Photocatalytic synthesis of substituted furanones

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Over the last decades, photochemistry has established itself as a valuable and versatile tool complementary to thermally driven chemistry, enabling transformations previously unattainable through traditional methods via more sustainable processes.[1,2] The research presented here is focused on the selective organic synthesis of oxygen heterocycles (Figure 1**A**) and their application as precursors for the preparation of pharmaceuticals and other bioactive materials (Figure 1**B**). A novel method for the oxidative dehalogenation of brominated heterocycles (**1**) through LED irradiation coupled with an organic photocatalyst and aerial oxygen has been developed (**2**).[3] The work is further extended towards a halogen-shuffling reaction delivering densely functionalized halogenated building blocks (**3**).

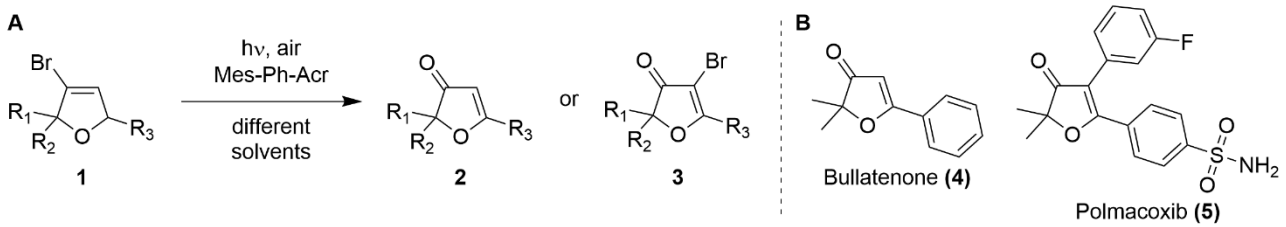

Figure 1. A: Photooxidation investigated in this research. **B:** bioactive target molecules.

A working protocol for the two photooxidations was established and the substrate scope of both reactions was probed. Mechanistic studies regarding the formation of **2** were performed utilizing kinetic measurements on selected substrates, Hammett analysis, exclusion experiments, electrochemical measurements, intermediate trapping as well as isotope labeling experiments (^{2}D, ^{18}O) and KIE measurements. Computational studies were performed to evaluate the energetic characteristics of reaction intermediates.

These reactions present easy ways to access the two furanone scaffolds **2** and **3**. Understanding the catalytic photooxidations in detail is of great value, as they offer a new method to access functionalized bioactive compounds through a more sustainable process.

1 S. Mai, L. González, *Angew. Chem. Int. Ed.* **2020**, *59*, 16832.
2 P. T. Anastas, J. C. Warner, Green chemistry. Theory and practice, Oxford University Press, Oxford, **1998**.
3 “Investigations into photocatalytic oxidations of halogenated 5-membered O-heterocycles” – Manuscript in preparation as of March 2025.