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Conference Report

14th Edition of the Nacional Organic Chemistry Meeting and 7th Edition of the Nacional Therapeutic Chemistry Meeting

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14th Edition of the Nacional Organic Chemistry Meeting and 7th Edition of the Nacional Therapeutic Chemistry Meeting †

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Abstract: Once more under the auspices of the Sociedade Portuguesa de Química, two important fields of Chemistry are brought together into a single event, the 14th National Organic Chemistry Meeting and the 7th National Medicinal Chemistry Meeting. These conferences brought together both long-recognized experts and newcomers.

Keywords: organic synthesis; drug design; natural compounds; drug discovery; bioactive molecules; structure–activity relationship; Medicinal Chemistry; anticancer agents; photosensitizers

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1. Aim and Scope of the Meeting

The Scientific Committee brought together a wide range of specialists in the areas of Organic and Medicinal Chemistry, which allowed the high quality of the meeting that was evident in the scientific excellence of the works presented. The contributions include plenary lectures, invited oral communications, oral communications, keynotes, flash, and poster communications, where the main topics focused on organic synthesis, drug design, natural compounds, drug discovery, drug metabolism, and Medicinal Chemistry.

This approach between scientists is of great importance for the exchange of experiences and recent knowledge as well as different perspectives in the various areas of study, and it enhances collaboration between teams. This environment of scientific sharing took place in the relaxed atmosphere by the sea at Costa da Caparica.

2. Plenary Presentations

2.1. Incursions into Anticancer Drug Design and Drug Toxicity Elucidation: Strategies and Challenges

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Two major research avenues in our group are the design, synthesis and evaluation of new anticancer drugs and the elucidation of mechanisms of toxicity elicited by xenobiotic agents of therapeutic or environmental relevance. Selected recent examples from both approaches will be presented and discussed.

Emphasis will be placed on the combined use of in silico tools, chemical synthesis and proof-of-concept biochemical and biological testing to tackle epigenetic pathways

great importance for obesity management and control. Polyphenols are naturally occurring and structurally diverse compounds and have diverse biological activities, such as anti-inflammatory, antioxidant, neuroprotective, antidiabetic and anti-obesity activities [5], which highlights their potential as lead compounds for the treatment of obesity. In the present study, a panel of structurally related polyphenols, including flavonoids, chalcones and 2-styrylchomones (2-SC), presenting hydroxyl (-OH), chloro (-Cl) and alkyl groups were chosen, and its inhibitory effects against the presented enzymes as well as its structure–activity relationship were evaluated. The results obtained for PL showed that the studied 2-SC achieved higher inhibitory activity when compared to the corresponding flavonoids and chalcones. Results also indicate that an extended alkyl group in the C-ring seems to be relevant to the inhibitory activity. Similarly, for α-amylase, 2-SC appears to be the group of polyphenols studied with the highest inhibitory effects, and the increase in the number of -OH substituents as well as the presence of a catechol group on the B-ring seems to confer greater inhibitory effects to the compounds. This work indicates that some of the tested polyphenols should be further explored as potential anti-obesity molecules.

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7.40. Cosmeceutical Potential of the Green Macroalga Caulerpa Prolifera

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The present cosmeceutical industry has been gradually shifting its interest from products based on synthetic compounds to macroalgae-based products due to their interesting antiaging properties but also to their lower cytotoxicity and allergens content. Molecules

isolated from macroalgae already showed potential as either active cosmetic ingredients or key elements for the consistency of the cosmetic formulation [1]. In this regard, it is of foremost importance to keep studying the chemical composition of different algal species, aiming to find new compounds with cosmeceutical potential.

Caulerpa prolifera (Figure 1), a green macroalgae species which invaded the Azorean waters [2], is widely understudied in terms of phytochemical composition and cosmeceutical properties, so the present work aims to extract and determine the antiaging activities of *Caulerpa prolifera* components.

Figure 1. Underwater photo of *Caulerpa prolifera*.

The dry material was sequentially extracted by maceration with three solvents of increasing polarity (dichloromethane, acetone, and ethanol). The extracts obtained were then fractionated by solubility in different solvents, which was followed by fractionation with different chromatographic techniques, namely column chromatography (CC) and thin-layer chromatography (TLC). The extracts and fractions obtained were tested for their antioxidant and chelating activity and the inhibitory activity of elastase, collagenase, tyrosinase, and hyaluronidase.

The best result obtained was for the dichloromethane extract (CP1), which inhibited tyrosinase activity with an IC_{50} of 31.3 ± 0.37 μg/mL, which was followed by its ethyl acetate fraction (CP1.2) with an IC_{50} of 40.8 ± 0.21 μg/mL. In addition, fraction CP1.2.5 was active against elastase with an IC_{50} of 45.9 ± 0.75 μg/mL. Further experimental results and the respective discussion will be presented.

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7.41. Machine Learning Methods to Predict the Terrestrial and Marine Origin of Natural Products

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