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COM O ALTO PATROCÍNIO DE SUA EXCELÊNCIA



O Presidente da República

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10º Encontro de Cromatografia

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PC3	Fatty acid profile of seaweeds from the North Portuguese Coast	70
	<i>Sara Sousa, Susana Machado, Cristina Soares, Elsa Vieira, Valentina F. Domingues, Ana P. Carvalho, Manuela Correia, M. João Ramalhosa, Teresa Oliva-Teles, Simone Morais, Cristina Delerue-Matos</i>	
PC4	GC-MS identification of oligosaccharides produced by nonenzymatic transglycosylation reactions	71
	<i>Soraia P. Silva, Ana S.P. Moreira, M. Rosário M. Domingues, Dmitry V. Evtuygin, Elisabete Coelho, Manuel A. Coimbra</i>	
PC5	Chemical characterization of three <i>Thymus</i> species: <i>T. herba-barona</i>, <i>T. pseudolanuginosus</i> and <i>T. caespititius</i>	72
	<i>Andrea F. Afonso, Olívia R. Pereira, Artur M.S. Silva, Susana M. Cardoso</i>	
PC6	Phytochemicals of <i>Salvia africana</i> and <i>Salvia elegans</i> and <i>Salvia officinalis</i> 'Icterina'	73
	<i>Andrea F. Afonso, Olívia R. Pereira, Artur M.S. Silva, Susana M. Cardoso</i>	
PC7	Applying an API HPLC Related Substances Monograph Method to an Inhalation Drug Product	74
	<i>Andreia Costa, Rúben Chaves, Sofia Silva</i>	
PC8	Perfil cromatográfico em ácidos gordos de seis génotipos de <i>Portulaca olerace</i> L.: uma fonte alternativa de ómega-3	75
	<i>Ângela Fernandes, Spyridon A. Petropoulos, Anestis Karkanis, Lillian Barros, Georgia Ntatsi, Konstantinos Petrotas, Christos Lykas, Ebrahim Khah, Isabel C.F.R. Ferreira</i>	
PC9	Fatty acids profile contribution for the discrimination of olive oil production year	76
	<i>Nuno Rodrigues, Susana Casal, António M. Peres, José A. Pereira</i>	
PC10	Monitoring fructooligosaccharides production using <i>Aspergillus aculeatus</i> by HPLC-ELSD	77
	<i>Aelina Lama, Sara Silvério, Ana C.A. Veloso, Lígia R. Rodrigues, Teresa Dias, António M. Peres</i>	
PC11	Selection of SPME fiber for the identification of the pheromone rhynchophorol by GC/MS	78
	<i>Arão C. Viana, Ingrid G. Ramos, Ananda M. Carvalho, Edeilza L. dos Santos, Janice I. Druzian</i>	
PC12	Similaridade da farinha da casca do maracujá amarelo (<i>Passiflora edulis flavicarpa</i>) com pectina e ácido galacturônico comerciais por CLAE/IR	79
	<i>Emanuela M. Coelho, Arão C. Viana, Luciana C. de Azevedo, Janice I. Druzian</i>	
PC13	Optimization of an analytical method for the determination of underivatized triclosan and related compounds by gas chromatography-triple quadrupole mass spectrometry	80
	<i>Cátia Magro, Davide Mendes, Marco Silva, Alexandra Ribeiro, Eduardo Mateus</i>	
PC14	Development and validation of an HPLC method for quantification of the biocide Econeal®	81
	<i>Cátia Vilas-Boas, Sara Cravo, Emilia Sousa, Madalena Pinto, Marta Correia-da-Silva</i>	
PC15	Efeito do processamento no perfil lipídico do feijão mangalô (<i>Phaseolus lunatus</i>) germinado	82
	<i>Clicia M.J. Benevides, Sónia Soares, Maria A. Nunes, Rita C. Alves, Maria Beatriz P.P. Oliveira</i>	
PC16	Vitamin E profile of green (<i>in natura</i>) seeds from different species of legumes	83
	<i>Cátia Araújo, Rita C. Alves, Sílvia Bessada, Anabela S.G. Costa, Clícia M.J. Benevides, Graça Soveral, M. Beatriz P.P. Oliveira</i>	
PC17	RP-HPLC analysis of 21 amino acids in edible seaweeds from the Portuguese coast after OPA/FMOC derivatization	84
	<i>Cristina Soares, Elsa Vieira, Susana Machado, Manuela Correia, M. João Ramalhosa, Valentina F. Domingues, Ana P. Carvalho, Teresa Oliva-Teles, Simone Morais, Cristina Delerue-Matos</i>	
PC18	Ion source-MS parameters optimization for pharmaceuticals compounds	85
	<i>Paula Paíga, Luís M.S. Silva, Cristina Delerue-Matos</i>	

PC-09

Fatty acids profile contribution for the discrimination of olive oil production year

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Olive oil is a highly appreciated food product mainly due to its nutritional and healthy properties. Olive oils (cv. Arbequina) produced during 4 consecutive crop years were evaluated regarding some quality attributes, fatty acids (GC-FID), and tocopherol (HPLC-FLD) compositions, total phenols contents (Folin-Ciocalteu) and radical scavenging activities (DPPH and ABTS). The results showed that, based on all parameters it was possible to split the olive oil according to the production year, using Principal Component Analysis (PCA). Also, Linear Discriminant Analysis (LDA) together with the simulated annealing (SA) variable selection meta-heuristic algorithm showed that the contents of C16:0, C16:1, C17:0, C18:1, C18:2, C18:3, C20:0, C20:1, SFA and PUFA allowed discriminating the olive oil according to the production year (Figure 2), pointing out that fatty acids composition was greatly affected by the production year. Indeed, a predictive overall mean sensitivity of 99.6% was achieved using a repeated K-fold cross-validation procedure (4 folds × 10 repeats).

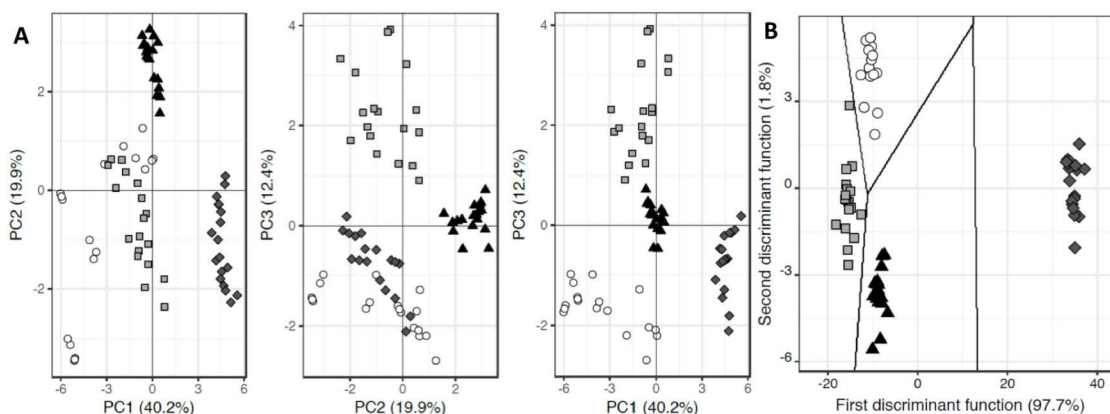


Figure 1. (A) PCA showing the olive oil split according to the production year, using all variables evaluated. (B) LDA: olive oil grouped by production year based on the fatty acids profile (C16:0, C16:1, C17:0, C18:1, C18:2, C18:3, C20:0, C20:1, SFA and PUFA)

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INTRODUCTION

- ✓ Olive oil is a highly appreciated food product mainly due to its nutritional and healthy properties.
- ✓ Olive oil composition and olive trees productivities are strongly influenced by edaphoclimatic conditions, olive tree density, olive grove age and olive tree variety.
- ✓ In this work, the possibility of assessing olive oil production year based on physicochemical quality attributes, fatty acids and tocopherol profiles, total phenols contents and radical scavenging activities (DPPH and ABTS)
- ✓ cv Arbequina olive oils produced in a high-density olive grove, installed in a non-traditional olive production region in **Valladolid Province (Spain)** during 4 consecutive crop years, were evaluated.



Olive oil analysis

Physicochemical Analysis

Free Acidity (FA)
Peroxide Value (PV)
UV-Vis Extinction Coefficients (K_{232} , K_{270} , ΔK)

Oxidative resistance (Rancimat)

Fatty acids profile (GC-FID)

SFA: C16:0; C17:0; C18:0; C20:0; C22:0; C24:0
MUFA: C16:1; C17:1; C18:1; C20:1
PUFA: C18:2; C18:3

Tocopherol profile (HPLC-FLD)

α -, β - and γ -tocopherol

Total phenol content (Folin-Ciocalteu)

Radical scavenging activities

DPPH
ABTS*



AIMS

OLIVE OILS PHYSICO-CHEMICAL COMPOSITION AND PROPERTIES

Establishment of olive oils' physicochemical putative *fingerprint*

Chemometric tools

- Principal component analysis (PCA)
- Linear discriminant analysis (LDA)
- Simulated annealing (SA) variable selection algorithm
- Leave-one-out cross-validation (LOO-CV)

Predictive performance for assessing cv Arbequina olive oils production year:

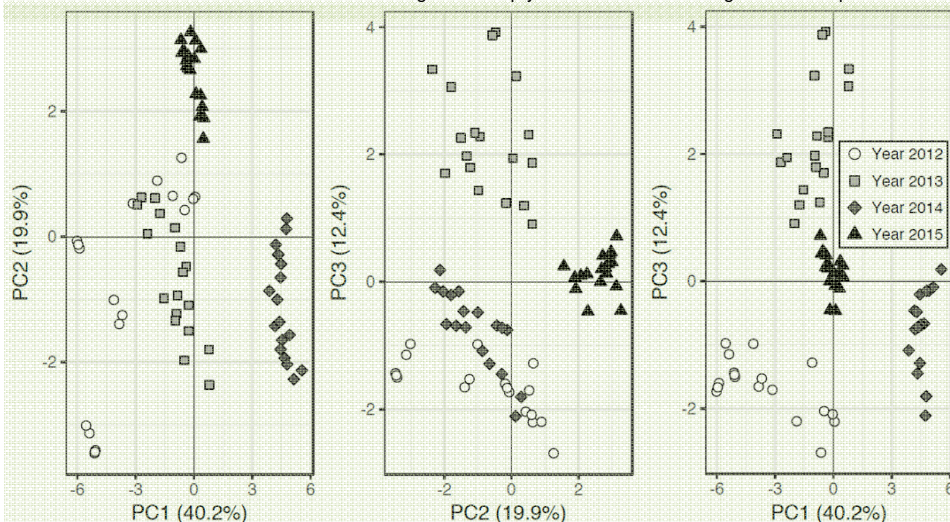
Repeated K-fold-CV (10 repeats; 4 folds → 25% of the original data for internal validation purposes)

RESULTS

PCA:

3 first PCs → explained 72.5% of the data variability

Allowed the differentiation of olive oils according to the crop year → BUT need a huge amount of parameters



LDA-SA:

- Selection of sub-set of parameters using the SA algorithm
- Minimum number of parameters
- Maximum correct classification, LOO-CV
- Internal-validation: repeated K-fold-CV

2 first DFs

- explained 99.5% of the data variability
- discriminant model based on only fatty acids

C16:0, C17:0, C20:0

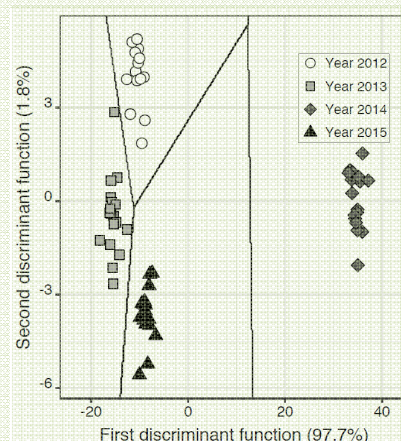
C16:1, C18:1, C20:1

C18:2, C18:3

SFA, PUFA

Correct classifications:

100% original data
100% LOO-CV
99.6±1.4% repeated K-fold-CV



CONCLUSIONS

- All cv Arbequina olive oils evaluated fulfilled the physicochemical thresholds for being classified as EVOO.
- The olive oils' compositions varied with the crop year, allowing to naturally split them according to the crop year (PCA results).
- LDA-SA models based only on fatty acids composition could be successfully applied to discriminate olive oils according to the crop year, pointing out that of fatty acids may be used as putative fingerprints for assessing olive oil production year.

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