MODELING AND PREDICTING SECOND and THIRD-ORDER FLUORESCENCE SPECTROSCOPY DATA AS A NOVEL QUALITY CONTROL STRATEGY FOR MAYONNAISE

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INTRODUCTION

- In order to evaluate/verify the quality of mayonnaise, it is necessary to perform physical, chemical and microbiological analysis. In this matter, the techniques routinely used became expensive, time-consuming and could require trained analysts.
- Due to straightforward sample preparation and fast acquisition time, fluorescence spectroscopy has found wide applications in food analysis as well as food area research. Besides, this technique allows to simultaneously evaluate multiple components in a sample.
- The combination between a noninvasive system, such us fluorescence spectroscopy, and the proper chemometric modeling, it is possible to obtain valuable information about the quality of food samples.
- In this work, to showcase the potential of fluorescence data in combination with chemometric, the spoilage of mayonnaise was evaluated by using classification analysis based on storage time.

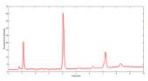
EXPERIMENTAL

Sample preparation

Homemade and commercial mayonnaise samples were maintained at 5 and 37°C. No prior sample processing was performed.

Eggs
Sunflower oil
Salt
Lemon juice

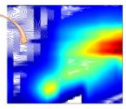
HPLC analysis



To identify compounds related to the spoilage of mayonnaise

Spectrofluorimetric analysis

Front face fluorescence system was used. EEMs were recorded at different times along 4 days



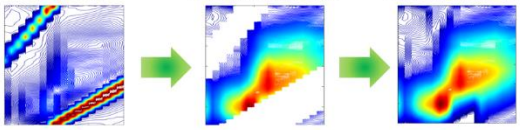
λ Excitation: 230-400 nm
λ Emission: 300-600 nm

DATA ANALYSIS

Removing Scattering

Rayleigh scatter was corrected by using a method based on interpolation in the affected area

Raw Data → Scattering Removed → Interpolated Data

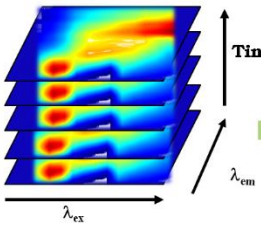


PARAFAC was used to obtain the component profiles and evaluate changes in the data
PLS-DA was applied to perform discriminant analysis

RESULTS and DISCUSSION

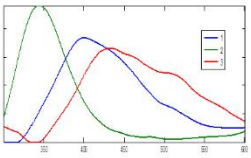
PARAFAC

EEMs for 1 samples

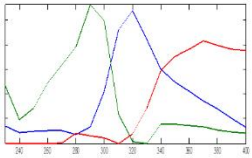


Profiles of three main compounds can be extracted with PARAFAC describing the quality evolution over time

Emission profiles

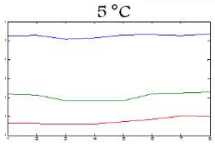


Excitation profiles



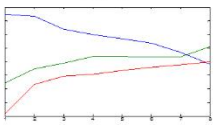
Relative concentrations

5 °C



No changes were observed for all components

37 °C



Changes describe the evolution of the compounds along time, indicating a mayonnaise spoilage

PLS-DA

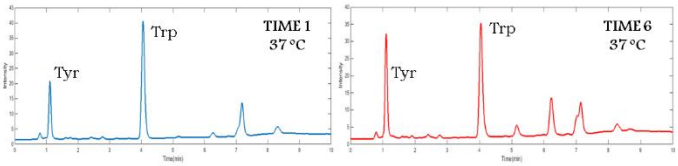
Mayonnaise samples stored at 37 °C for up to 4 days were classified by storage time.
3 factors were necessary for FLS modelling.

Groups	Training					% Correct classification
	0	1	2	3	4	
0	8	0	0	0	0	100
1	0	8	0	0	0	100
2	0	0	8	0	0	100
3	0	0	0	8	0	100
4	0	0	0	0	8	100

Rows: observed classification.
Columns: predicted classification.

Discriminant model of training and prediction data set reached 100% classification rate

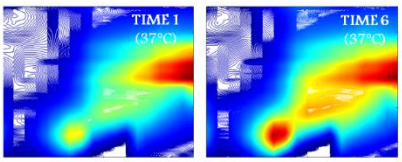
HPLC and fluorescence data evaluation



Tyrosine (Tyr) and tryptophan (Trp) were present in all the samples analyzed
Additionally, unidentified compounds were observed at higher storage time

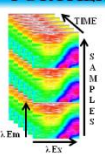
Chromatographic analysis allowed to confirm the storage time dependency of the Trp (decrease) and Tyr (increase) concentration.

Changes the both in spectra as contribution can be observed by visual inspection of EEMs



FURTHER ANALYSIS

Commercial mayonnaise samples



EEMs were obtained using a spectrofluorometer equipped with a plate reader accessory coupled to an optical fiber and a gated photomultiplier. Samples were irradiated for two minutes, 10 times per sample.

Third-order data analysis will be performed to evaluate the fat content among other quality parameters of different mayonnaise samples.
Degradation kinetics of different mayonnaise components will be studied by applying classification methods by using EEM data, evaluating differences between mayonnaises samples and predicting their quality.

CONCLUSION

Evolution profiles obtained by front face fluorescence of fluorescent components that are native and/or generated as mayonnaise spoils can be extracted by second and third-order algorithms and used for obtaining information about the quality of the mayonnaise.

ACKNOWLEDGEMENTS

Universidad Nacional del Litoral
Universidad Nacional de La Pampa
Consejo Nacional de Investigaciones Científicas y Técnicas
Agencia Nacional de Promoción Científica y Tecnológica