Chemical variation of sugar beet subjected to long-term storage by Vis-NIR spectroscopy, Hyperspectral Imaging and chemometric methods

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SuChAQuality

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I. INTRODUCTION

Twenty percent of the world's sugar production is obtained from sugar beets, whose manufacturing efficiency depends mainly on the quality of the raw material [1]. Prior to processing, sugar beets are subjected to long-term storage, which promotes the degradation of some compounds, especially inversion of sucrose to glucose and fructose, which reduces their quality [2,3]. Tools are needed for quick and easy characterization of beet quality. Spectroscopy techniques in visible and IR range are powerful tools that allow to quickly characterize samples based on their interaction with radiation. Hyperspectral Imaging (HSI) provides simultaneous spatial and spectral information of the samples [4]. **The objective of this research was to analyze the chemical variation (composition and distribution) of beet subjected to a long-term storage, through IR spectroscopy techniques enhanced with chemometric techniques.**

II. METHODOLOGY

Beet sampling Ñuble region, Chile → Storage at 20°C (1 day: D1; 1 month: D2; 1.5 month: D3; 2 months: D4) → Middle slice

Vis/NIR
USB4000
Range: 400-1000 nm
Resolution: 0.2 nm
Scans: 5

1st derivative (95)
MC
PCA
$X=TP^T+E$
PLS-Toolbox
(Eigenvector Inc)

HSI
Resonon Pika-L
Range: 400-1000 nm
Spectral channels: 281
Spatial resolution: 900 pixels per line

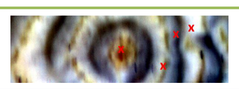
Smoothing (19)
Hypercube Unfolding
MCR-ALS
Initial estimation: spectra
No negativity for concentration (ffnls)
Iterations: 80 Error allowed: 0.5
$D=CS^T+E$
MCR-ALS GUI 2.0 Toolbox

ATR-FTIR
Diamond cristal
Range: 4000-400 cm^{-1}
Scans: 32
Resolution: 4 cm^{-1}

SNV, 2nd derivative (15)
MC
PCA
$X=TP^T+E$
PLS-Toolbox
(Eigenvector Inc)

Distribution Maps ← **Pure spectra**

Selection of **reference spectra** of each component of **D4** beet



Classification method
Spectral Angle Mapper (SAM)

$$\alpha=\cos^{-1}\frac{\Sigma XY}{\sqrt{\Sigma(X)^2\,\Sigma(Y)^2}}$$

Spectronon Pro

Model applied on D1-D2-D4 beets

III. RESULTS

1. PCA of Vis/NIR spectra

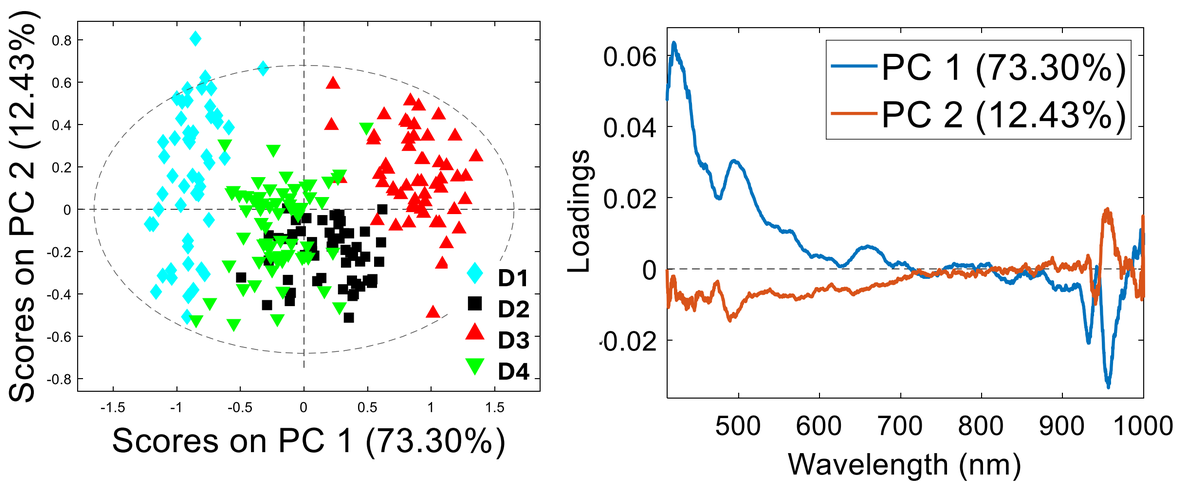


Figure 1. Scores and loadings plot of PC1 and PC2 for Vis-NIR spectra between D1, D2, D3 and D4 beets

2. MCR-ALS of HSI

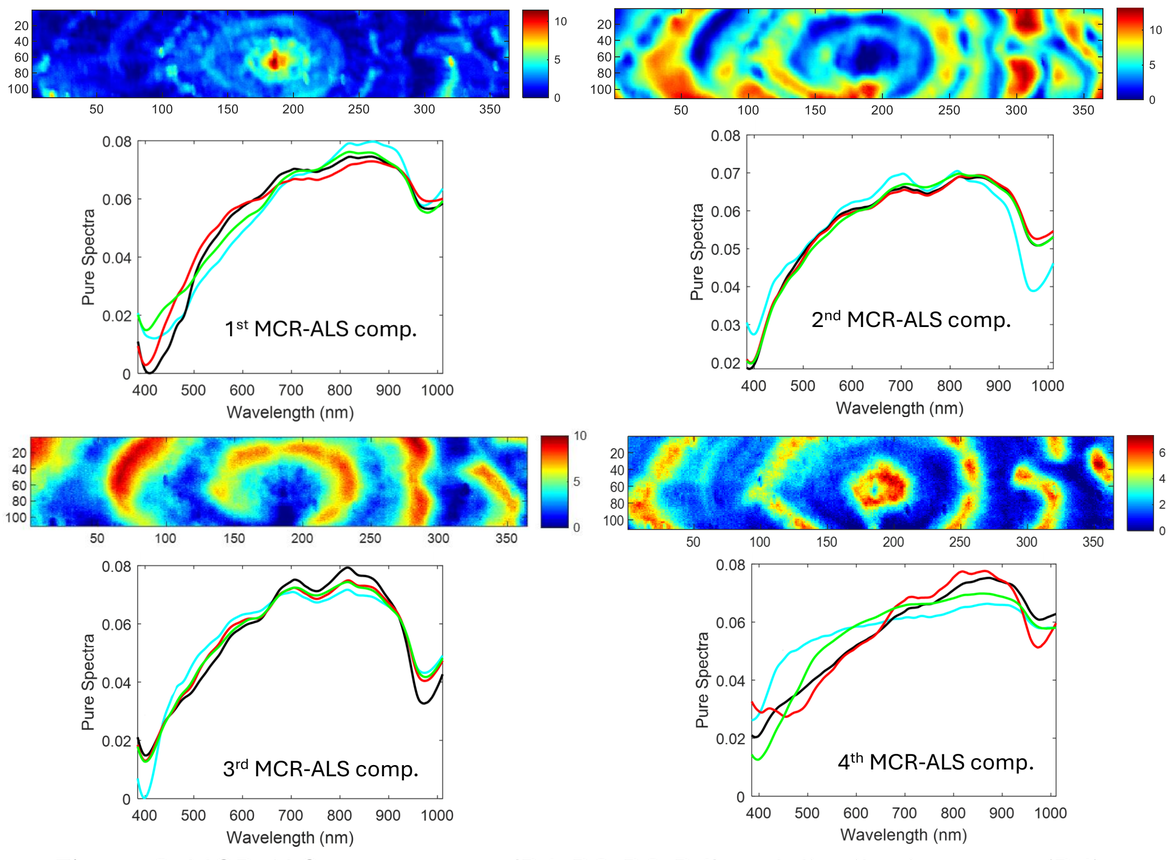


Figure 2. MCR-ALS pure spectra (D1-D2-D3-D4) and distribution maps (D4)

3. Classification by SAM

Figure 3. Raw and 2nd derivative of reference spectra of each MCR-ALS component and the clasification maps of beet

4. PCA of ATR-FTIR spectra

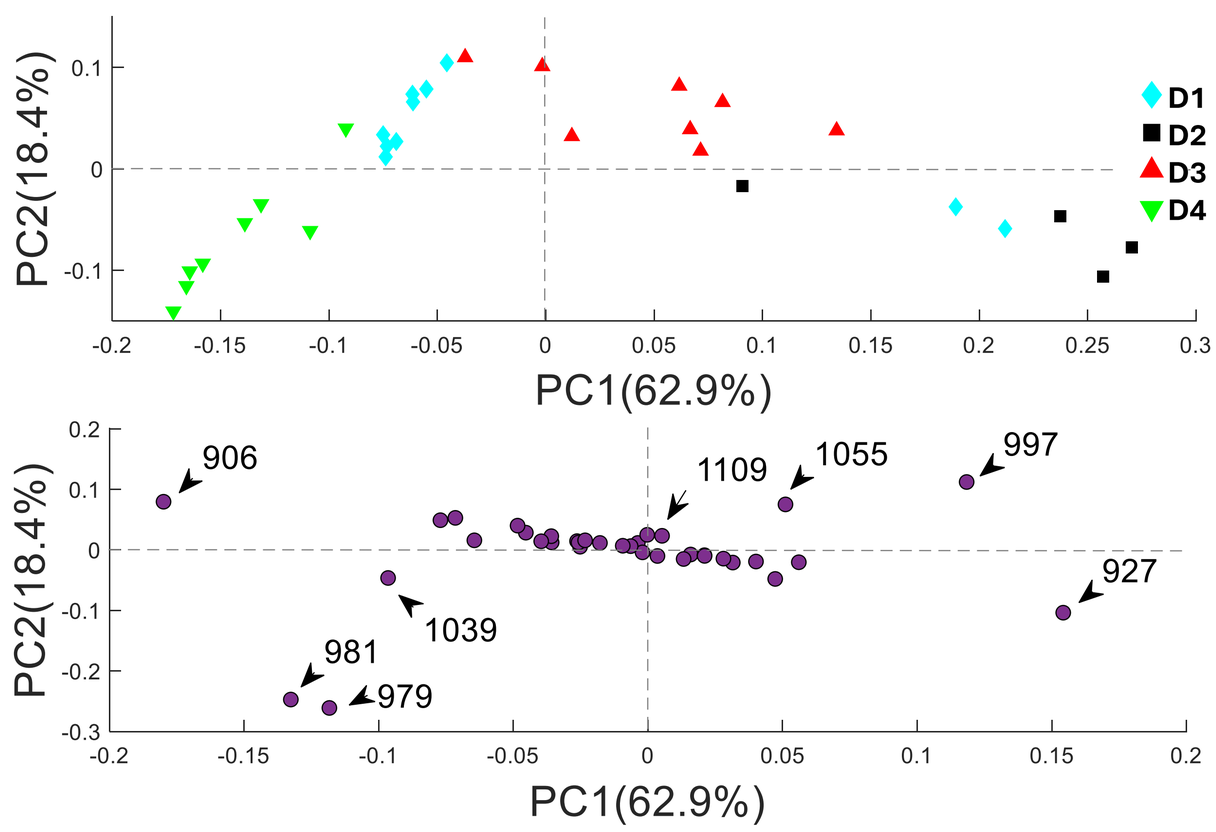


Figure 4. Scores and loadings of ATR-FTIR spectra of beets with different storage time

IV. DISCUSSION AND CONCLUSIONS

- Exploratory analysis of Vis/NIR spectra allowed to detect that there are chemical variations due to storage time.
- The application of MCR-ALS on HSI was a successful method to determine the number of components present in the beets, allowing to obtain their respective reference spectra to develop SAM classification methods.
- The mid-IR analysis allowed us to obtain chemical information associated with storage time. It is assumed that a longer storage time decreases the sucrose content, increasing the glucose and fructose content. After 2 months the glucose content would tend to decrease due to beet respiration.
- Spectral data could provide information about the chemical state of samples for a quality control of biomass during the storage

V. REFERENCES

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