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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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† Presented at the 14th National Organic Chemistry Meeting and the 7th National Medicinal Chemistry Meeting, Caparica, Portugal, 20–22 April 2022.

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

measures and regulations for herbal products, their sources, manufacturing and plastic packaging. The alternative hypothesis is that phthalates are indeed biosynthesized by *Diopyros batocana*. The published literature indicates that they are also natural compounds and serve as biologically active substances for competitive selection with a claimed allelopathic activity that could facilitate the dominance of plants or algae capable of producing them [1,3–6]. These phthalate derivatives are probably synthesized through the shikimic acid pathway and are a barrier against biotic and abiotic factors [8]. In conclusion, synthetic and natural phthalates are widely distributed around us, and they deserve special attention regarding their origin, possible use or reduction in toxic production and environmental contamination.

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7.25. Kaempferol Derivatives from Hedychium gardnerianum—Unveiling the Potential of an Invasive Plant

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The therapeutic properties of plants and of their secondary metabolites are a current research topic of great interest. Considering that Hedychium species are used in folk medicine around the globe [1], Hedychium gardnerianum Sheppard ex Ker Gawl., an extremely aggressive invasive plant in Hawaii [2] and in Azores [3], was selected and phytochemically studied in order to search for natural compounds with interesting biological activities. Maceration of the dried aerial parts of the plant (200 g) took place with ethanol 96% (2 L) as solvent, providing an ethanolic extract of 14.30 g. Through liquid–liquid partition, fractionation of the extract originated the hexane, ethyl acetate and aqueous fractions. The hexane fraction was subjected to column chromatography and

thin layer chromatography (TLC), leading to the isolation of three pure compounds that were analyzed by nuclear magnetic resonance (NMR) and mass spectrometry (MS). The ethanolic extract and its fractions were tested regarding their antioxidant properties (ABTS and DPPH assays), with only the ethanolic extract (IC_{50} = 34.18 ± 0.97 µg/mL in ABTS assay and IC50 = 6.21 ± 1.04 µg/mL in DPPH assays) and the ethyl acetate fraction (IC_{50} = 20.38 ± 0.47 µg/mL in ABTS) reporting interesting results. The NMR and MS data enabled the identification of three flavonols (Figure 1), two of them new in the Hedychium genus, i.e., kaempferol 7,4′-dimethyl ether (1) and kaempferol 3,7,4′-trimethyl ether (2), and one new in the Zingiberaceae family, i.e., kaempferol 3,5,7,4′-tetramethyl ether (3). Flavonols are known for their bioactive activities; e.g., kaempferol 7,4′-dimethyl ether (1) has reported antioxidant activity of 187.28 ± 1.82 µg/mL IC_{50} value in DPPH assay [4], and kaempferol 3,5,7,4′-tetramethyl ether (3) demonstrated antidiabetic properties [5]; thus, the continuing study of Hedychium gardnerianum fractions is promising in the near future.

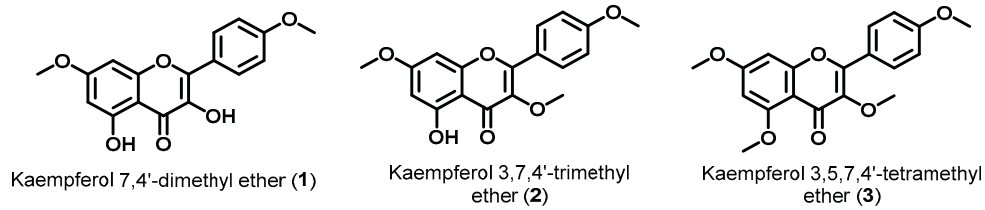

Figure 1. The three flavonols isolated from *Hedychium gardnerianum*.

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7.26. Synthesis and Characterization of Polymersomes with a Glycosylated Xanthone for Glioma

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