



# 10º Encontro Nacional de Cromatografia

Bragança 2017 – 4 a 6 de dezembro

**Abstracts book / Livro de resumos**



SOCIEDADE PORTUGUESA DE QUÍMICA



INSTITUTO POLITÉCNICO DE BRAGANÇA Centro de Investigação de Montanha

COM O ALTO PATROCÍNIO DE SUA EXCELÊNCIA



*O Presidente da República*

## Title

10th Chromatography Meeting

## Título

10º Encontro de Cromatografia

## Authors / Autores

António M. Peres (Instituto Politécnico de Bragança, Portugal)

Lillian Barros (Instituto Politécnico de Bragança, Portugal)

Luís G. Dias (Instituto Politécnico de Bragança, Portugal)

Isabel C.F.R. Ferreira (Instituto Politécnico de Bragança, Portugal)

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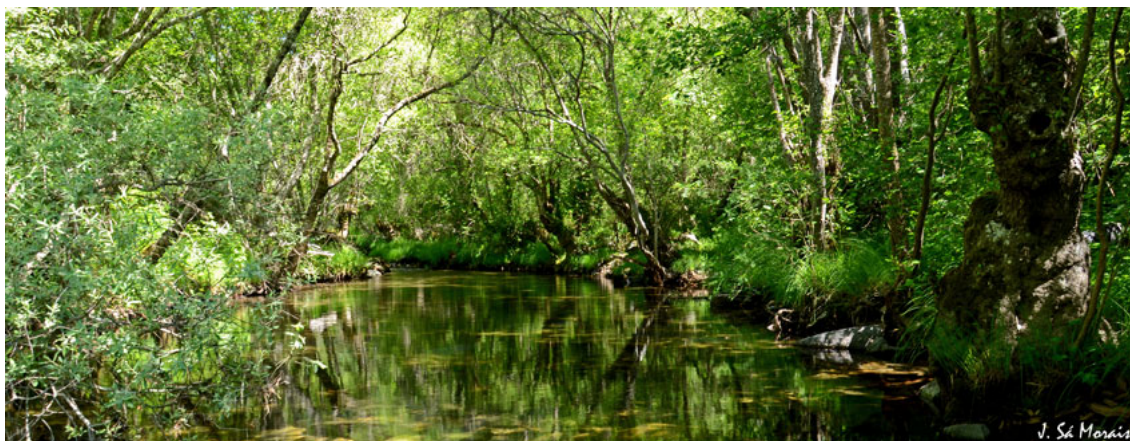
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Raquel Aires Barros (Universidade de Lisboa)  
Sílvia M. Rocha (Universidade de Aveiro)



## Program / Programa

Time	December 4	
8:00-9:00		• Registration
9:00-10:00		• Opening session in <i>Auditorium Dionísio Gonçalves</i>
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>Isabel C.F.R. Ferreira</b> ( <i>Instituto Politécnico de Bragança</i> )		
10:00-11:00	PL-01	<b>In-tube SPME from open tubular column (in-tube SPME-LC) to directly coupled to mass spectrometry</b> <b>Maria Eugênia Costa Queiroz</b> <i>Universidade de São Paulo, Brasil</i>
11:00-11:30		• Coffee Break and panel session
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>Sílvia M. Rocha</b> ( <i>Universidade de Aveiro</i> )		
11:30-12:00	IC-01	<b>Different Strategies Based on Micro(extraction) Followed by GC-MS/MS and LC-MS/MS for the Determination of Personal Care Products in Cosmetics and Environmental Samples</b> <b>Maria Llompart</b> <i>University of Santiago de Compostela, Espanha</i>
12:00-12:30	EC-01	<b>LCMS Technologies: Introducing the Orbitrap for Ultrahigh Resolution Exact Mass and Unequivocal ID</b> <b>Daniel Ettlin</b> <i>Thermo Unicam Sistemas Analíticos</i>
12:30-14:30		• Lunch
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>Nuno Mateus</b> ( <i>Universidade do Porto</i> )		
14:30-15:00	IC-02	<b>Back to Basics: Considerations in eco-user-friendly/cost-effective micro-extraction techniques</b> <b>José Nogueira</b> <i>Universidade de Lisboa, Portugal</i>
<b>15:00-16:30</b>	<b>Oral session 1A / Sessão Oral 1A</b>	
	OC-01	<b>A multiresidue targeting approach for pesticide detection in olive oil: the role of dual-layer solid-phase extraction based on molecular imprinting technology</b> <b>Raquel Garcia</b>
	OC-02	<b>New brush-type chiral stationary phases based on xanthone derivatives for liquid chromatography</b> <b>Carla Fernandes</b>
	OC-03	<b>Chromatographic techniques to assess the profile of biomolecules in different mycorrhizal mushroom species</b> <b>Filipa Reis</b>
	OC-04	<b>Multicolumn based liquid chromatography processes for the separation of nadolol racemates</b> <b>António Ribeiro</b>
	OC-05	<b>An expanded bed chromatography approach for improving human mesenchymal stem cells purification</b> <b>Ricardo Silva</b>

OC-06 [Chromatographic analysis of biological samples using monolithic columns](#)  
**Marcela Segundo**

**Moderator / Moderador - Auditorium B**

**Marco Gomes da Silva** (Universidade Nova de Lisboa)

**15:00-16:30**

**Oral session 1B / Sessão Oral 1B**

OC-07 [Avaliação da qualidade do ar em espaços de um edifício de ciências](#)  
**Sara Santos**  
[Engineered polymer particles for the valorization of phenolic compounds present in mixtures obtained through supercritical extraction](#)

OC-08 [Thermostability studies of oil-soluble cyanidin-3-glucoside dyes](#)  
**Catarina Gomes**

OC-09 [Adsorption equilibrium and kinetics of CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub> on zeolite BETA with different cations and SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> ratio](#)  
**Adriano Henrique**

OC-10 [Seawater degradation studies of gallic acid persulfate, a promising synthetic antifouling agent](#)  
**Cátia Vilas Boas**

OC-11 [BeerOmics: how can advanced gas chromatography help to understand beer aroma properties?](#)  
**Cátia Martins**

16:30-17:00

- Coffee Break + Poster session

**Moderator / Moderador - Auditorium Dionísio Gonçalves**

**José Manuel F. Nogueira** (Universidade de Lisboa)

[Nexera UC Online SFE-SFC-MS System](#)

17:00-17:30

EC-02 **José Manuel Macias**  
*Izasa Scientific*

**17:30-18:00**

**Oral session II / Sessão Oral II**

OC-13 [Phenolic composition, antioxidant and biological activities of Portuguese vine shoot from \*Touriga Nacional\* and \*Tinta Roriz\* varieties](#)  
**Manuela Moreira**

OC-14 [Caracterização química e bioatividades de \*Hibiscus sabdariffa\* L.](#)  
**Inès Jabeur**

19:30

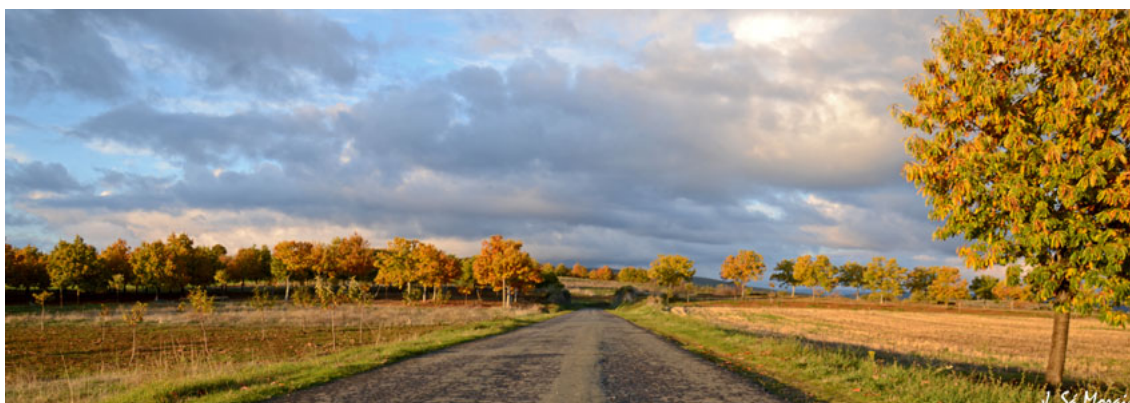
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Time	December 5
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>Marcela Segundo</b> (Universidade do Porto)	
9:00-10:00	PL-02 <b>Green Foodomics: new strategies towards the discovery of functional food ingredients with biological activity</b> <b>Elena Ibanez</b> Institute of Food Science Research – CIAL, Espanha
10:00-10:30	IC-03 <b>Multicolumn Continuous Countercurrent Chromatography for Downstream Processing of Biopharmaceuticals</b> <b>Paulo Mota</b> University Nova de Lisboa, Portugal
10:30-11:00	• Coffee Break + Poster session
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>M. Beatriz Oliveira</b> (Universidade do Porto)	
<b>11:00-12:30</b>	<b>Oral session IIIA / Sessão Oral IIIA</b>
OC-15	Selective capillary coatings for in-tube SPME off-line or on-line with LC-MS/MS for bioanalysis <b>Israel Souza</b>
OC-16	Preparative separation of nadolol racemates by fixed-bed liquid chromatography using C18 columns <b>Rami Arafah</b>
OC-17	Hollow fiber microextraction (HF $\mu$ E) - A new hybrid microextraction technique for trace analysis <b>Alessandra Ide</b>
OC-18	Tape Adsorptive Microextraction - A new analytical approach for sample enrichment <b>Nuno Neng</b>
OC-19	Multidimensional chromatographic techniques applied to chemical ecology <b>Eduardo Mateus</b>
OC-20	Síntese de fase estacionária monolítica e posterior imobilização térmica de polidimetilsiloxano (PDMS) sobre a superfície porosa para aplicação em cromatografia líquida capilar <b>Carla Bottoli</b>
<b>Moderator / Moderador - Auditorium B</b> <b>Helena Soares Costa</b> (Instituto Nacional de Saúde Dr. Ricardo Jorge)	
<b>11:00-12:30</b>	<b>Oral session IIIB / Sessão Oral IIIB</b>
OC-21	Permeation of caffeine, CQA and HMF from Coffee silverskin extracts on EpiSkin™ 3D model <b>Diana Pinto</b>
OC-22	NTME/GC-qMS: a powerful strategy for selection sets of cancer-specific VOMs with potential for cancer differentiation <b>Priscilla Figueira</b>
OC-23	Validation of a dSPE-HPLC methodology for the determination of biogenic amines in wines <b>Juliana Ferreira</b>
OC-24	Looking for new contributions in asthma biomarkers - a chromatographic-based approach <b>José Câmara</b>

	OC-25	Gas-chromatography mass spectrometry analysis of <sup>13</sup> C-labeled fatty acids revealed new information about the ruminal biohydrogenation of linolenic acid <b>Susana Alves</b>
	OC-26	Multidetecção de antibióticos em tecidos comestíveis: evolução de estratégias analíticas <b>Andreia Freitas</b>
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>M. Beatriz Oliveira</b> (Universidade do Porto)		
12:30-13:00	EC-03	A new, fast, simple, and ultra-sensitive determination of semi-volatile organic compounds in water samples by GC-MS/MS Triple Quadrupole system <b>Miguel Ángel Pérez</b> Bruker Applications Development Laboratory
13:00-14:30		• Lunch
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>Victor Freitas</b> (Universidade do Porto)		
14:30-15:00	IC-04	Polyphenols identification. Has LC-MS killed HPLC-DAD <b>Celestino Santos-Buelga</b> University of Salamanca, Espanha
<b>15:00-16:30</b>	<b>Oral session IVA / Sessão Oral IVA</b>	
	OC-27	Chromatographic analysis of nutritional and bioactive compounds in vegetative parts of <i>Fragaria vesca</i> L. obtained by in vitro culture <b>Maria Inês Dias</b>
	OC-28	Liquid by-products from canned fish industry as sources of omega-3 polyunsaturated fatty acids <b>Ana Carvalho</b>
	OC-29	Fingerprinting of volatome profile of lemon ( <i>Citrus limonum</i> ) based on a new analytical approach - NTME/GC-MS analysis <b>José Figueira</b>
	OC-30	Perfil fenólico e bioatividades de maçã portuguesa da variedade "Bravo de Esmolfe" <b>Tânia Pires</b>
	OC-31	The volatile profile for discrimination of lavender and heather honey, using solid phase microextraction and gas chromatography-mass spectrometry <b>Soraia Falcão</b>
	OC-32	<i>Geranium robertianum</i> L. phenolic compounds: individual characterization of stems and leaves profile <b>Marcelo Catarino</b>
<b>Moderator / Moderador - Auditorium B</b> <b>Cristina Delerue Matos</b> (Instituto Politécnico do Porto)		
<b>15:00-16:30</b>	<b>Oral session IVB / Sessão Oral IVB</b>	
	OC-33	Ácido 4-hidrazinobenzoico como agente derivatizante para a determinação de aldeídos por HPLC-UV e LC-MS <b>Pedro Brandão</b>
	OC-34	Effects of natural colourants on the fatty acids profile of different ice cream formulations <b>Custódio Roriz</b>
	OC-35	High Throughput Bar Adsorptive Microextraction (HT-BA $\mu$ E): A novel cost-effective tool for monitoring psychotropic drugs in biological matrices <b>Samir Ahmad</b>

	OC-36	Caracterização do perfil fenólico de agrião por HPLC-DAD-ESI/MS e otimização da extração por alta pressão hidrostática utilizando a metodologia de superfície de resposta <b>José Pinela</b>
	OC-37	Polyols based solvents for the extraction of phenolic compounds from <i>Juglans regia</i> L. leaves <b>Vanessa Vieira</b>
	OC-38	Oncolytic virus purification using multi-column chromatography <b>João Mendes</b>
16:30-17:00		• Coffee Break + Poster session
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>Manuela Pintado</b> (Universidade Católica)		
17:00-17:30	EC-04	Aplicações de cromatografia iónica e abordagem às técnicas de preparação em linha de amostras <b>Susana M. M. Pereira</b> MT Brandão Lda
<b>17:30-18:00</b>	<b>Oral session V / Sessão Oral V</b>	
	OC-39	Effects of e-beam irradiation on bioactive content of cherry tomatoes <b>Joana Madureira</b>
	OC-40	Otimização da extração de antocianinas de cereja madura através da metodologia de superfície de resposta <b>Carla Pereira</b>
18:00-19:00	Reunião Grupo de Cromatografia SPQ /Meeting	
20:00	Meeting Dinner / Jantar do Encontro	



Time		December 6	
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>Manuel António Coimbra</b> (Universidade de Aveiro)			
9:00-10:00	PL-03	Comprehensive two-dimensional liquid chromatography in food and natural products analysis <b>Paola Dugo</b> Università di Messina, Itália	
10:00-10:30	IC-05	Separation and concentration of nutraceuticals, active compounds and essential oils from Agro-Food sources using supercritical carbon dioxide <b>Juan Francisco Rodríguez</b> TQUIMA, Espanha	
10:30-11:00		• Coffee Break + Poster session	
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>Alírio Rodrigues</b> (LSRE/LCM, Faculdade de Engenharia, Universidade do Porto)			
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OC-41		Efeito da radiação gama e feixe de eletrões na concentração de ergosterol em <i>Agaricus bisporus</i> (J.E. Lange) Imbach <b>Ângela Fernandes</b>	
OC-42		Optimization of the extraction of triterpenes from <i>Ganoderma lucidum</i> <b>Miguel Angel Prieto</b>	
OC-43		Unveiling the chemical composition of willow added-value lipophilic extractives by gas chromatography-mass spectrometry <b>Patrícia Ramos</b>	
OC-44		Application of anti-hail net in apple orchards: effects on fruits chemical characteristics <b>Carlos Gomes</b>	
<b>Moderator / Moderador - Auditorium B</b> <b>José Câmara</b> (Universidade da Madeira)			
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OC-47		Characterization of phospholipids, including plasmalogens, in bivalves of the Portuguese coast using solid-phase extraction followed by gas-liquid chromatography <b>Rui Bessa</b>	
OC-48		Characterization and Identification of Four Essential Oils by GC-MS <b>Ana Marques</b>	
<b>Moderator / Moderador - Auditorium Dionísio Gonçalves</b> <b>Luís Pais</b> (Instituto Politécnico de Bragança)			
12:00-12:30	EC-05	Successful generic approaches for heartcutting 2DLC with focus on user friendliness <b>Isabelle François</b> Waters	
12:30-13:00		Closing Session / Sessão de Encerramento	

- PL Plenary communication / Comunicação plenária
- IC Invited oral communication / Comunicação oral convidada
- EC Enterprise oral communication / Comunicação oral de empresa
- OC Oral communication / Comunicação oral



J. Sá Morais

EC - Enterprise oral communications / Comunicações orais de empresas

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## OC-34

# Effects of natural colourants on the fatty acids profile of different ice cream formulations

Custódio Lobo Roriz<sup>a,b</sup>, João C.M. Barreira<sup>a</sup>, Patricia Morales<sup>b</sup>, Lillian Barros<sup>a</sup>, Isabel C.F.R. Ferreira<sup>a,\*</sup>

<sup>a</sup>Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Portugal

<sup>b</sup>Dpto. Nutrición y Bromatología II. Facultad de Farmacia. Universidad Complutense de Madrid, Spain

\*iferreira@ipb.pt

Ice cream is a complex food colloid formed of air bubbles, fat globules, ice crystals and a serum unfrozen phase [1]. Although presenting a complex composition, including milk, sweeteners, emulsifiers, stabilizers, colourants and flavouring agents, ice cream is very poor in some essential components such as natural antioxidants, dietary fibres, minerals and vitamins, all representing features desired by consumers [2]. Nevertheless, the addition of a natural food colourant to ice cream, besides fulfilling its main colouring function, might be an effective way to functionalize it, due to the antioxidant activity of most natural colourants (e.g., anthocyanins, carotenoids or betacyanins). *Gomphrena globosa* L. is a good example of an alternative source of colouring compounds of natural origin, namely betacyanins, which present a threefold higher colouring capacity than its commercial analogue (anthocyanins), additionally possessing antioxidant, antiviral, and antimicrobial properties [3]. Therefore, betacyanins extracted from the purple flowers of *G. globosa* were evaluated as colouring/functionalizing agents in ice-cream formulations, aiming to verify potential improvements on fatty acids profile, analysed by gas chromatography (GC) coupled to a flame ionization detector (FID). In order to acquire comprehensive conclusions, other ice-cream formulations (IF) were prepared and analysed in 5 storage times (ST). Besides the ice cream containing *G. globosa* extract, three formulations were prepared: control ice cream (without colourants), ice cream with commercial betalain and ice cream with *Beta vulgaris* extract (E-162). The profiles in fatty acids were especially sensitive to ST, which induced a significant effect in all cases except C18:1 ( $p=0.271$ ) and MUFA ( $p=0.108$ ), in contrast with IF, which was only significant in the cases of C14:0, C16:1, C18:1 and MUFA. In general, the new colouring approach allowed maintain the most relevant fatty acids unchanged.

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