



Metabolomic fingerprinting of Moroccan Argan kernels using two platform techniques UPLC-TOF/MS and UPLC-DAD: A geographic classification

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Introduction

Argan culturing has a great economic and social importance in the Southwestern Moroccan area. Moreover, Argan oil is worldwide one of the more expensive cosmetic and edible oils. Currently, in Morocco the Argan forest covers an area of 840 000 ha, including the fertile Souss valley region, the foothills of the Anti-Atlas mountains, and the coastal region between Essaouira and Agadir [1-2].

Information about food's origin is necessary to verify its specifications and to guarantee its quality, because foods from different origin have distinct qualities. Quality traceability and authenticity of Argan oil is the object of interest of the Moroccan authorities for protecting this heritage and to increase its economic value. The characterization of its origin, composition and quality has a great interest to ensure the quality for consumers.

Aims

Phenolic-compounds? profiling from food has been an area of intensive research because of their nutritional value and biological activities. Information about food's origin is necessary to verify specifications and to guarantee quality because food from different origin may have distinct qualities.

Two untargeted fingerprinting techniques, UPLC-MS and UPLC-DAD, were comparatively investigated to trace the geographical origin of one-hundred and twenty Argan fruit kernels from five regions ('Agadir' (A), 'Ait-Baha' (A-B), 'Essaouira' (E), 'Tiznit' (Tiz) and 'Taroudant' (T)). Argan-kernels polyphenols-containing extracts were subjected to UPLC-MS, UPLC-DAD, and the obtained fingerprints subsequently to multivariate classification tools. The UPLC-DAD fingerprint data were directly used, while UPLC-MS data were decomposed by metabolomic tools, such as multivariate curve resolution alternating least squares (MCR-ALS). Each chromatographic data set was pretreated and prepared separately using the chemometric pretreatment tools.

Results and Discussion

Classification of Argan kernels origin based on UPLC/DAD

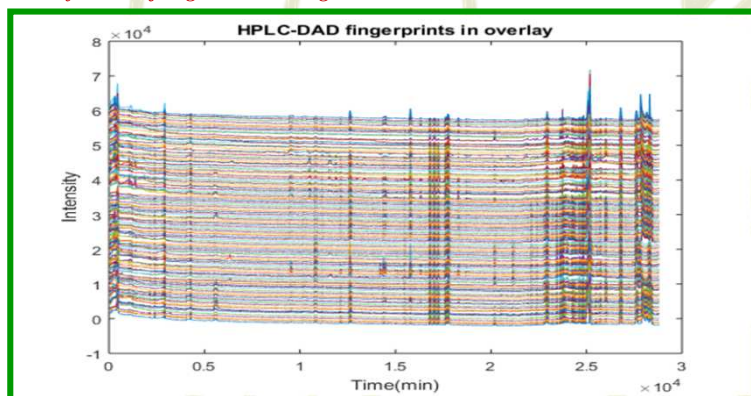


Fig. (1). Overlay UPLC-DAD chromatograms at 280 nm after COW alignment,

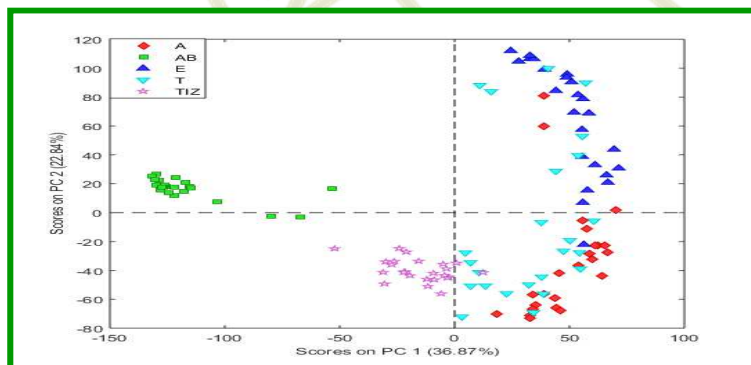


Fig. (2). PCA-scores (PC1-PC2) from UPLC-DAD data at 280 nm,

Classification of Argan oil based on UPLC-ESI-TOF/MS fingerprinting

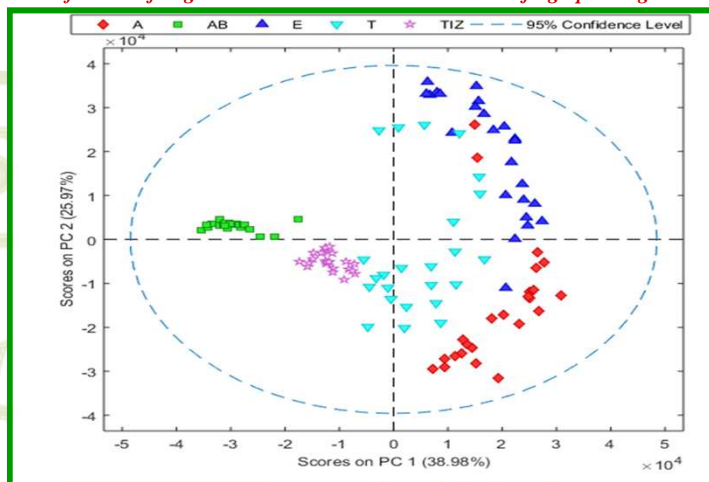


Fig. (3). PCA scores plot (PC1-PC2) based on UPLC-ESI-TOF/MS data

Table. (1). % correct classification of Argan kernels polyphenols with different multivariate methods using cross-validation

Data	Chemometric tools	Classes					
		A	A-B	E	T	Tiz	
UPLC/DAD	PLS-DA	100	100	100	100	100	
	SVM	C-SVM	100	100	100	100	100
		nu-SVM	100	100	100	100	100
	SIMCA	100	100	100	100	100	
	KNN	90	92	100	88	95	
UPLC/TOFMS	PLS-DA	100	100	100	100	100	
	SVM	C-SVM	100	100	100	100	100
		nu-SVM	95	98	100	100	100
	SIMCA	100	100	100	100	100	
	KNN	85	92	95	92	98	

Conclusions

Principal component analysis (PCA) was applied as exploratory technique to distinguish the five origins from the chromatographic data. On the other hand, three multivariate classification techniques, Partial Least Squares Discriminant Analysis (PLS-DA), Soft Independent Modeling of Class Analogies (SIMCA), and Support Vector Machine (SVM), were used to classify the samples in the predefined classes. The classification models and their abilities were highlighted.

The approaches applying either DAD or MS detection were compared. For the different classification techniques, either the results based on UPLC-DAD fingerprinting or UPLC-MS metabolomic profiling allowed classifying and categorizing the samples with high accuracy.

Summarized, the developed fingerprints and their metabolomics-based data handling was successfully applied for the geographical traceability evaluation of Moroccan Argan kernels and their extracted polyphenols.

References

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- [2] Manthaus, B., Guillaume, D., Gharby, S., Haddad, A., Harhar, H., & Charrouf, Z. Effect of processing on the quality of edible argan oil. *Food chemistry*, 120(2), 426-432, 2010.

