XXII Encontro Luso-Galego

Química

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Chromone derivatives as novel dienes in Diels–Alder reactions

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Chromones are a group of heterocyclic compounds widespread in Nature and an interesting scaffold because they have been involved in a range of chemical transformations [1]. Following our previous studies on Diels–Alder (DA) reactions of chromone derivatives [2], novel 2-[(1*E*,3*E*)-4-arylbuta-1,3-dien-1-yl]-4*H*-chromen-4-ones **1** were synthesized to further study the reactivity of their two diene systems (α,β:γ,δ versus 2,3:α,β) in DA reactions (Fig.1).

A series of dienophiles were reacted with chromones **1** under microwave-assisted conditions. The best yields of adducts **2** were achieved using *N*-methylmaleimide as dienophile and $Sc(OTf)_3$ as Lewis acid in solvent-free conditions. The crucial role of $Sc(OTf)_3$ relies on the chelation with carbonyl group of adducts **2** avoiding both the occurrence of a second DA reaction and the formation of bisadducts **6**. The α,β:γ,δ-diunsaturated system of chromones **1** showed to be the most reactive diene for maleimides, dicarboxylates and azo-dicarboxylates, affording adducts **2**, **4** and **5**, respectively. Adducts **2** were dehydrogenated to the corresponding flavone derivatives **3** using DDQ as oxidizing agent (Fig.1).

Computational calculations confirmed the experimental findings on DA reactions and helped to explain the unexpected lack of reactivity of some dienophiles.

All the experimental procedures and extensive 1D and 2D NMR characterization of the final adducts and intermediates will be presented and discussed.

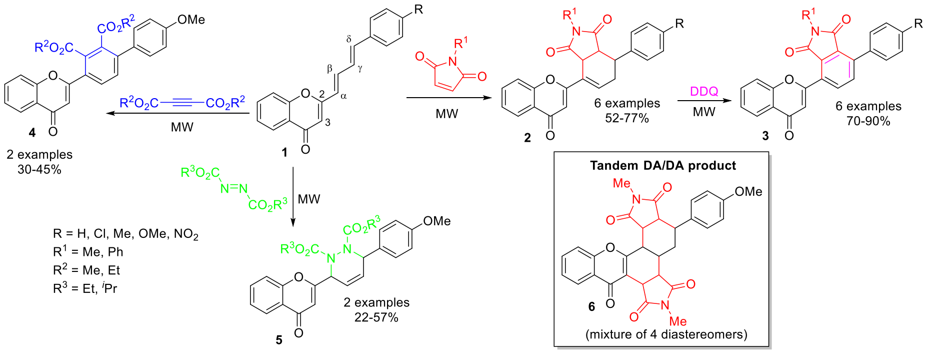

Fig.1. Microwave-assisted Diels–Alder reactions on chromones derivatives **1**

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