PREDICTION OF BEER SHELF-LIFE USING AN HS-MS e-NOSE

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Introduction

Flavor, which is the combination of aroma and taste, is one of the most determinant factors of quality of any foodstuff, including beer. During its shelf-life, beer is subjected to several chemical reactions that can affect both aroma and taste resulting in decreased sensory quality [1].

Generally, a sensory panel in combination with common analytical tools, such as gas chromatography, are used to evaluate beer flavor. An alternative to this expensive and time-consuming approach is to use an electronic nose (e-nose) based on the use of a mass spectrometer detector (MS) over the whole volatile fraction of the samples (HS-SPME), which is a faster and more objective method [2].

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Aim of study

- To build a prediction model of beer shelf-life by comparing the changes occurred in the volatile matrix of the samples during one year when kept under optimal storage conditions.
- To differentiate between aluminium cans and glass bottles packaging.

Materials and Methods



- 44 samples of a commercial Lager beer, packaged in aluminium cans and glass bottles (alcohol content of 5.4% v/v).
- Samples were naturally aged for 12 months at 14 °C.
- Samples were analysed by HS-SPME-MS (e-nose). The analytical column (HP-5MS) was kept at the

suitable temperature to guarantee transfer of volatiles in less than 5 minutes to the MS and to avoid chromatographic separation.

- Partial Least Squares Discriminant Analysis (PLS-DA) was used to discriminate between fresh and aged beers, and Partial Least Squares Regression (PLSR) was used to build a prediction model relating mass spectra to aging months.
- <u>Software</u>: MATLAB and PLS toolbox.

Results

MASS SPECTRA



1) PLS-DA

CONFUSION TABLE	ACTUAL CLASS	
	CLASS 1	CLASS 2
PREDICTED AS CLASS 1	12	0
PREDICTED AS CLASS 2	0	37
PREDICTED AS UNASSIGNED	0	0
	ACTUAL CLASS	
	ACTUA	L CLASS
CONFUSION TABLE CV	ACTUA CLASS 1	L CLASS CLASS 2
CONFUSION TABLE CV PREDICTED AS CLASS 1	ACTUA CLASS 1 12	L CLASS CLASS 2 0
CONFUSION TABLE CV PREDICTED AS CLASS 1 PREDICTED AS CLASS 2	ACTUA CLASS 1 12 0	CLASS CLASS 2 0 37
CONFUSION TABLE CV PREDICTED AS CLASS 1 PREDICTED AS CLASS 2 PREDICTED AS UNASSIGNED	ACTUA CLASS 1 12 0 0	CLASS 2 0 37 0

PLS-DA allows discriminating fresh from aged beers, with a 100% of correct classification.

PLS-DA models were not able to discriminate samples packaged in aluminium cans or in glass bottles. This was confirmed by further sensory analysis (no differences were found).

3) PLSR (Predicted vs Reference plot)



The prediction error in aging time (RMSECV)

2) PLSR (Scores plot)





No differences are observed between aluminium cans and glass bottles, but there are groupings related to aging time (6 and 11 months). The group of aged beers appears more compact than the group of fresh beers (fresh and 3 months aged).

was found to be around 1.1 months, for a model with 5 LVs.

This means that with our model a beer aged less than 11 months can be safely predicted as being within its shelf-life (1 year).

Conclusions

- HS-SPME-MS coupled to multivariate analysis seems to be a useful tool for discriminating beer samples based on the time of storage.
- PLS-DA applied to the data obtained when analysing the samples all through a year under optimal storage conditions is able to discriminate fresh from aged beer samples.
- PLSR was able to relate the whole mass spectra of the samples to the aging time (fresh, 3-, 6-, and 11-month-aged) and predict aging time with an error of 1.1 months.



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Acknowledgements

Grant PID2019-104269RR-C33 funded by MCIN/AEI/10.13039/501100011033.



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Generalitat de Catalunya for the PhD fellowship of

Ana Carolina de Lima (2019 FI_B 00851).