

# Successful geographical discrimination of Argan oil from four Moroccan regions based on their vibrational spectroscopic fingerprints, proper preprocessing and supervised classification

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## 1 Introduction

Argan oil is a valuable oil that has numerous nutritional and cosmetic properties [1]. Given its high value, the national and international demand increased in recent years. As a result, determining its geographical origin, which is usually done using slower and more expensive chromatographic techniques [2], has become a necessary task for the authentication and quality control of this product. In the last few years, attention on authentication and quality control has also been focused using spectroscopic techniques that offer fast, non-destructive and cost-effective methods for food analysis. Mid-Infrared [4], Near Infrared [5] and Raman [6] spectroscopy, combined to multivariate data analysis, have shown to be successful analytical approaches for quantitative and qualitative analysis. In this study, the abilities of two spectroscopic techniques, NIR and MIR, as fast and non-invasive techniques in combination with multivariate data analysis were evaluated to discriminate between Argan oil from four different Moroccan regions. Preprocessing was applied for a better classification with SIMCA and PLS-DA discrimination techniques.

## 2 Material and methods

93 Argan oil samples were collected from four Moroccan regions, Taroudant, Essaouira, Agadir and Tiznit, and extracted mechanically. From each sample, three separate samplings were scanned, which gives a total of 279 spectra for each instrument. NIR spectral data were collected in transflection mode using small glass petri dishes as sample holder with a reflector placed in the axis of the light beam, above the sample, using the NIRA accessory with an FT-IR/ NIR spectrometer, (PerkinElmer). For MIR spectra collection, a universal ATR accessory (UATR) was used on an FT-IR/NIR spectrometer (PerkinElmer) in the diffuse reflection mode. The PCA and PLS-DA in this study were performed using the PLS\_Toolbox software V8.2.1 (Eigenvector, Wenatchee, WA, USA) running on MATLAB (R2018b) (The MathWorks, Natick, MA, USA), and SIMCA algorithm was downloaded from the Freeware Classification toolbox, version 5.3 [7].

## 3 Results and discussion

This study investigates the potential of spectroscopic fingerprinting for the discrimination of Argan oils according to their geographical origin. No clear difference was seen by visual examination

of the recorded NIR and MIR spectra. Then PCA was carried out for the NIR and MIR fingerprints of the 93 Argan oil samples after applying mean centering and Generalized Least Squares Weighting (GLSW) preprocessing. The score plots of the first three PCs explained about 70% and 40% of the total spectral variance for NIR and MIR, respectively, and four distinct groups were seen.

For the discrimination, a PLS-DA and SIMCA models were built for each technique. A venetian-blinds cross validation with six splits was used to evaluate the predictive properties of the models, and the recorded data were split into a training (70%) and a test set (30%). Different preprocessings were tested and the best models were obtained using mean centering and GLSW for both NIR and MIR spectra. The PLS-DA built model had coefficients of determination ( $R^2$ ) higher than 99% and 96%, for NIR and MIR, respectively. For both datasets, the PLS-DA models exhibit 100% specificity and selectivity. For the SIMCA model, the spectral data was forced to be attributed to one of the four classes by choosing distance as assignation criterion. The  $R^2$  was 96 % and 94% for the training set, and 92 % and 91% for the test set for NIR and MIR, respectively. Models built showed achieved a sensitivity of 87%-100.00% and 71%-100.00% and a specificity of 88%-100.00% and 86%-100.00% for NIR and MIR, respectively. Both chemometric approaches showed good discrimination patterns, but the PLS-DA models outperformed SIMCA.

## 4 Conclusion

This study shows the potential of NIR and MIR spectroscopy, in combination with chemometric data analysis, to classify Argan oils according to their geographical origin. Mean centering and GLS Weighting as pre-processings yielded the best results. PCA was used for the initial visualization of the pre-processed data, and it allowed clearly distinguishing the various groups. Then, applying PLS-DA, a good discriminative model was built, with high  $R^2$  values. Finally, SIMCA enabled the construction of class models with a good sensitivity and specificity, as well as an acceptable accuracy. However, when comparing the two chemometric tools, it can be concluded that PLS-DA provides superior classification models. Comparing the results of the models obtained with the NIR and MIR spectra, no significant differences were observed. Consequently, NIR and MIR spectroscopy can be used for the quality control and authentication of Argan oils.

## 5 References

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