Potential of NIR Spectroscopy and Chemometrics as Predictive Tools for Products and Processes in the Leather Industry

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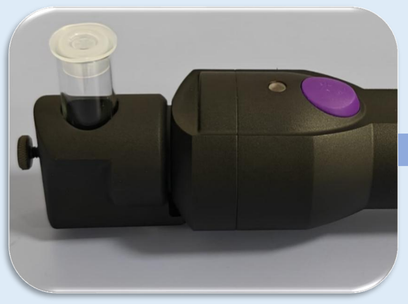
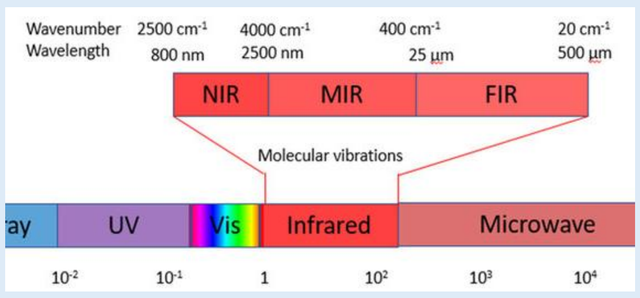
Abstract

Chemometric techniques are based on the construction of **predictive models** built on a database of known samples with different characteristics. **Near infrared (NIR) spectroscopy,** is already used in many industrial sectors from pharmaceuticals to agrifoods for the characterisation of product quality, directly in the production line. In the tanning sector, NIR instrumentation is currently not used in process and product control. Furthermore, few studies in the literature evaluate its application to tanning products. In this research, we highlighted the versatility of NIR in acquiring reliable and robust spectral information from both solid and liquid samples. Through the application of principal component analysis (PCA), it was possible to demonstrate how **NIR discriminates different samples based on their tanning origin** from both classical (chrome, glutaraldehyde, vegetable, carbamoyl sulphonate) and experimental (dialdehyde starch) tanning.

Subsequently, by means of **multivariate partial least square regression (PLSR)** model based on spectroscopic analysis, it was possible to construct models for the **quantitative analysis** of **unknown amounts of tanning agents in solutions** simulating tanning drums conditions. Encouraging results were obtained for the use of this technique in process control to assess the tanning agent concentration in the drum in real time to evaluate the possible use of these sensors for in-line tanning agent control. Furthermore, through these chemometrics models, it was possible to evaluate the removal of chromium by means of innovative adsorbents such as zeolites, obtaining quantitative results in the removal of chromium from water.

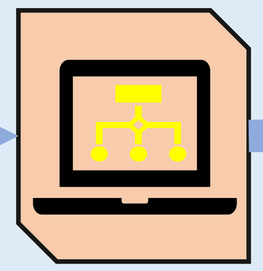


Near Infrared



NIR spectroscopy is a non-destructive analytical technique that analyses molecular vibrations—mainly **C-H, O-H, and N-H** bonds—through light-matter interaction in the near-infrared region.

It is especially suited for studying organic and biological materials.



Multivariate Chemometric Models

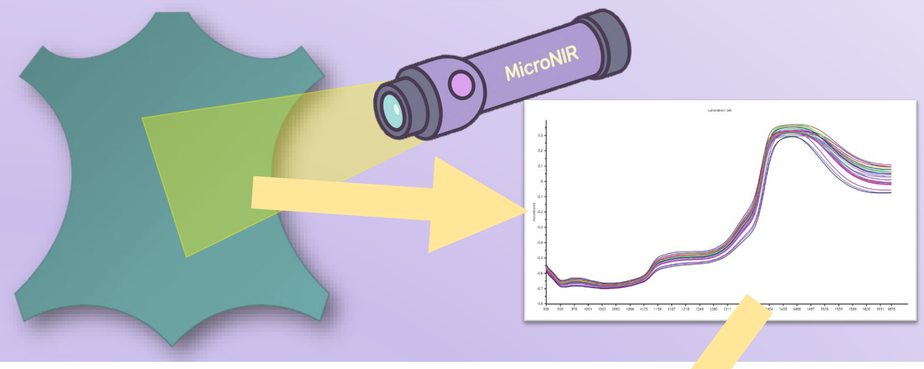
Chemometrics combines statistical and mathematical tools **to extract relevant information from spectroscopic data**.

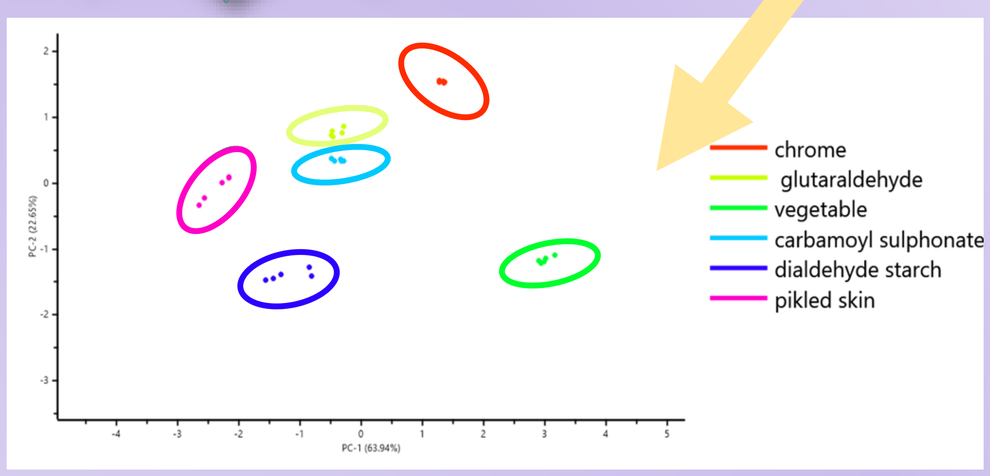
Principal Component Analysis (PCA) is used to reduce data dimensionality, **detect hidden patterns**, and identify outliers by projecting spectra into a lower-dimensional space that retains most of the original variance.

Partial Least Squares Regression (PLSR) enables the development of **predictive models** correlating NIR spectra with key **chemical** and **physical properties**, supporting real-time process monitoring.

Product and Process Control

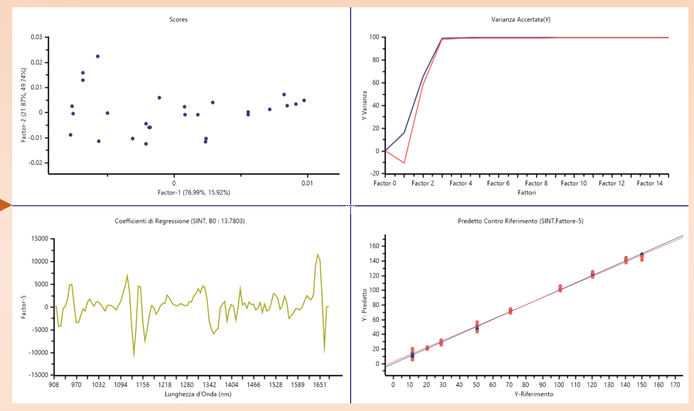
PCA
Differentiation of Tanning Methods





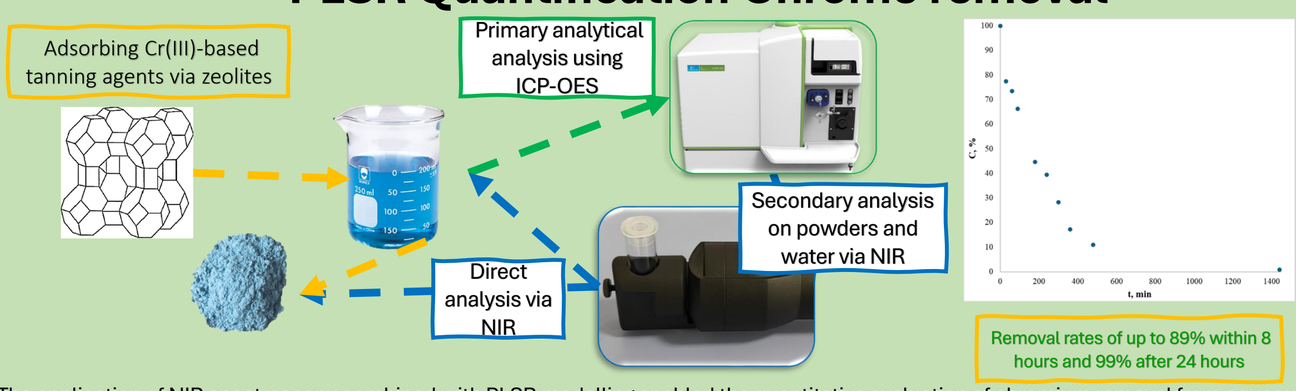
To assess the **discriminating power of NIR-based chemometrics,** leather samples processed with different tanning methods (traditional and innovative) were analysed.
PCA (Principal Component Analysis) was used to reduce spectral data dimensionality and highlight chemical and structural differences.
This **microNIR–PCA workflow robustly differentiate industrial tanning systems**, even accounting for natural biological variability, and confirms its value for real-time classification and quality control.

PLSR
Quantification of Tanning Agents



Partial Least Squares Regression (PLSR) was used to develop quantitative models capable of estimating the concentration of tanning agents in aqueous phase. Models were built using standard solutions under controlled conditions to simulate the actual tanning process.
Results showed good predictive accuracy, highlighting the potential of PLSR for **real-time quality control**.
Score plots were used to visualize sample distribution in principal component space.
Loading plots identified key wavelengths influencing the prediction of chemical parameters.

PLSR Quantification Chrome removal



Removal rates of up to 89% within 8 hours and 99% after 24 hours

The application of NIR spectroscopy combined with PLSR modelling enabled the quantitative evaluation of chromium removal from aqueous solutions using innovative adsorbent materials such as zeolites.

Conclusion

NIR spectroscopy combined with PCA and PLSR proved to be an effective, non-destructive tool for **monitoring leather tanning processes**.
The methods allowed:
•**Discrimination** between traditional and innovative tanning systems.
•**Real-time estimation** of tanning agent concentrations.
•**Evaluation** of chromium removal using zeolites.
These results support the use of NIR-chemometric approaches for quality control and sustainability in the tanning industry.
Future work will focus on model expansion, in-line monitoring, and integration of advanced data analysis techniques.

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