



XXII Encontro Luso-Galego
Química

9 a 11 novembro 2016

Instituto Politécnico de Bragança | BRAGANÇA - PORTUGAL



Livro de Resumos

<http://xxiilgq.eventos.chemistry.pt>



SOCIEDADE
PORTUGUESA
DE QUÍMICA



Colegio Oficial de
Químicos de Galicia



9 a 11 novembro 2016

**Instituto Politécnico de Bragança
BRAGANÇA – PORTUGAL**



TÍTULO

Livro de Resumos do XXII Encontro Luso-Galego de Química

EDITORES

Helder T. Gomes, Maria Olga A. S. Ferreira, João Barreira, Joana Amaral

EDIÇÃO

Sociedade Portuguesa de Química
Av. da República, 45 – 3º Esq
1050-187 Lisboa – Portugal

DATA

Novembro de 2016

EXECUÇÃO GRÁFICA

IPB, Soraia Maduro (design)
Sersilito – Maia (impressão)

FOTO DE CAPA

Rami Arafah

CATALOGAÇÃO RECOMENDADA

Livro de Resumos do XXII Encontro Luso-Galego de Química
Instituto Politécnico de Bragança, Bragança, Portugal, 2016, 336 páginas

ISBN

978-989-8124-17-3

TIRAGEM

350 exemplares

@ Sociedade Portuguesa de Química

Direitos reservados. Proibida a reprodução deste livro por qualquer meio, total ou parcialmente, sem autorização expressa da Sociedade Portuguesa de Química.

Os Editores declaram que o conteúdo dos resumos científicos é da inteira responsabilidade dos respetivos autores.

XXII ENCONTRO LUSO-GALEGO DE QUÍMICA

Organizado sob os auspícios de
Sociedade Portuguesa de Química
Colégio Oficial de Químicos de Galicia

COMISSÃO DIRETIVA

Baltazar Romão de Castro (FCUP)
José Luís Costa Lima (FFUP)
José Luís Figueiredo (FEUP)
Pelayo Rubido Muñiz (COLQUIGA)
Juan Mogin del Pozo (COLQUIGA)
Antonio Macho Senra (COLQUIGA)

COMISSÃO CIENTÍFICA

Joaquim Luís Faria (FEUP)
Artur Silva (UA)
Victor Freitas (FCUP)
Mario Ferruzzi (NCSU, USA)
Ignacio Pérez Juste (UVigo)
Moisés Canle López (UdC)
Pilar Bermejo Barrera (USC)

COMISSÃO ORGANIZADORA

Helder Gomes (IPB) - Presidente
Ana Isabel Pereira (IPB)
Ana Vera Machado (UM)
Baltazar Romão de Castro (FCUP)
Filomena Barreiro (IPB)
Isabel Ferreira (IPB)
Joana Amaral (IPB)
João Barreira (IPB)
José Alcides Peres (UTAD)
José Luís Costa Lima (FFUP)
José Luís Figueiredo (FEUP)
Lillian Barros (IPB)
Manuel Coimbra (UA)
Olga Ferreira (IPB)

QAMA52	Phenolic extraction from almond hulls: effect of time, temperature and ultrasound <u>I. Prgomet</u> , B. Gonçalves, R. Domínguez-Perles, N. Machado, N. Pascual-Seva, A. Barros
QAMA53	Raw material influence in mead production <u>Regina Santos</u> , Ana Paula Pereira, Letícia Estevinho, Ilda Caldeira, Ofélia Anjos
QAMA54	Direct analysis of vitamin A, vitamin E, carotenoids, chlorophylls and free sterols in animal and vegetable fats by NP-HPLC-DAD/FD <u>R. Cruz</u> , S. Casal
QAMA55	Estudo da composição química de seis génotipos de <i>Portulaca oleracea</i> L. <u>Ângela Fernandes</u> , Spyridon A. Petropoulos, Anestis Karkanis, Lillian Barros, Georgia Ntatsi, Konstantinos Petrotos, Christos Lykas, Ebrahim Khah, Isabel C. F. R. Ferreira
QAMA56	Caracterização físico-química da flor de <i>Borago officinalis</i> em dois estados de floração <u>L. Fernandes</u> , S. Casal, J. A. Pereira, J. A. Saraiva, Elsa Ramalhosa
QAMA57	Effect of <i>Fucus vesiculosus</i> powder addition on colour and textural properties of gluten-free cookies based on chestnut flour <u>R. Moreira</u> , F. Chenlo, J. Sineiro, M. D. Torres, S. Arufe
QAMA58	Chemical composition and oxidative stability of Algerian <i>Moringa oleifera</i> whole seed and kernel oils <u>S. Boukandoul</u> , S. Casal, N. Hassissène, F. Zaidi
QAMA59	Evaluation of the antioxidant and antibacterial activity of spearmint (<i>Mentha spicata</i> L.) <u>Cláudia S. Moreira</u> , Ana Sofia Artilheiro, Maria João Afonso, Joana S. Amaral
QAMA60	Evaluation of Tunisian olive oils from different cultivars Souihli Slim, <u>Nuno Rodrigues</u> , Luís G. Dias, Ana C. A. Veloso, José A. Pereira, Souheib Oueslati, António M. Peres
QAMA61	Water adsorption and desorption isotherms of <i>Undaria pinnatifida</i> brown seaweed <u>F. Chenlo</u> , J. Sineiro, M. D. Torres, S. Arufe, R. Moreira
QAMA62	Estimation of water sorption of sucrose from glucose and fructose data <u>M. D. Torres</u> , D. M. Prieto, F. Chenlo, R. Moreira
QAMA63	<i>In silico</i> and experimental analysis of DNA markers for <i>Citrus aurantium</i> identification in herbal medicines Inês Sousa, Joana Costa, <u>Joana S. Amaral</u> , M. Beatriz P. P. Oliveira, Isabel Mafra
QAMA64	Potencial antioxidante de <i>Stevia rebaudiana</i> Bertoni cultivada em Portugal e conservada em diferentes condições térmicas Marisa R. Barroso, <u>Lillian Barros</u> , M. Ângelo Rodrigues, Maria João Sousa, Celestino Santos-Buelga, Isabel C. F. R. Ferreira
QAMA65	Estudo da hidrólise do pigmento natural Curcumina presente na planta <i>Curcuma longa</i> <u>V. Martins</u> , M. Valero
QAMA66	Phenolic compounds content, antioxidant and antimicrobial activities of juniper (<i>Juniperus communis</i> L.) <u>Isabel Bacém</u> , Maria João Afonso, Joana S. Amaral
QAMA67	Mixing properties of gluten-free dough based on chestnut flour enriched with <i>Fucus vesiculosus</i> brown seaweed <u>S. Arufe</u> , M. D. Torres, F. Chenlo, J. Sineiro, R. Moreira
QAMA68	Air drying kinetics modelling of brown seaweed <i>Undaria pinnatifida</i> <u>J. Sineiro</u> , F. Chenlo, M. D. Torres, S. Arufe, R. Moreira
QAMA69	Tratamento de <i>Melissa officinalis</i> L. com irradiação gama e feixe de elétrons aumenta a concentração de compostos fenólicos Eliana Pereira, <u>João C. M. Barreira</u> , Amílcar L. Antonio, Celestino Santos-Buelga, Lillian Barros, Isabel C. F. R. Ferreira
QAMA70	Nutritional profile of <i>Phaseolus lunatus</i> and <i>Cajanus caja</i> seeds A. S. G. Costa, C. M. J. Benevides, <u>M. B. P. P. Oliveira</u>

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. Pereira⁸, Souheib Oueslati², António M. Peres^{9,*}**

¹ESA, Instituto Politécnico de Bragança, Campus Santa Apolónia, 5300-253 Bragança, Portugal

²Université Libre de Tunis, 32 Bis avenue Kheireddine Pacha, 1002 Tunis, Tunisia

³REQUIMTE-LAQV/CIMO, ESA, Instituto Politécnico de Bragança, Campus Santa Apolónia, 5300-253 Bragança, Portugal

⁴Universidad de León, Departamento de Ingeniería Agrária, Av. Portugal, nº 41, 24071 León, España.

⁵CQ-VR, Centro de Química – Vila Real, UTAD, 5001-801 Vila Real, Portugal

⁶Instituto Politécnico de Coimbra, ISEC, DEQB, Rua Pedro Nunes, Quinta da Nora, 3030-199 Coimbra, Portugal

⁷CEB - Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal

⁸REQUIMTE-LAQV, ESA, Instituto Politécnico de Bragança, Campus Santa Apolónia, 5300-253 Bragança, Portugal

⁹Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), ESA, Instituto Politécnico de Bragança, Campus Santa Apolónia, 5300-253 Bragança, Portugal

*peres@ipb.pt

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

This work was financially supported by Project POCI-01-0145-FEDER-006984 – Associate Laboratory LSRE-LCM and by Project UID/QUI/00616/2013 – CQ-VR both funded by FEDER through COMPETE2020 - Programa Operacional Competitividade e Internacionalização (POCI) – and by national funds through FCT - Fundação para a Ciência e a Tecnologia. Strategic funding of UID/BIO/04469/2013 unit is also acknowledged. Nuno Rodrigues thanks FCT, POPH-QREN and FSE for the Ph.D. Grant (SFRH/BD/104038/2014).

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.



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. Pereira⁸, Souheib Oueslati², António M. Peres⁹

1: ESA, Instituto Politécnico de Bragança, Bragança, Portugal; **2:** Université Libre de Tunis, Tunis, Tunisia; **3:** Universidad de León, Departamento de Ingeniería Agrária, León, España; **4:** REQUIMTE-LAQV/CIMO, ESA, Instituto Politécnico de Bragança, Bragança, Portugal; **5:** CQ-VR, Centro de Química – Vila Real, Universidade de Trás-os-Montes e Alto Douro, Vila Real, Portugal; **6:** Instituto Politécnico de Coimbra, ISEC, DEQB, Coimbra, Portugal; **7:** CEB, University of Minho, Braga, Portugal; **8:** REQUIMTE-LAQV, ESA, Instituto Politécnico de Bragança, Bragança, Portugal; **9:** LSRE-LCM, ESA, Instituto Politécnico de Bragança, Bragança, Portugal

(*) peres@ipb.pt

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

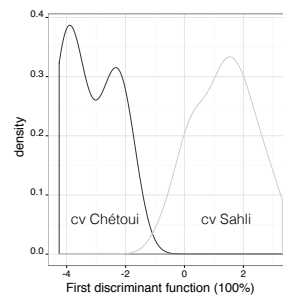
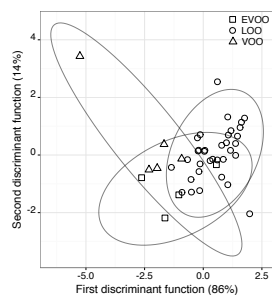
Variations (P-value > 0.06)

t-Student test

Physicochemical parameter	Tunisian autochthonous cultivar cv Chétoui	cv Sahli	P-value	Physicochemical parameter	Tunisian autochthonous cultivar cv Chétoui	cv Sahli	P-value
PV	↓	↑	0.0393 [‡]	FA			0.2144 [‡]
Total phenols	↓	↑	0.0388 [‡]	K_{232}			0.0636 [‡]
OS	↓	↑	0.0013 [‡]	K_{270}			0.0845 [‡]
DPPH	↓	↑	0.0101 [‡]	ΔK			0.3914 [‡]
SFA	↓	↑	<0.0001 [‡]	C14:0	Contents statistically equal		0.0815 [‡]
C16:0	↓	↑	<0.0001 [‡]	C15:0			0.1526 [‡]
C18:0	↓	↑	0.0001 [‡]	C17:0			0.0663 [‡]
C20:0	↓	↑	0.0089 [‡]	C21:0			0.4406 [‡]
C24:0	↓	↑	0.0097 [‡]	C22:0	(5% significance level)		0.0914 [‡]
MUFA	↓	↑	<0.0001 [‡]	C14:1			0.1361 [‡]
C18:1	↓	↑	<0.0001 [‡]	C17:1			0.4548 [‡]
PUFA	↓	↑	0.0076 [‡]	C22:1			0.0746 [‡]
β -tocopherol	↓	↑	0.0328 [‡]	C24:1			0.3900 [‡]
γ -tocopherol	↓	↑	0.0003 [‡]	C18:2			0.0807 [‡]
				C18:3			0.3150 [‡]
				Vitamin E			0.3332 [‡]
							0.2282 [‡]

[‡] Student test equal variances
[‡] 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

Acknowledgements

This work was financially supported by Project POCI-01-0145-FEDER-006984-Associate Laboratory LSRE-LCM and by Project UIDB/QUI/00616/2013-CQ-VR both funded by FEDER - Fundo Europeu de Desenvolvimento Regional through COMPETE2020-Programa Operacional Competitividade e Internacionalização (POCI) - and by national funds through FCT-Fundação para a Ciência e a Tecnologia, Portugal. Strategic funding of UIDB/BIQ/04469/2013 unit is also acknowledged. Nuno Rodrigues thanks FCT, POPH-OREN and FSE for the Ph.D. Grant (SFRH/BD/104038/2014).

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