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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

M. Matilde Marques

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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

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6.8. Laurus Azorica Leaves: Sesquiterpene Lactones and Antiaging Activity

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Plants are a relevant source of biologically active compounds for skin protection [1]. *Laurus azorica* (Seub.) Franco, an endemic species from Azores, was traditionally used as a disinfectant, and the oil from its berries was used to treat wounds [2,3]. This species is barely studied concerning its chemical constituents and biological activities.

In this study, three sesquiterpene lactones, costunolide (**1**), 11,13-dehydrosantonin (**2**) and reynosin (**3**) (Figure 1), were isolated for the first time on the hexane fraction of the ethanol extract from *Laurus azorica* leaves by chromatographic techniques. The chemical structure of the compounds was elucidated, using spectroscopic techniques, such as NMR 1D (^{1}H, ^{13}C, DEPT 90 e 135) and 2D (COSY, HSQC, HMBC e H2BC) and ESIMS. These compounds have already been isolated and identified in the species *Laurus nobilis*, and in *Laurus novocanariensis*, only costunolide and reynosin were identified [4,5]. The three sesquiterpene lactones have been described as having cytotoxic activity [4].

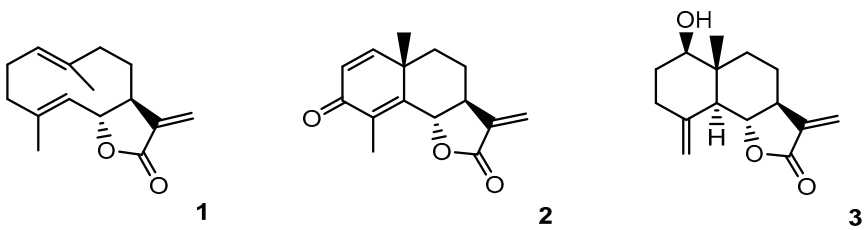

Figure 1. Chemical structure of compounds isolated from *Laurus azorica* leaves.

The in vitro antiaging activity was also evaluated. The ethanol extract exhibited an excellent antioxidant activity in ABTS and β-carotene bleaching assays (IC_{50} = 6.78 μg/mL and IC_{50} = 10.41 μg/mL, respectively) and moderate inhibition activity of tyrosinase

enzyme (IC_{50} = 12.04 μg/mL). In β-carotene bleaching assay, hexane fraction exhibited an IC_{50} = 14.74 μg/mL, which was comparable to the gallic acid used as standard (IC_{50} = 14.56 μg/mL), while costunolide was shown to be very active (IC_{50} = 4.08 μg/mL).

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6.9. Dual Inhibition of Carbohydrate-Hydrolyzing Enzymes α-Amylase α-Glucosidase by Flavonoids

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Type 2 diabetes (T2D) is characterized by the presence of insulin deficiency and/or resistance, leading to the progressive development of complications such as neuropathy, nephropathy, and retinopathy. According to the latest data released by the International Diabetes Federation, about 537 million adults are living with diabetes, and this disease is responsible for 6.7 million deaths in 2021 [1]. One class of antidiabetic agents currently available is the α-glucosidase inhibitors, which also inhibit α-amylase. Both enzymes are key carbohydrate hydrolases that regulate blood glucose levels by sequentially hydrolyzing starch to produce glucose. Therefore, the inhibition of α-glucosidase and α-amylase activity is a strategy to retard the absorption of glucose and reduce the postprandial hyperglycemia. Acarbose, voglibose and miglitol are clinically approved α-glucosidase inhibitors used for the management of T2D. These agents, as strong inhibitors of α-glucosidase and α-amylase, are however associated with frequent gastrointestinal adverse effects, including flatulence, diarrhea, and abdominal distention, which limit their clinical application. However, it was shown that only a mild inhibition of pancreatic α-amylase is required in order to avoid gastrointestinal side effects as a result of excessive bacterial fermentation of carbohydrates in colon. Based on this background, numerous efforts have been carried out to discover new and selective α-glucosidase inhibitors. Flavonoids are heterocyclic phenolic compounds