XXII Encontro Luso-Galego

Química

9 a 11 novembro 2016

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TIRAGEM
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Evaluation of Tunisian olive oils from different cultivars

Souihli Slim[1,2], Nuno Rodrigues[3,4], Luís G. Dias[1,5], Ana C. A. Veloso[6,7], José A. Pereira[8], Souheib Oueslati[2], António M. Peres[9,*]

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Olive oil is a highly appreciated food product due to sensory and healthy attributes, being quite prone to frauds. So, physicochemical evaluation of olive oils is legally required. In this study, 43 olive oil samples produced in Tunisia from different olive cultivars (groups: Sahli cv – 11 samples; Chetoui cv- 26 samples; and, Other cvs – 4 samples including Leguim cv and Arbequina cv) were physicochemically evaluated taking into account: (i) free acidity (FA), K_{232} and K_{270} extinction coefficients, ΔK, and, peroxide values (PV), required for quality level classification (i.e., extra-virgin, virgin and lampante olive oil: EVOO, VOO and LOO); and (ii) other useful data for olive oil overall characterization (total phenols (TP); antioxidant capacity (DPPH); and, oxidative stability (OS)). Based on the levels found for FA, PV and extinction coefficients (K_{232}, K_{270} and ΔK), the 43 olive oils were classified as: EVOO (4 samples), VOO (5 samples) and LOO (33 samples). It was verified that TP, DPPH and OS levels of EVOO, VOO and LOO samples were statistically similar (*P*-value ≥ 0.2340 for one-way ANOVA). Also, the olive cultivar (i.e., Sahli cv, Chetoui cv and other cvs) did not statistically influenced the mean levels of the FA, PV, TP, K_{232} and DPPH evaluated (*P*-value > 0.05), and slightly influenced the mean levels of K_{270} and OS (*P*-value < 0.05). Finally, as expected an almost linear tendency could be established between DPPH and OS or TP. The possibility of using the 8 physicochemical parameters for classifying olive oils according to cultivar; as well as TP, DPPH and OS for differentiating among olive oil quality levels was assessed through a fusion physicochemical data-chemometric tools approach and further evaluated using a repeated K-fold cross-validation procedure. The results from the linear discriminant analysis (LDA) coupled with a simulated annealing (SA) variable selection algorithm pointed out that the physicochemical data evaluated did not possess the aimed discrimination potential (sensitivities around 80% for cross-validation). So, for these olive oils, the identification of potential putative markers for the recognition of olive oil cultivar and quality level must be performed. Alternatively, the potential use of other analytical procedures like electrochemical analysis should be evaluated considering the satisfactory results already achieved by the research team [1].

Acknowledgments
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References

[1] L.G. Dias, A. Fernandes, A.C.A. Veloso, A.A.S.C. Machado, J.A. Pereira, A.M. Peres, Food Chemistry, 160 (2014) 321.

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EVALUATION OF TUNISIAN OLIVE OILS FROM DIFFERENT CULTIVARS

Souihli Slim[1,2], Nuno Rodrigues[3,4], Luís G. Dias[1,5], Ana C.A. Veloso[6,7], José A. Pereira[8], Souheib Oueslati[2], António M. Peres[9]

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INTRODUCTION

✓ Olive oil commercialization has a great impact in the regional economy of Tunisia

✓ It is a high-value food product, quite prone to frauds.

✓The physical-chemical characterization of olive oils produced from autochthonous Tunisian olive cultivars allow to minimize the risk of usual adulterations

✓In this work, Tunisian olive oils (namely from Chétoui and Sahli cultivars) are evaluated aiming to propose putative classification biomarkers

CHEMOMETRICS

Establishment of the best LDA-SA models using physicochemical fingerprints of olive oils:

→ variable selection with simulated annealing (SA) algorithm

→ linear discriminant analysis (LDA)

→ sub-set with minimum number of parameters => maximum correct classification

✓ Leave-one-out cross validation (LOO-CV)

✓ Repeated *K*-fold-CV (4 folds×10 repeats): **25% data internal validation**

OBJECTIVES

Prospective physicochemical characterization of TUNISIAN olive oils

→ Monovarietal olive oils from autochthonous Tunisian cultivars: cv Chétoui and cv Sahli

→ Olive oils physicochemical quality level assessment (edible and inedible olive oils):

- Extra virgin olive oil (EVOO)
- Virgin olive oil (VOO)
- Lampante olive oil (LOO)

➢ **TO FIND:** olive oils' putative biomarkers → to define the best physicochemical *fingerprints*

➢ **TO ALLOW:** olive oils' discrimination according to:

1) Olive oil physicochemical quality (EVOO, VOO or LOO)

2) Olive cultivar (cv Chétoui or cv Sahli)

SAMPLES

Olive oil samples produced in TUNISIA (olive variety)

- cv Sahli (26 olive oils: autochthonous)
- cv Chétoui (11 olive oils: autochthonous)
- cv El Leguim (2 olive oils: autochthonous)
- cv Arbequina (1 olive oil: introduced)
- cv Koroneiki (1 olive oil: introduced)

RESULTS

1) Tunisian olive oils quality evaluation

ACCORDING TO PHYSICOCHEMICAL DATA

(European Regulation 2568/91 and subsequent amendments)

Extra-virgin olive oils (EVOO) - 4 samples; Virgin olive oils (VOO) - 6 samples; Lampante olive oils (LOO) - 33 samples

2) Monovarietal olive oils evaluation

ACCORDING TO OLIVE CULTIVARS

(Label information)

Monovarietal cv Sahli olive oils - 26 samples;

Monovarietal cv Chétoui olive oils - 11 samples

Physicochemical analytical assays

- Free acidity (FA)
- Peroxide values (PV)
- K_{232} and K_{270} extinction coefficients and ΔK
- Oxidative stability (OS, *Rancimat* determinations)
- Antioxidant activity (DPPH)
- Total phenols (TP)
- Tocopherols (α-, β- and γ-)
- Vitamin E
- Fatty acids profile (including SFA, MUFA and PUFA)

One-way ANOVA (+ Tukey's test)

C15:1 (*P*-value = 0.0191):

$[C15:1]_{EVOO} > [C15:1]_{VOO} = [C15:1]_{LOO}$

All other parameters: no statistical significant Variations (*P*-value > 0.06)

t-Student test

Physicochemical parameter	Tunisian authocthnous cultivar cv Chétoui	cv Sahli	*P*-value
PV	↓	↑	0.0393 $
Total phenols	↑	↓	0.0388 $
OS	↑	↓	0.0013 $
DPPH	↑	↓	0.0101 $
SFA	↓	↑	<0.0001 $
C16:0	↑	↓	<0.0001 $
C18:0	↑	↓	0.0001 $
C20:0	↑	↓	0.0068 $
C24:0	↓	↑	0.0097 $
MUFA	↑	↓	<0.0001 $
C18:1	↑	↓	<0.0001 $
PUFA	↑	↓	0.0076 $
β-tocopherol	↑	↓	0.0328 #
γ-tocopherol	↑	↓	0.0003 $

$t-Student test equal variances

#t-Student test unequal variances (Welch's correction)

Physicochemical parameter	Tunisian authocthnous cultivar cv Chétoui	cv Sahli	*P*-value
FA			0.2144 $
K_{232}			0.0636 $
K_{270}			0.0845 $
ΔK			0.3914 #
C14:0	Contents		0.0815 #
C15:0	statistically		0.1526 $
C17:0	equal		0.0663 #
C21:0			0.4406 $
C22:0	(5% significance level)		0.0914 #
C14:1			0.1361 $
C17:1			0.4548 #
C22:1			0.0746 #
C24:1			0.3900 $
C18:2			0.0807 $
C18:3			0.3150 #
α-tocopherol			0.3332 $
Vitamin E			0.2262 $

$t-Student test equal variances

#t-Student test unequal variances (Welch's correction)

LDA-SA classification models:

Olive oils' quality level discrimination: EVOO, LOO & LOO

↓

LDA-SA model (7 parameters):

C17:0, C24:0, C17:1, C24:1, PUFA, trans total and total trans linoleic-linolenic

↓

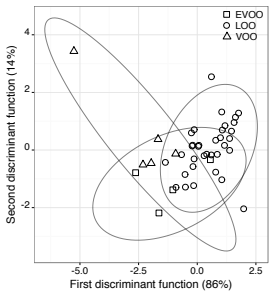
LOO-CV:

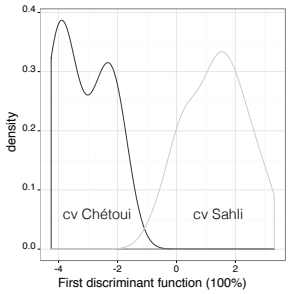
79% of predictive correct classifications

↓

Repeated K-fold-CV:

80% ± 10% of predictive correct classifications





Olive oils' discrimination by olive cultivars: cv Chétoui & cv Sahli

↓

LDA-SA model (10 parameters):

PV, TP, C17:0, C20:0, C22:0, PUFA, C18:2cc, trans total, total trans oleic acid and γ-tocopherol

↓

LOO-CV:

95% of predictive correct classifications

↓

Repeated K-fold-CV:

94% ± 7% of predictive correct classifications

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CONCLUSIONS

Statistical analysis pointed out that:

→ Olive cultivar has a high effect on several physicochemical parameters of Tunisian olive oils

→ Olive oil quality level did not significantly affect the physicochemical parameters of Tunisian olive oils

LDA-SA models could be used to:

→ Tunisian olive oils' predictive classification according to olive cultivar;

→ Tunisian olive oils' predictive classification according to quality grade

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CERTIFICADO

Certifica-se que

Nuno Miguel Sousa Rodrigues

apresentou a Comunicação em Painel intitulada

Evaluation of Tunisian olive oils from different cultivars

no XXII Encontro Luso-Galego de Química, realizado no Instituto Politécnico de Bragança, de 09/11/2016 a 11/11/2016.

Pel´A Comissão Organizadora

Instituto Politécnico de Bragança,

11 de Novembro de 2016