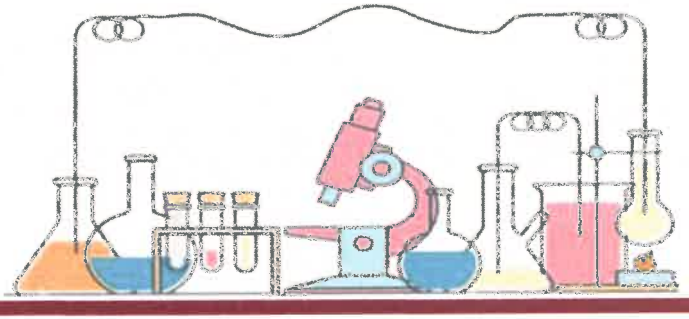

3rd Symposium on Medicinal Chemistry of University of Minho

May 26th, 2017

School of Science, Chemistry Department

University of Minho, Campus of Gualtar

Scientific Committee

Fernanda Proença - Department of Chemistry, University of Minho
Isabel Ferreira - Polytechnical Institute Bragança
M. Alice Carvalho - Department of Chemistry, University of Minho
A. Gil Fortes - Department of Chemistry, University of Minho
Luís S. Monteiro - Department of Chemistry, University of Minho

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Juliana Rocha (MSc student of Medicinal Chemistry)
Mónica Fernandes (MSc student of Medicinal Chemistry)
Pedro Figueiredo (MSc student of Medicinal Chemistry)

Symposium Programme

8h00 **Registration**

9h00 **Opening Session**
Session 1. Chairperson – **Luís S. Monteiro**

9h30 **PL1** *Discovery and Development of Opicapone: A Potent and Peripherally Selective Catechol O-methyltransferase (COMT) Inhibitor for the Adjunctive Treatment of Parkinson's Disease.*
Läszlo Kiss, Medicinal Chemist Manager, Laboratory of Chemical Research, Department of Research & Development, BIAL - Portela & Ca., S. A

10h15 **IC1** *Making the Use of Protein-Ligand Docking in Drug Discovery More Effective.*
Sérgio Sousa, REQUIMTE, Faculty of Sciences, University of Porto.

10h45 **OC1** *Metal ion complexes with pyridine-bis-oxazole ligands.*
A. Carvalho, Department of Chemistry, University of Minho.

11h00 **OC2** *Dietary supplements phenolic profile and closely related bioactivity.*
C. Pereira, Mountain Research Centre (CIMO), ESA, Polytechnic Institute of Bragança.

11h15 **Coffee break and Poster Session**
Session 2. Chairperson – **A. Gil Fortes**

11h45 **IC2** *How to discover and develop innovative medicines in Portugal? The example of redaporfin.*
Luís Arnaut, Chemistry Centre of Coimbra, Department of Chemistry, University of Coimbra.

12h15 **OC3** *A computational study on the transesterification reaction; modeling the reaction between scopine and MDTG.*
L. M. S. Sobral, Hovione FarmaCiencia SA.

12h30 **Lunch**
Session 3. Chairperson – **M. Fernanda Proença**

14h00 **PL2** *Biotransformation-induced toxicity. Challenges in drug design.*
Maria Matilde S. D. Marques, Centre of Structural Chemistry, Department of Chemical Engeneering, Technical Superior Institute

14h45 **OC4** *Cationic phthalocyanines as a promising new approach for the inactivation of multi-resistant microorganisms.*
Rafael T. Aroso, CQC, Department of Chemistry, University of Coimbra.

Plenary Lectures

Invited Communications

Oral Communications

OC2

Dietary supplements phenolic profile and closely related bioactivity

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Medicinal plants are recognized since ancient times as therapeutic agents with several beneficial properties for human health. Herein, the phenolic profile of three formulations (infusions, pills and syrups) based on artichoke, milk thistle and borututu was analysed as well as their bioactivity, namely the antioxidant, hepatoprotective and antimicrobial activities.

In what concerns the phenolic composition, the studied plants proved to represent a good source of bioactive compounds, especially phenolic acids and flavonoids. Regarding artichoke and milk thistle, phenolic compounds were higher in the infusion preparations when compared to the other formulations, but in the case of borututu, the syrup revealed the highest contents. Luteolin-7-*O*-glucuronide was the major flavonoid found in artichoke infusion, protocatechuic acid was the main constituent of borututu infusion, and isorhamnetin-*O*-deoxyhexoside-*O*-hexoside was the most abundant compound in milk thistle syrup.

Regarding the bioactivity of these formulations, the samples containing the highest amounts of phenolic compounds also presented the most potent bioactivities at the tested concentrations, which could be explained by the well-known therapeutic properties of these compounds [1]. In a general way, all the samples revealed good antioxidant properties, but infusions and syrups showed higher antioxidant activity than pills. Despite artichoke presented the best results in antitumor activity, its infusion also revealed some toxicity for normal cells in similar concentrations. Borututu infusion and milk thistle syrup gave the best results in the antioxidant activity with similar EC_{50} values, but regarding the capacity to inhibit the proliferation of HepG2 cell line, the infusion showed best results than the syrup. All the formulations revealed antimicrobial properties, with the exception of the syrups based on artichoke and borututu. From the present study, it can be concluded that these plants represent important natural sources of phytochemicals with antioxidant, hepatoprotective and antimicrobial properties, which can easily be included in diet, namely in the form of supplements, thereby contributing to prevent chronic diseases.

Acknowledgments:
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References:
*[1] A. Garbetta et al., J. Funct. Foods, **2014**, 10, 456.*