four beers in the region selected for PCA (1200−800 cm^{-1}) (i.e., the fingerprint region of the mid-infrared wavelength range). In the three top spectra, as well as in the spectra of most beers analyzed, the most intense bands appear at 1151−1155, 1079−1085, 1045−1043, and 879 cm^{-1}. These bands reflect mainly the contributions of beer carbohydrates and of ethanol, as seen by comparison with the reference spectra shown in **Figure 1B**; ethanol strongly absorbs at 879, 1045, and 1085 cm^{-1}, while maltose and malto-oligosaccharides show several overlapping bands ranging from 998 to 1155 cm^{-1}. On the other hand, the spectrum shown at the bottom of **Figure 1A** does not show the ethanol band at 879 cm^{-1} and shows much lower intensity for the 1045 cm^{-1} band, in agreement with the fact that it belongs to an alcohol-free beer. In this spectrum, the contribution of maltose/dextrins is thus clearly visible, as indicated by the similarity with the reference spectra shown in **Figure 1B**.

To compare the beers analyzed in a more systematic way and look for the main sources of variability present in their FTIR spectra, PCA has been applied to the 1200−800 cm^{-1} spectral region. **Figure 2A** shows the scores scatter plot of the first two PCs, which together account for 93% of the total variability. Two groups may be suggested based on the distribution of samples along PC1, which explains most of the variability (77%): one group with negative PC1 scores (A), and another group with scores located in the positive side of PC1 (B). The examination of the loadings is useful to understand the basis of the observed separation of samples. The PC1 loadings profile (**Figure 2B**) shows negative values at absorption bands characteristic of ethanol (879, 1045, and 1085 cm^{-1}), indicating that higher amounts of this compound characterize the samples with

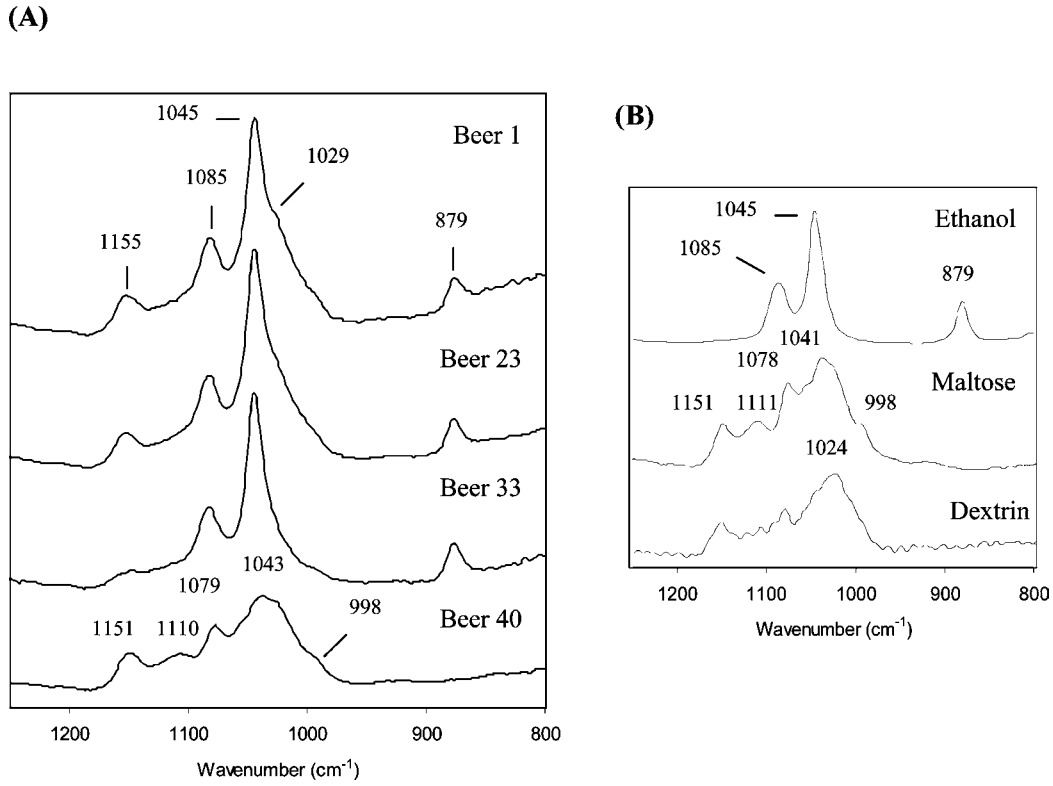

Figure 1. 1250–800 cm^{-1} region of the FTIR-ATR spectra of (A) four different beers, numbered according to **Table 1**, and of (B) ethanol, maltose, and potato starch dextrin aqueous solutions.

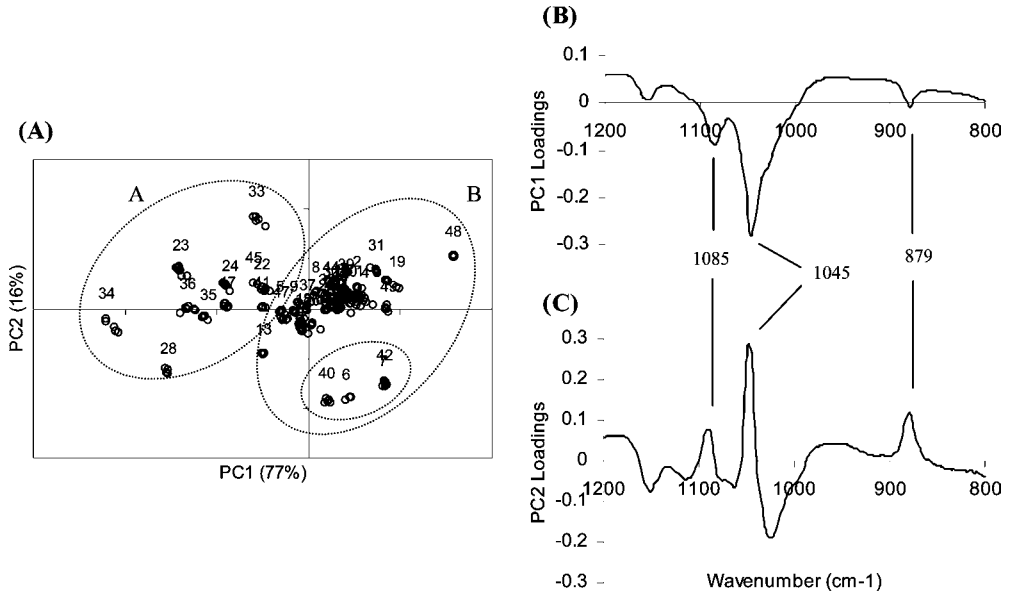

Figure 2. PCA of the FTIR-ATR spectra of 49 beers (1200–800 cm^{-1}): (A) scores scatter plot of PC1 vs PC2 (groups are highlighted by the circles manually drawn), (B) PC1 loadings profile, and (C) PC2 loadings profile. Circle A, > 6% alcohol; circle B, < 6% alcohol; sub-circle in B, alcohol-free.

negative PC1 scores. Indeed, samples of group A are ales containing more than 6.0% alcohol, whereas group B comprises beers with lower alcohol contents. On the other hand, the four alcohol-free beers (samples 6, 7, 40, and 42) are roughly separated from those within group B along PC2, showing scores lying in the negative side of this axis. The positive PC2 loadings (**Figure 2C**) show the contribution of ethanol bands to that separation; in addition, negative PC2 loadings, corresponding to characteristic bands of maltose/dextrins, suggest some contribution from variations in the carbohydrate composition.

Principal Component Analysis (PCA) of ^{1}H NMR Spectra. **Figure 3** shows the 1D ^{1}H NMR spectra of four beer samples, recorded at 600 MHz with suppression of ethanol (δ 1.17 and 3.65 ppm) and water (δ 4.77 ppm) resonances in the case of the three top spectra, and of water in the alcohol-free sample. The assignment of many of the signals observed, carried out by both 2D NMR and LC NMR/MS, has been reported in recent publications (*1*−*3*), enabling the detailed characterization of beer composition to be made. In the aliphatic region of the spectra (0−3 ppm), peaks from alcohols (e.g., propanol, isobutanol, isopentanol), organic acids (e.g., citric, malic, pyruvic, acetic, succinic), amino acids (e.g. alanine, γ-aminobutyric, proline), and fatty acids are observable. The mid-field region (3−6 ppm) shows the contribution of beer carbohydrates, which normally

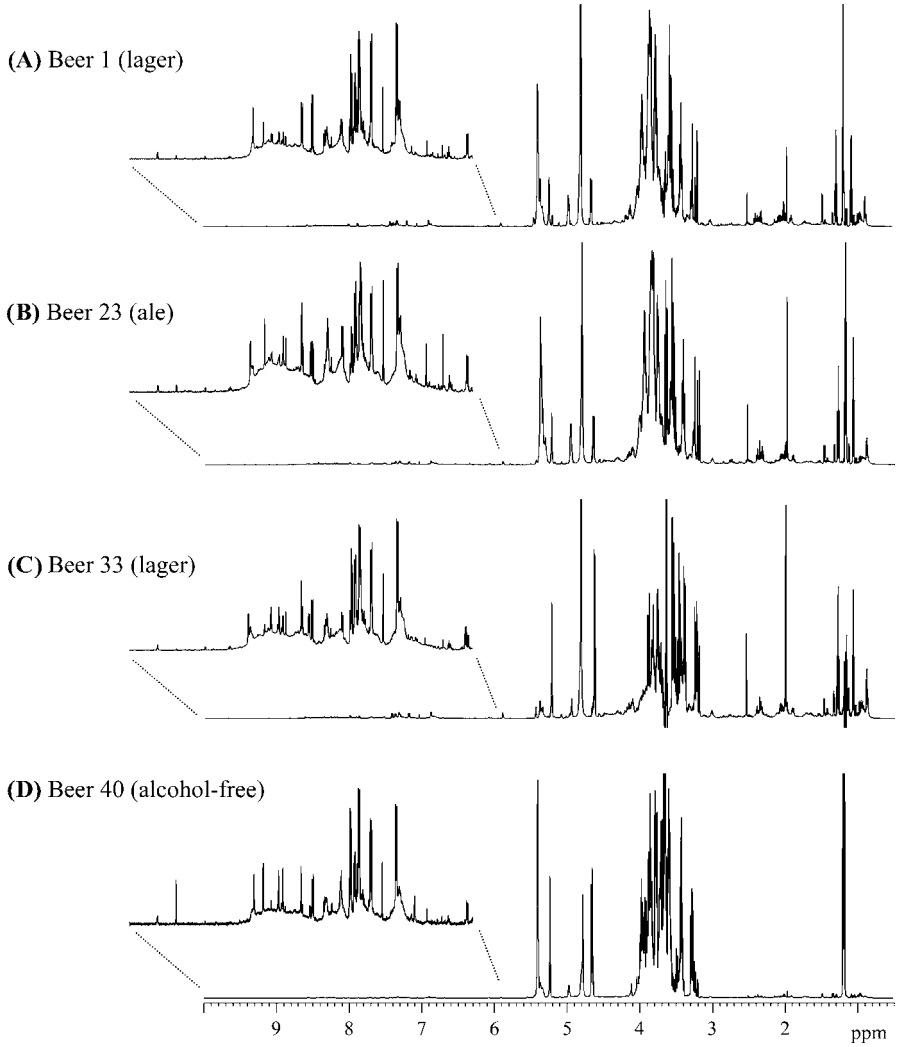

Figure 3. 600 MHz ^{1}H NMR spectra of four beer samples, numbered according to **Table 1**.

comprise fermentable sugars (e.g., glucose, maltose) and dextrins (glucose oligomers with varying degrees of polymerization and branching). As previously reported (*1*), the structural characterization of beer carbohydrates by ^{1}H NMR is severely hindered by strong signal overlap, a problem that can be successfully tackled by hyphenated NMR methods (LC-NMR/MS) (*2*). The signals in the aromatic region (6−10 ppm), vertically expanded in the figure inserts, show the presence of aromatic amino acids (tyrosine, phenylalanine, tryptophane), nucleosides (cytidine, uridine, adenosine/inosine), aromatic alcohols (2-phenylethanol, tyrosol, tryptophol) and polyphenolic compounds that give rise to underlying broad humps between 6.7 and 8.7 ppm (*1*, *3*). Although many of the components mentioned above are present in all beer samples, they significantly differ in quantitative levels and proportions, thus significantly influencing the beer organoleptic properties. For instance, the samples shown in **Figure 3** clearly differ in their carbohydrate compositions, whereas the two top spectra (**Figure 3**, parts **A** and **B**) show intense and relatively broad signals arising from dextrins, the two bottom spectra (**Figure 3**, parts **C** and **D**) show well resolved sugar regions due to the predominance of low molecular weight carbohydrates, namely glucose in beer 33 and maltose in beer 40. In the aliphatic and aromatic regions, spectral differences between samples may also be noted, but their full interpretation is hindered by both low intensity and strong overlapping of the signals. The compositional differences shown by the spectra should reflect properties such as beer type, production process and origin; hence, the question that arises is whether the NMR spectrum may be consistently correlated to one or more of those properties, to be able to be used as a new tool for beer quality control. Given the high spectral complexity and the large number of samples to be compared, PCA has been applied to the ^{1}H NMR spectra of the beers analyzed in this work.

PCA was first performed using the 3.0−6.0 ppm region (excluding water and ethanol signals), which is the region where the major beer components (carbohydrates) resonate. The scores scatter plot of the first two PCs, which together express 50% of the total variability (PC1 = 26%, PC2 = 24%), is shown in **Figure 4A**. Four groups of samples are noted: a large group comprising 36 samples (A), a group of 8 samples (B), the two beers 6 and 40 (C), and the two beers 33 and 48 (D). In the PC1 loadings profile (**Figure 4B**), positive values are found for broader signals corresponding to dextrins (5.38, 4.96, 3.5−4.0 ppm), indicating that these compounds predominate in beers of group A (with positive PC1 scores). On the other hand, PC1 loadings show negative values at positions corresponding to glucose (5.20, 4.60, and 3.2−3.8 ppm) and to maltose (5.41, 5.24, 4.66, and 3.2−4.0 ppm), suggesting that beers with scores lying in the negative side of PC1, namely those of groups C and D, contain relatively higher contents of one or both of these sugars. PC2 loadings (**Figure 4C**) may be used to interpret the separation of group C (beers 6 and 40) from the remaining ones, as their scores are strongly negative in the PC2 axis. Negative loadings are found for signals at 5.41, 5.24, 4.66, and 3.2−4.0

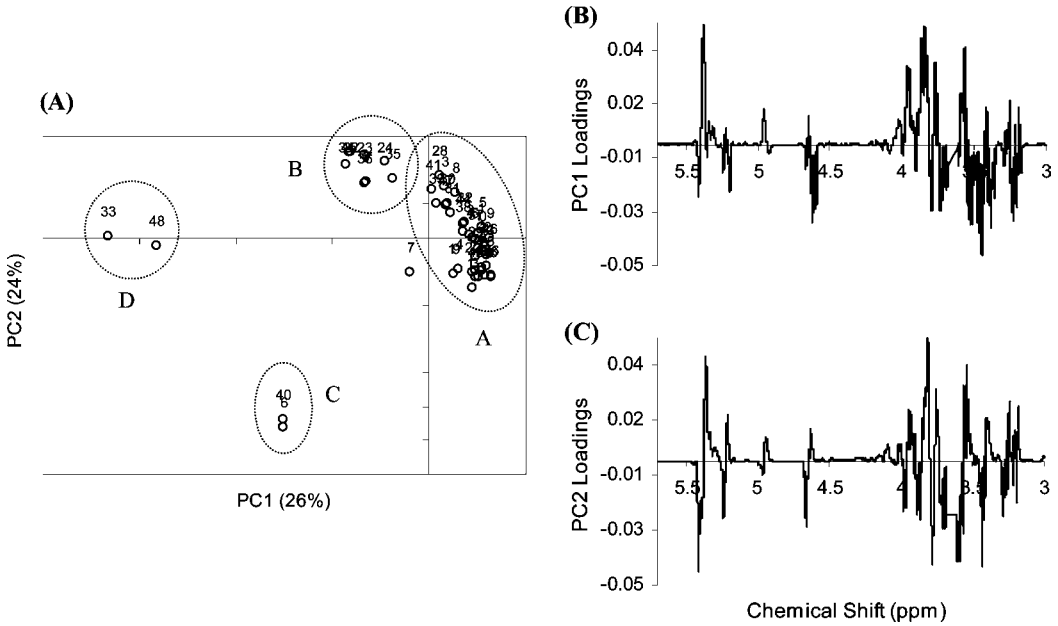

Figure 4. PCA of the ^{1}H NMR spectra of 49 beers in the 3.0–6.0 ppm range (excluding the segments containing ethanol and water signals at 3.65 and 4.80 ppm, respectively): (A) scores scatter plot of PC1 vs PC2 (groups are highlighted by the circles manually drawn), (B) PC1 loadings profile, and (C) PC2 loadings profile.

ppm, which arise from maltose, therefore, beers 6 and 40 seem to be characterized by an important contribution of this disaccharide rather than other carbohydrates. Inspection of the ^{1}H NMR spectra shows that samples of group A correspond, indeed, to the predominance of dextrins, and so do those of group B; however, with basis on the 1D spectra only, it does not become clear why PCA separates these two groups; it is possible that this distinction reflects small differences in the nature and proportion of the dextrins present. The spectrum of beer 40 (**Figure 3D**) is dominated by the signals of maltose, and the same may be observed in the spectrum of beer 6 (not shown). On the other hand, glucose clearly predominates in beer 33 (**Figure 3C**) as well as in beer 48 (spectrum not shown), confirming the observations of the PCA approach.

Relating the PCA results (**Figure 4**) with the known characteristics of the samples presented in **Table 1**, it is interesting to note that group B comprises all the ale beers containing more than 6.0% alcohol, except for beer 33, which, despite its high alcoholic content (9.0%), is separated along with beer 48 (group D), according to the above-mentioned similarity of their carbohydrate profiles. The remaining ales are in group A together with most lagers, which also contain less than 6.0% alcohol. On the other hand, group C is composed by two alcohol-free beers, whereas the third alcohol-free sample analyzed (beer 7) is not included in the same group. Inspection of the ^{1}H NMR spectra of these three beers in the 3.0−6.0 ppm region may help understanding the reasons for this separation. The carbohydrate profile of beer 7 is actually very similar to those of beers 6 and 40, all being characterized by the clear predominance of maltose. However, in the spectrum of beer 7, the sugar signals show small shifts ($\Delta\delta$ 0.002−0.003 ppm) compared to the positions measured in the spectra of beers 6 and 40, although the TSP-d_4 reference signal has been calibrated to the same chemical shift value (δ 0.000 ppm) in all spectra. These shifts may arise from differences in samples pH (4.28, 4.05, and 4.58 for beers 6, 40, and 7, respectively), metabolite concentration and/or instrumental instabilities (e.g., temperature), and constitute artifacts that may lower the classification ability and the stability of the multivariate data analysis. To attempt masking these shifts, higher values of line broadening (LB) factor have been used for exponential multiplication of the free-induction-decays (10, 30, and 50 Hz), and PCA has been applied to the new data matrixes. When the spectra are processed with an LB factor of 10 Hz, the shifts are not totally masked, and beer 7 is still separated from beers 6 and 40. However, when 30 and 50 Hz LB's are used, the small shifts are no longer observed, and the three alcohol-free samples become grouped in the PC1 versus PC2 scores scatter plot (not shown); this indicates that the separation of beer 7 from beers 6 and 40 shown in **Figure 4A** does not correspond to true differences in the composition of the samples but rather to the effect of very small peak shifts. However, it is also found that the separation of group B comprising ales with more than 6.0% alcohol (**Figure 4A**) is no longer observed for LB factors greater than 0.3 Hz (results not shown). This loss of information is obviously caused by the decrease in spectral resolution, which masks the small differences between the dextrins profiles of groups A and B. It is clear, therefore, that much care should be taken when interpreting results obtained by analysis of line-broadened spectra.

To account for the contribution of minor components to the variability within the beers analyzed, PCA has also been performed on data matrixes constructed for NMR aliphatic (0−3.0 ppm) and aromatic (6.0−10.0 ppm) regions. The scores scatter plot of PC1 versus PC2 obtained when only the aliphatic regions of the spectra (processed with 0.3 Hz LB) are considered for PCA shows considerable dispersion (**Figure 5A**), and so do the plots of subsequent PCs. This dispersion may be related to shifts in the positions of some signals, as suggested by the first-derivative-like effects observed in the PC1 loadings profile (**Figure 5B**). In particular, the signals of organic acids resonating in this region are very sensitive to differences in sample pH (e.g., the singlets of acetic and succinic acids show shifts between spectra of up to 0.05 and 0.06 ppm, respectively). Similarly to the approach used for the sugar region, LB factors higher than 0.3 Hz have been used to mask these shifts. The PC1 versus PC2 scores scatter plots, obtained for LB 10 and 30 Hz, and the corresponding PC1 loadings are shown in **Figure**

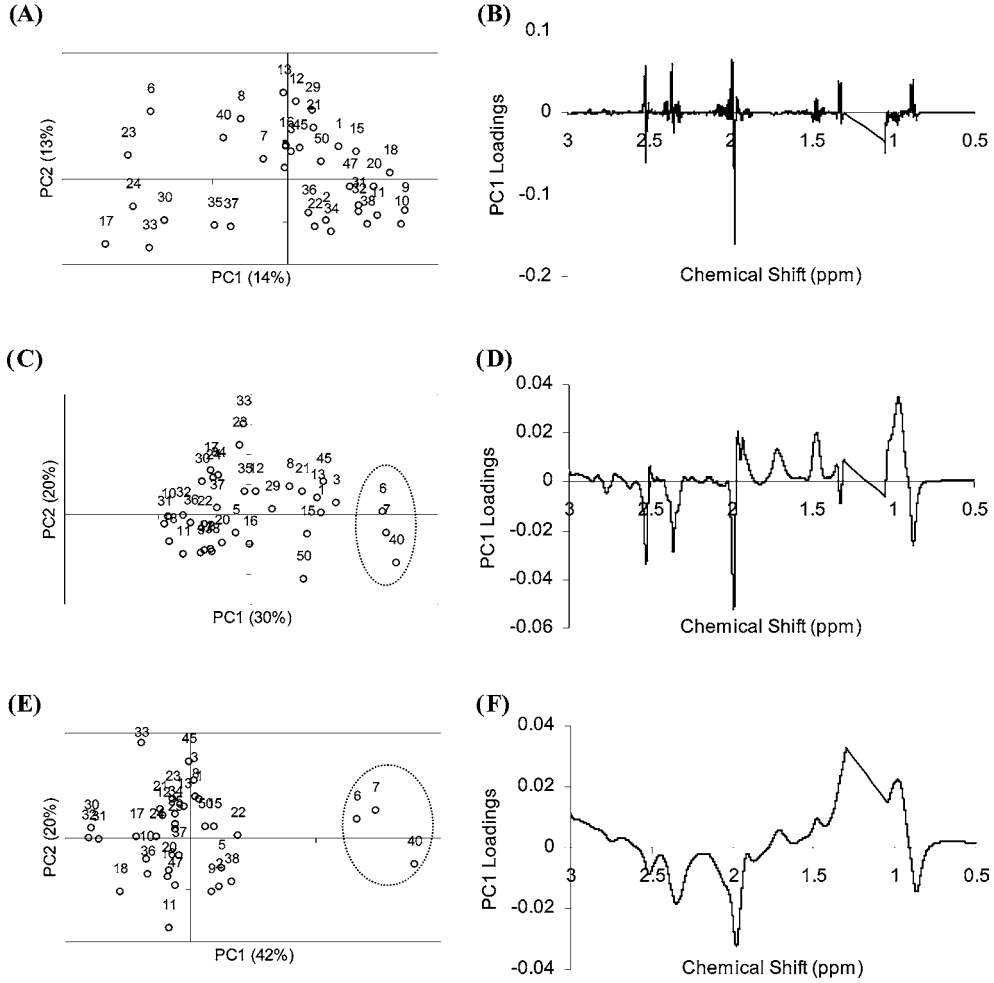

Figure 5. PCA of aliphatic NMR spectral regions (0.5–3.0 ppm) processed with different LB factors: (A) PC1 vs PC2 scores scatter plot and (B) PC1 loadings obtained for LB 0.3 Hz, (C) PC1 vs PC2 scores scatter plot and (D) PC1 loadings obtained for LB 10 Hz, (E) PC1 vs PC2 scores scatter plot and (F) PC1 loadings obtained for LB 30 Hz. In the loadings graphs, the cutoff between 1.05 and 1.30 ppm corresponds to the ethanol absorption region left out of the PCA calculations.

5, parts **C**−**F**. The separation of the three alcohol-free beers from the remaining samples is already suggested for spectra with 10 Hz LB (**Figure 5C**) and becomes clearer for LB 30 Hz (**Figure 5E**). The respective PC1 loadings (**Figure 5F**) show negative values for the signals of propanol/isobutanol/isopentanol (0.87 ppm), acetic acid (1.98 ppm), pyruvic acid (2.35 ppm), and succinic acid (2.52 ppm), suggesting their lower abundance in the alcohol-free beers, which show positive PC1 scores. Indeed, this observation was confirmed by inspection of a selection of spectra and calculation of the integral ratio of each of the above-mentioned peaks relative to the TSP peak; these calculations clearly showed lower amounts of the corresponding compounds in the alcohol-free beers (samples 6, 7, and 40). Although the PC1 loadings also suggest positive contributions (e.g., at 1.46 and 1.70 ppm), namely for higher LB values (**Figure 5**, parts **D** and **F**), the strong signal overlap in that region hinders any objective interpretation of such variations.

When only the aromatic regions of the spectra are considered for PCA, the PC1 versus PC2 scores scatter plot suggests separation of samples into three groups (**Figure 6A**). The scores lying toward the negative side of PC1 (group A) correspond to the majority of the ale beers analyzed, whereas the scores near zero or in positive PC1 (group B) correspond mostly to lager beers, although three ales (beers 4, 46, and 49) are also included in this group. The PC1 loadings profile, shown in **Figure 6B**, gives an indication of which aromatic compounds are responsible for this separation. However, this analysis should be done in tandem with close inspection of individual spectra, to identify first-derivative-like effects, which result from peak shifts and not from real changes in sample composition. The negative PC1 loadings that contribute to the ale aromatic profiles (group A) seem to arise mainly from the broader peaks at 6.84, 7.50, and 7.67 ppm (indicated with arrows in **Figure 6B**). These may arise from polyphenolic species, suggesting that such compounds may be more abundant in the ale beers. Interpretation of the positive PC1 loadings is seriously complicated by the strong first derivative appearance of most signals in **Figure 6B**. Indeed, only the peak at 6.87 ppm (part of the tyrosine/tyrosol multiplet) and the multiplets at 7.36 and 7.17 ppm (2-phenylethanol) seem to show a clearer positive nature, thus indicating that these compounds may be slightly more abundant in the lager beers (group B). The scores scatter plot obtained for the aromatic regions (**Figure 6A**) also shows the separation of two samples along PC2, explaining 17% of the total variability (group C). The two samples have positive PC2 scores and correspond to the alcohol-free beers 6 and 40, indicating that these beers also differ from the bulk of the samples in terms of their aromatic composition. However, the PC2 loadings profile (not shown) does not clearly show which aromatic components cause this distinction, due to the strong first-derivative-like effect observed for most signals. Again, the third alcohol-free sample analyzed

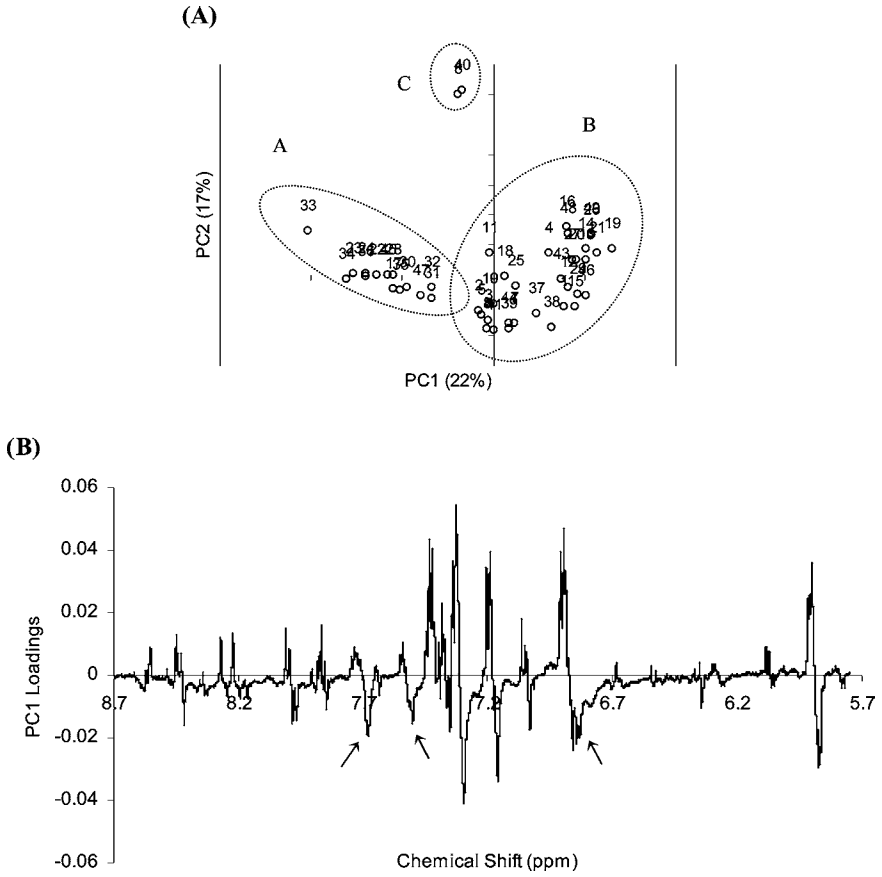

Figure 6. PCA of the ^{1}H NMR spectra of 49 beers in the 6.0–10.0 ppm range: (A) scores scatter plot of PC1 vs PC2 (groups are highlighted by the circles manually drawn), (B) PC1 loadings profile.

(beer 7) is only grouped with beers 6 and 40 when a 30 Hz LB is used, although in this case, the suggested separation according to ale/lager type becomes unclear. These results, as well as those obtained by PCA of the sugar regions, demonstrate that the attempt made here to correct for shifts by decreasing the spectral resolution may help to highlight true compositional similarities/differences between some samples but also carries a significant loss of information, and it would be more useful to carry out spectral alignment without reducing the resolution; some preprocessing algorithms such as the partial linear fit (*5*) and the dynamic time warping (*25*) seem to be promising in this respect. It is also worth noting that the line broadening manipulation may be used to mimic the effects of a lower field instrument, an important point to consider if cost-effective industrial applicability is to be explored.

In conclusion, PCA of spectroscopic data of beer resulted in the separation of samples according to some of their different compositional properties, showing the potential of this approach to provide rapid information about several factors affecting beer production. PCA of FTIR spectra (1200−800 cm^{-1}) gave direct information about ethanol content, separating beers with more than 6.0% alcohol from those with lower percentages, and among the latter, the alcohol-free beers. PCA of ^{1}H NMR spectra provided much richer information regarding components other than ethanol. In particular, PCA of the carbohydrate region of the spectra resulted in separation of beers according to their composition in dextrins, maltose and glucose; in addition, an indirect correlation between carbohydrate profile and ethanol content was found, reflecting the different production processes employed. When PCA was performed on spectral regions where minor components resonate, the aromatic region (6.0−10.0 ppm) was found to be particularly sensitive to the types of beer analyzed (ale, lager, and alcohol-free), thus being potentially useful for their distinction. An important point to make relates to the applicability of these results to the beer industry, where the speed of measurement becomes determinant. Although experiment lengths of 30 min per sample were used here to observe minor (aromatic) components, recording lengths may be reduced down to 10 min (using 8 scans instead of 128) if only carbohydrate composition is to be analyzed. Additional features such as flow injection and optimization of number of scans and recycle time for specific samples should enable experiment times to be shortened further.

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