


XXV ENCONTRO NACIONAL

Sociedade Portuguesa de Química



Book of Abstracts



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Joana Carvalho (UL)

Ricardo Lopes (UL)

Margarida Espadinha (UL)

Rafael Gomes (UL)

João Ravasco (UL)

Lídia Cavaca (UL/UNL)

Ângelo Rocha (IST)

Raquel Teixeira (UL)

João Rosa (UL)

Sterline Moneus (UPMC)

Elisa Forte (Uni. Torino)

19.00	FC4 Cecília Roque (FCT-UNL, Portugal) <i>Affinity materials for medical and biotechnological applications</i>	FC9 Vera Lucia (QOPNA-UA, Portugal) <i>Ohmic Heating Assisted Synthesis of 1,3-Disubstituted-quinolin-4(1H)-ones by C-C Cross Coupling Reactions in Aqueous Media</i>	19.00	FC11 António Ribeiro (IPB) <i>Separation of Nadolol Racemates by Fixed-bed and Continuous Preparative Liquid Chromatography using C18 Columns</i>
19.10	FC5 Ana C. Santos (IST-UL, Portugal) <i>Smart Polymer Fibers for Stem Cell Cultivation</i>	FC10 Luís Fernandes (FCT-UE, Portugal) <i>Alpha-glucosidases and cholinesterases inhibition</i>	19.10	FC12 Ricardo Branco (FCT-UNL) <i>De novo computational design of a protein catalyst for the Beckmann rearrangement reaction</i>
20.00- Sunset Party & Conference Dinner				

Wednesday, July 19th, 2017

Session 10 | Chairman: Carlos Romão (FCT-UNL) | Auditorium – Environmental Challenges – *Sponsored by Bruker*

9.00	PL10 David Milstein (Weizmann Institute of Science, Israel) <i>Design and Applications of Sustainable Catalytic Reactions for Synthesis and Energy</i>
9.50	PL11 Armando Pombeiro (IST-UL, Portugal) <i>Inert Alkanes as Potential Feedstocks for Synthesis?</i>

10.40-11.40 Coffee break and poster session 5

Session 11 | Chairman: Beatriz Royo (ITQB-UNL) | Auditorium – Environmental Challenges – *Sponsored by Bruker*

11.40	PL12 Paul Chirik (Princeton University, USA) <i>Catalysis with Earth Abundant Transition Metals</i>
12.30	PL13 Antonio Echavarren (ICIQ, Spain) <i>Gold-Catalysis for the Synthesis of Biologically Active Natural Products</i>

13.20-15.00 Lunch

Session 12 | Chairman: José Cavaleiro, Carlos Afonso (Auditorium) – *Sponsored by Paralab*; Joaquim Faria, Carla Morais (Amphitheatre A) – *Sponsored by ChemPubSoc Europe*

	Auditorium A Sea of Opportunities		Amphitheatre A Teaching Challenges
15.00	KN19 Anake Kijjoa (CIIMAR-UP, Portugal) <i>Marine-Derived Fungi: A Promising Source of Bioactive Compounds for Drug Discovery</i>	15.00	KN22 José Gomes (FC-UP, Portugal) <i>A Química no ensino básico e secundário: Um desafio para os alunos?</i>
		15.25	IOC10 Adelino Galvão (SG-SPQ, Portugal) <i>Aprendizagens Essenciais: Os novos desafios transdisciplinares no ensino da Química</i>

FC8 | *Synthesis and physical-chemical characterization of novel anthocyanin-lipophilic bioactives.*

Luis Miguel Neves Ferreira Serra Cruz

FC9 | *Ohmic Heating Assisted Synthesis of 1,3-Disubstituted-quinolin-4(1H)-ones by C-C Cross Coupling Reactions in Aqueous Media*

Vera Lúcia Marques da Silva

FC10 | *Alpha-glucosidases and cholinesterases inhibition*

Luís António Garrido Nunes Fernandes

FC11 | *Separation of Nadolol Racemates by Fixed-bed and Continuous Preparative Liquid Chromatography using C18 Columns*

António Manuel Esteves Ribeiro

FC12 | *De novo computational design of a protein catalyst for the Beckmann rearrangement reaction*

Henrique Daniel Figueiredo Carvalho

FC13 | *Characterization of the Chemiexcitation Step of Marine Imidazopyrazinone Chemiluminescence*

Luís Tiago da Costa Pinto da Silva

FC14 | *Development of Chemistry Education Research in Portugal: The Emerging Picture from the Papers Published in the Journal of Chemical Education*

Célia Faustino

FC15 | *Science outreach activities from early grades to high school*

Marta Corvo

Health Challenges Poster Communications

HC1 | *Determination of fluoxetine in hair by high-pressure liquid chromatography with fluorescence detection*

Adriana Patrícia Fernandes Ribeiro

HC2 | *A quality-by-design approach for the understanding of the effect of model antigen mannose on PLGA nanoparticles*

Ainhoa Teresa Cardoso Coelho

HC3 | *Bioactivation of the anti-HIV drug etravirine to reactive metabolites: in vivo and in vitro approaches*

Ana Lúcia Aguiar Godinho

HC4 | *Ionic Liquids as functional ingredients in Lipidic Implants*

Ana Luísa Gomes Júlio

Separation of Nadolol Racemates by Fixed-bed and Continuous Preparative Liquid Chromatography using C18 Columns

Ribeiro A. E.,^a Arafah R. S.,^a Rodrigues A. E.,^b Pais L. S.^a

Laboratory of Separation and Reaction Engineering, Associate Laboratory LSRE/LCM

a) School of Technology and Management, Polytechnic Institute of Bragança; Campus de Santa Apolónia, Apartado 1134, 5301-857 Bragança, Portugal.; b) Department of Chemical Engineering, Faculty of Engineering, University of Porto; Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal

Email: aribeiro@ipb.pt

Nadolol is a pharmaceutical drug marketed as a mixture of four stereoisomers, used to treat cardiovascular diseases. However, its prescription is also related with some severe risks such as heart failure. Its chemical structure has three stereogenic centers which allows for eight possible stereoisomers. However, the two hydroxyl substituents on the cyclohexane ring are fixed in the cis-configuration, which precludes four stereoisomers. Nadolol is presently marketed as an equal mixture of the four stereoisomers.

It is well known that pure enantiomer separation is important to control chiral drugs safety. Recently, our research group reported the pseudo-binary separation of nadolol by simulated moving bed (SMB) chromatography using both coated Chiralpak AD and Chiralpak IA immobilized chiral stationary phases (CSP).^{1,2} This technology is generally based on the use of chiral adsorbents which must have enough recognition for all the chiral species.

In this work it is proposed an alternative strategy, implementing a first achiral separation step, to be followed by two subsequent parallel chiral separation steps.^{3,4} In this first achiral step, C18 columns are used to perform the separation of the two pairs of nadolol enantiomers ("racemate A" from "racemate B") under reversed-phase mode. The C18 achiral adsorbent allows the separation of the two pairs of nadolol diastereomers, i.e., the first racemate (composed by the nadolol compounds 2 and 3) co-eluting in the raffinate, and the second racemate (composed by the nadolol compounds 1 and 4) to be obtained in the extract SMB stream. After this preliminary achiral separation step, two parallel SMB runs must be carried out using a chiral stationary phase to achieve the complete separation of all the four nadolol stereoisomers.

Extensive experimental and simulation results will be presented including solvent screening, measurement of equilibrium and kinetic data, and both fixed-bed and SMB preparative separations.

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References:

1. Ribeiro A. E.; Rodrigues A. E.; Pais, L. S. *Chirality* **2013**, 25, 197.
2. Arafah R.S.; Ribeiro A.E.; Rodrigues A. E.; Pais L. S. *Chirality* **2016** 28, 399.
3. Gheysens E. T.; Ribeiro A.E.; Rodrigues A. E.; Pais L. S. *Proc of XXIV Encontro Nacional da Sociedade Portuguesa de Química*, Coimbra, Portugal, **2015**, 157.
4. Arafah R. S.; Ribeiro A. E.; Rodrigues A. E.; Pais L. S. *Proc of XXII Encontro Luso-Galego de Química*, Bragança, Portugal, **2016**, 259.