Programme RDay 2017

08:45 - 9:00 – Reception

09:00 - 09:30 – Intervention by the Rector and Vice-Rector for Research

09:30 - 10:30 – Invited Talks: Carlos Borrego (http://www.cesam.ua.pt/index.php?tabela=pessoaldetail&menu=198&user=41) (U. Aveiro) | Asad J. Khattak (http://cee.utk.edu/people/asad-khattak/) (U. Tennessee)

10:30 - 11:00 – Coffee break

11:00 -12:00 – Soumodip Sarkar (http://www.uevora.pt/pessoas/(id)/27652) (U. Évora) | Humberto Delgado Rosa (http://ec.europa.eu/environment/archives/greenweek2015/speaker-h-delgado.html) (European Commission)

12:00 - 13:00 – Round table (Moderator – Eduarda Maio)

13:00 - 14:00 – Lunch

14:00 - 14:30 – Intervention by the Vice-President of FCT: Miguel Castanho

14:30 - 15:30 – Short talks

15:30 - 17:30 – Poster session

17:30 - 18:00 – Concert and awards

18:00 - Closin

Posters: Authors and Titles | Underground location

Ciências		Authors/Títles
CIDMA	1	**Pedro V.P. Cunha, C. Herdeiro and E. Radu** *Fundamental Photon orbits: black hole shadows and spacetime instabilities*
	2	**Filipa Santana, Diego Napp and Raquel Pinto** *Convolutional codes for network coding. Fast error-correction for streaming aplications*
	3	**Ana Helena Tavares, Vera Afreixo and Paula Brito** *Distance distributions between words: a mathematical descriptor of DNA sequences*
	4	**Daniel Figueiredo, Manuel Martins and Madalena Chaves** *Differential dynamic logic for reasoning about biological regulatory networks*
	5	**Aurineide Fonseca** *Fractional Integral Transforms*
	6	**Anabela Silva and Luís Castro** *Integral Operators on Spaces with Variable Integrability*
IBI-MED	7	**Rita Coimbra, Andreia Reis, Ana R Bezerra and Gabriela Moura** *Exploratory transcriptomics in Candida rugosa by next-generation sequencing*
	8	**Ana Oliveira, Susan Lage and Alda Marques** *Validity and reliability of computerised adventitious respiratory sounds in COPD*
	9	**Maria João Freitas, Cameron Brothag, Joana Vieira Silva, Srinivasan Vijayaraghavan and Margarida Fardilha** *Unraveling isoform-specific functions of GSK3 in male fertility*
	10	**Ana Rita Ferreira, Ana Cristina Magalhães, Sílvia Gomes, Marta Vieira, Ana Gouveia, Isabel Valença, Markus Islinger, Rute Nascimento, Michael Schrader, Jonathan C. Kagan, Daniela Ribeiro** *Cytomegalovirus' evasion of the peroxisome-dependent antiviral immune response*
	11	**Edgar Lopes, Carla Oliveira, Rita Bezerra and Manuel Santos** *Candida albicans gene mistranslation as a modulator of host-pathogen interactions and pathogenesis*
	12	**Filipa Martins, Cátia D. Pereira, Odete A. B. da Cruz e Silva and Sandra Rebelo** *BRI2 is a novel player in neuronal differentiation*
CINTESIS	13	**Sara Guerra, Álvaro Mendes and Liliana Sousa** *Affective meanings of inheriting and "donating" a late onset neurological genetic illness: an exploratory qualitative study*
	14	**Catarina Rosa, Miguel M. Gonçalves, Rafael Araújo, Pedro Bem-Haja and Carlos F. Silva** *Rumination Room: A procedure that combines executive control activation and exposure to ruminative thoughts.*
	15	**Natália L. Fernandes, Josefa N. S. Pandeirada, Sandra C. Soares and James S. Nairne** *Remind myself not to touch it, it's contaminated!": Memory and contamination*
	16	**Pedro Bem-Haja, Isabel M. Santos, Hugo de Almeida, Mariana L. Carrito, Beatriz Oliveira and Carlos F. Silva** *Early brain detection of false memories in eyewitness testimony*
	17	**Ana Bártolo, Sara Monteiro and Isabel M. Santos** *Reproductive concerns and psychosocial outcomes in young adult female cancer survivors: A systematic review*
CESAM	18	**Nuno Canha, Joana Lage, Marta Almeida and Célia Alves** *Indoor air quality while sleeping: under different ventilation patterns*
	19	**Ana Cristina Esteves, Fernanda Lima, Carina Félix, Rute Terezinha, Rui Vitorino, Pedro Domingues and Artur Alves** *A proteomics approach to understand biocontrol mechanisms of Trichoderma species*
	20	**Sandra Valente, Celeste Coelho and Jan Jacob Keizer** *Social valuation of forest ecosystem services: Exploratory study in the Central region of Portugal*
	21	**Ángela Fontán Bouzas, P. Baptista, P. A. Silva, L. Tubarão, C. Ferreira, J. Barbosa and C. Bernardes** *Impact of wave climate in dune erosion of Poço da Cruz-Mira coastal stretch (NW Portugal)*
	22	**Isabel G. Teixiera, Pedro Cermeño, Francisco G. Figueiras, Vanessa Balagué, Ramón Massana and Henrique Queiroga** *Seasonal dynamics of picoplankton in the NW Iberian upwelling system: a metagenomics approach*
	23	**Maria Pavlaki, Rui G. Morgado, Joana Neves, Amadeu M.V.M. Soares and Susana Loureiro** *Bioaccumulation patterns copper-based pesticides in soil organisms: comparing nano- and non-nano agrochemicals*
	24	**Heliana Teixeira, Ana I. Lillebø, Mariana Morgado and António J. A. Nogueira** *Integrated management of the aquatic continuum supported by causalities between biodiversity, ecosystem functions and services*
	25	**Milene Matos and Carlos Fonseca** *From scientific knowledge to sustainability: strategies for valuing natural resources through public participation*
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	67	**Emanuel V. Capela, Sara A.S.L. Rosa, João A.P. Coutinho, M. Raquel Aires-Barros, Ana M. Azevedo and Mara G. Freire** *Novel ionic-liquid-based strategies for the downstream processing of monoclonal antibodies*
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	83	**Pedro A. R. Fernandes, Sónia S. Ferreira, António Pinto, Manuel A. Coimbra, Dulcineia F. Wessela and Susana M. Cardoso** *Why should apple pomace be an industrial disposable?*
	84	**Raquel Nunes da Silva, Â. Cunha and A. C. Tomé** *Phthalocyanines bearing sulfonamide units as photosensitizers for the photodynamic inactivation of Gram positive and Gram negative bacteria*
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	88	**Simone Colombo, Giulia Coliva, Agnieszka Kraj, Jean-Pierre Chervet, Maria Fedorova, Pedro Domingues and M. Rosário Domingues** *Oxidative metabolism of phosphatidylethanolamines predicted by electrochemistry-mass spectrometry*
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	99	**Daniel Belo, Ricardo Correia, Pedro Pinho and Nuno Carvalho** *Efficient and Reconfigurable Wireless Power Transmitter Based on a Backscattered Pilot Signal*
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sciences

Conjugate additions of carbon nucleophiles to chromone derivatives towards nitrogen heterocycles

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Abstract

Conjugate additions of nitromethane to the extended π-system of chromone derivatives afforded the 1,6-conjugate addition products, together with structure complex oxygen heterocycles through *tandem* processes. Further functionalization of targeted adducts allowed the preparation of biological relevant nitrogen heterocycles such as styrylpyrrolidines, as well as pyrazole and bis-pyrazole derivatives.

Introduction

Following previous work of our research group,[1] herein, the reactivity of the extended 3,2:α,β:γ,δ-triunsaturated system of chromones **1** in conjugate addition reactions with several carbon nucleophiles and further functionalizations of the addition products, was addressed. In comparison with 2-styrylchromones, the presence of a third unsaturation extends the π-system on chromones **1** and allows δ-position to become a novel site for nucleophilic attack (possible 1,8-conjugate addition) (Figure 1). This feature enables the synthesis of multisubstituted heterocyclic derivatives with new stereocenters as well as their further functionalization to give novel nitrogen-containing heterocyclic compounds.

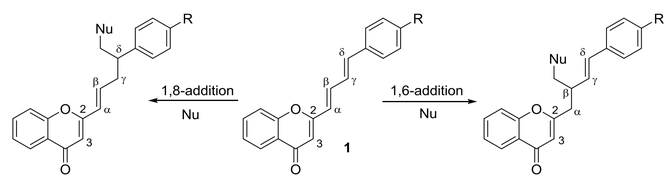
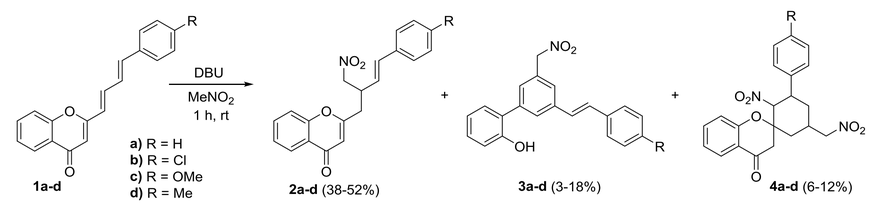


Fig. 1 - Possible sites of conjugate addition to 2-[(1*E*,3*E*)-4-arylbuta-1,3-dien-1-yl]-4*H*-chromen-4-ones (**1**). Nu = nucleophile.

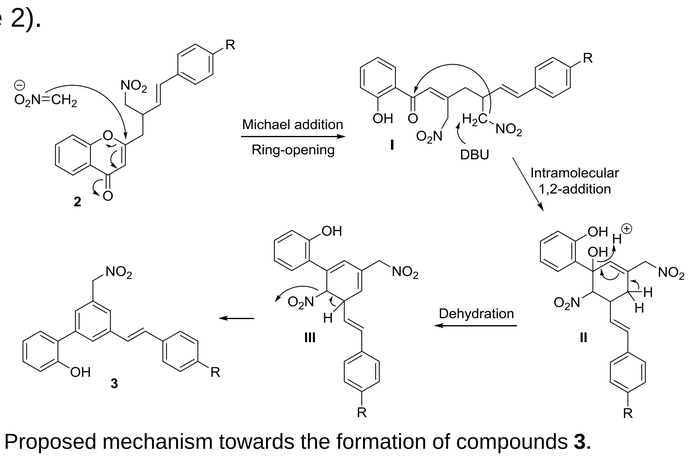
Nitromethane conjugate additions

The DBU-catalyzed addition reaction of nitromethane, in neat conditions, to chromones **1** afforded the β-(nitromethyl)chromones **2** (1,6-conjugate addition) as major products, together with (*E*)-5'-(nitromethyl)-3'-styryl-[1,1'-biphenyl]-2-ol and 3'-aryl-2'-nitro-5'-(nitromethyl)spiro[chromane-2,1'-cyclohexan]-4-one derivatives **3** and **4**, respectively, as minor products. These byproducts result from the addition of a second molecule of nitromethane, in *tandem* processes (Scheme 1).



Scheme 1. Nitromethane conjugate addition to chromones **1**.

The formation of derivatives **3** could be explained based on the Michael addition of a nitromethane anion to C-2 of β-(nitromethyl)chromones **2** along with chromone ring opening to give intermediates **I**. A DBU-catalyzed intramolecular 1,2-addition led to intermediates **II**, which upon dehydration affords intermediates **III**, that affords derivatives **3** after HNO_2 elimination (Scheme 2).



Scheme 2. Proposed mechanism towards the formation of compounds **3**.

Acknowledgements

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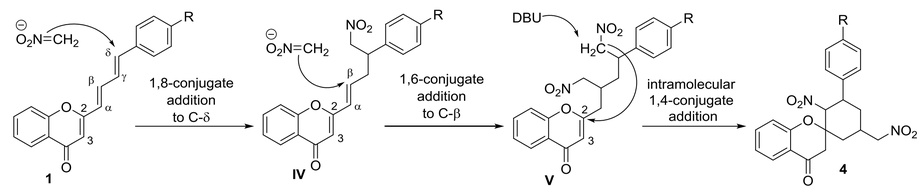
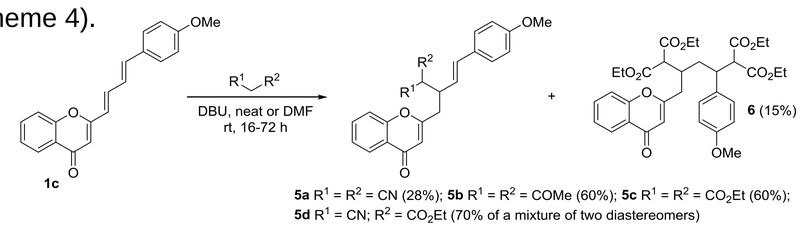
The plausible mechanism for the formation of derivatives **4** involves the 1,8-conjugate addition of a nitromethane anion to C-δ of chromones **1**, affording intermediates **IV**. Then, the 1,6-conjugate addition of another nitromethane anion to C-β of **IV** gives intermediates **V**, which undergoes DBU-catalyzed intramolecular 1,4-conjugate addition to C-2 leading to the formation of the spiro trisubstituted cyclohexanes **4** (Scheme 3).



Scheme 3. Proposed mechanism towards the formation of compounds **4**.

Nucleophile scope

The scope of the reaction was extended to malononitrile, acetylacetone, ethyl cianoacetate and diethyl malonate as carbon nucleophiles. The DBU-catalyzed reaction with these nucleophiles to chromone derivative **1c** gave the expected 1,6-addition products **5**, being also possible to isolate in the latest case, a minor product **6** formed via 1,8-/1,6-addition sequence (Scheme 4).

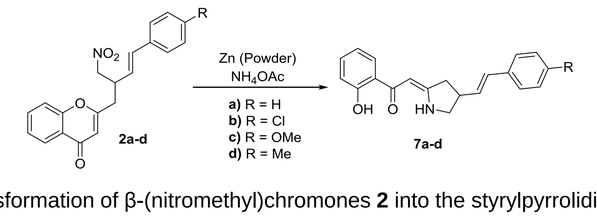


5a $R^1 = R^2$ = CN (28%); **5b** $R^1 = R^2$ = COMe (60%); **5c** $R^1 = R^2 = CO_2Et$ (60%); **5d** R^1 = CN; $R^2 = CO_2Et$ (70% of a mixture of two diastereomers)

Scheme 4. Nucleophile scope in conjugate addition reaction to chromone **1c**.

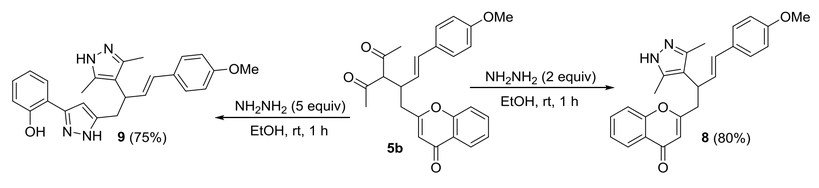
Functionalization of the 1,6-conjugate addition products

Reduction of the nitro group of the β-(nitromethyl)chromones **2** with Zn (powder)/NH_4OAc afforded primary amine derivatives, which underwent intramolecular aza-Michael addition to α,β-unsaturated system of the chromone core, followed by heterocyclic ring opening, leading to the styrylpyrrolidine derivatives **7** (Scheme 5).



Scheme 5. Transformation of β-(nitromethyl)chromones **2** into the styrylpyrrolidines **7**.

The reaction of **5b** with 2 equiv of hydrazine hydrate afforded the expected pyrazole derivative **8**. On the other hand, employing 5 equiv of hydrazine, a bis-pyrazole derivative **9** was obtained (Scheme 6).



Scheme 6. Transformation of **5b** into pyrazole **8** and bis-pyrazole **9**.

Conclusion

The conjugate addition reaction of nitromethane to chromones **1** afforded β-(nitromethyl)chromones **2** as major products, as well as compounds **3** and **4** as minor ones. The addition of other carbon nucleophiles resulted in the expected 1,6-conjugate addition products. Further functionalization of some adducts allowed the synthesis of styrylpyrrolidines and new pyrazole and bis-pyrazole derivatives.

References

(1) E. M. P. Silva, A. M. S. Silva, J. A. S. Cavaleiro, *Synlett* **2011**, 2740-2744;
(2) E. M. P. Silva, K. Grenda, I. N. Cardoso, A. M. S. Silva, *Synlett* **2013**, 24, 2375-2382.