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Meeting Report

11th National Meeting of Organic Chemistry and 4th Meeting of Therapeutic Chemistry

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Abstract: For the first time under the auspices of Sociedade Portuguesa de Química, the competences of two important fields of Chemistry are brought together into a single event, the 11st National Organic Chemistry Meeting and the the 4th National Medicinal Chemistry Meeting, to highlight complementarities and to promote new synergies. Abstracts of plenary lectures, oral communications, and posters presented during the meeting are collected in this report.

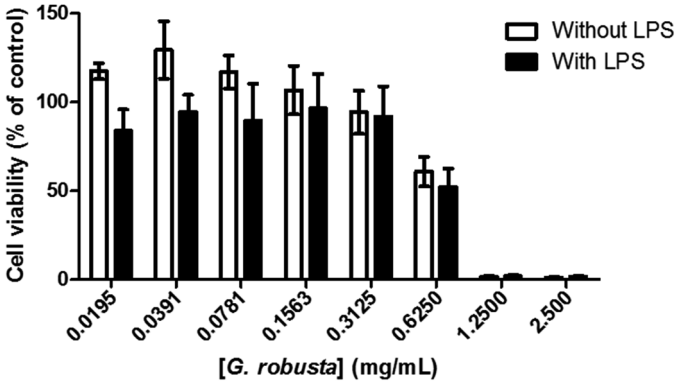
Keywords: organic synthesis; spectroscopic methods; natural compounds; drug metabolism and disposition; beyond small molecules; drug design; antitumor and anti-infective drugs; industrial applications

1. Aim and Scope of the Meeting

The Scientific Committee has put high expectations on the excellence of the scientific program, which includes plenary/keynote lectures from renowned scientists whose work has been an inspiration for researchers in Organic and Medicinal Chemistry. Oral communications focused on topics from the following main research fields: organic synthesis, spectroscopic methods, organic natural compounds, drug metabolism and disposition, beyond small molecules, computational methods and drug design, antitumor and anti-infective drugs, industrial applications.

This meeting is expected to bring together researchers with different expertise and perspectives, from senior to young scientists, to discuss and share their latest achievements in a stimulating

flavonoids can be highlighted. In this work, the ability of *Grindelia robusta* Nutt aqueous extract and of some of its flavonoids, to reduce nitric oxide (NO) levels in RAW 264.7 cells was assessed. Results revealed that the extract of *G. robusta* reduced cells' viability.



Cell viability of RAW 264.7 cells pre-treated for 2 h with *G. robusta* aqueous extract, followed by 22h co-treatment with LPS (1 μg/mL) with LPS or vehicle (culture medium). Results represent the mean ± standard deviation of four independent experiments performed in triplicate.

A tendency to reduce NO levels, in a dose-dependent way, was also observed. All flavonoids were able to decrease NO levels in a concentration-dependent manner, quercetin being the most effective one (IC_{50} values of 7.47 μM). The presence of quercetin, apigenin and luteolin derivatives in the extract of *G. robusta* can partially explain its capacity to decrease NO levels. In a general way, aglycones revealed to be more active than the respective glycosides. Furthermore, the catechol group on ring B and the hydroxyl group in C3 seem to be essential for the anti-inflammatory activity of these compounds.

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4.5. Antitumor Activities of Invasive Alien Species from the Azores (P6)

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Asparagopsis armata Harvey, *Asparagopsis taxiformis* (Delile) Trévisan Saint-Léon, *Codium fragile* subsp. *fragile* (Suringar) Hariot, *Microcosmus squamiger* Michaelsen, 1927, *Bugula neritina* (Linnaeus, 1758), *Tricellaria inopinata* d'Hondt & Occhipinti Ambrogi, 1985 and *Zoobotryon verticillatum* (Delle Chiaje, 1822) were collected in marinas from Santa Maria (SMA) and of S. Miguel (SMI) islands (Azores). Dichloromethane and methanol extracts of these organisms were assessed against HeLa (cervix tumor), A549 (lung), MCF-7 (breast) and Vero (control) cell lines using the MTT method (Barreto, M.C., *et al.* in *Determination of Biological Activities. A Laboratory Manual*, 2012. ISBN 978-972-8612-82-5).

None of the extracts was active against A549 cell line or against any cell line in log phase up to 200 μg/mL. In lag phase, the dichloromethane extract from *Z. verticillatum* presented the best activity against MCF-7 cells and was the only extract active against HeLa cells (with selectivity Index of 1.94 and 4.64, respectively).The results obtained show the potential of *M. squamiger*, *B. neritina* and *Z. verticillatum* as sources of antitumor agents.

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4.6. Following the Removal of Fluoroquinolones on the Environment: An HPLC-FD Method (P7)

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Antibiotic residues have been detected in various environmental matrices, such as surface and drinking waters. Although present at low levels (μg/L, ng/L), many antibiotics are bioaccumulative, pseudo-persistent and can promote resistance/alterations in bacterial populations (Doorslaer, V.X., *et al. Sci. Total Environ.* 2014, *500*, 250–269). In this work we present the biosorption of three widely used fluoroquinolones (FQ)—ofloxacin (OFL), norfloxacin (NOR) and ciprofloxacin (CPF)—to activated sludge (AS) and aerobic granular sludge (AGS). A HPLC-FD method was validated and optimized to follow the biosorption of the targeted FQ (Maia, A.S., *et al. J. Chrom. A* 2014, *1333*, 87–98). The validated method demonstrated good selectivity, linearity ($r^2 > 0.999$), intra-day and inter-day precisions (RSD < 3%) and accuracy. LOD and LOQ were, respectively, 0.7 ng/mL and 1 ng/mL for the three FQ. Several parameters that can affect biossorption kinetics, namely, contact time, pH, and biosortion mass were also studied. At pH 7 AS showed better performance to biosorb OFL, NOR and CPF. The equilibrium data for AS showed a better fit to the Langmuir model, while AGS showed a better fit to the Freundlich model. The FQ could be desorbed from AGS at pH 3, 8 and 9, whereas at pH 4 the biosorption process was promoted.

4.7. The Antioxidant Activity of Novel Polyhydroxylated 3-Hydroxy-2-Styrylchromones and 3-Hydroxyflavones (P8)

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Flavonoids are chemically based on a fifteen-carbon skeleton consisting of two benzene rings (ring A and ring B) joined by a linear three carbon chain (C_6-C_3-C_6) forming an oxygenated heterocycle pyran ring (ring C). 2-styrylchromones (2-SC), a small group of compounds characterized by the attachment of a styryl group to the 2-position of the chromone skeleton, have structural similarities with flavonoids, particularly those belonging to the class of flavones. Flavonoids possess many biological activities, from which the antioxidant properties are the best described. Considering the structural similarities of 2-SC and the fact that their styryl moiety may greatly contribute to their molecular stabilization under redox challenges, some of its biological activities are likely to be similar or even enhanced in comparison to flavonoids, although it needs to be experimentally confirmed. Thus, the purpose of the present study was to evaluate and compare the putative scavenging of reactive oxygen (ROS) and nitrogen (RNS)