

Direct Transformation of Esters into Heterocyclic Compounds: Synthesis of Fluorescent Dyes

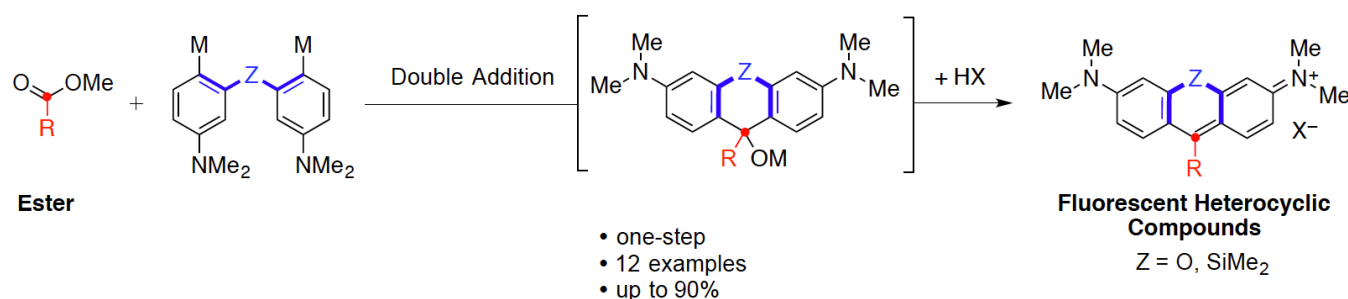
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Heterocyclic compounds are of considerable importance in material science as well as medicinal chemistry. Therefore, efficient and environmentally benign methods for the synthesis of heterocyclic compounds are required. Xanthylium based small-molecule fluorophores are a class of heterocycles which are known for over a century and have become essential for the visualization of biomolecules and biochemical events, e.g. to support the understanding of diseases. However, the synthesis of such small-molecule fluorophores bear unsolved syntheses issues and the currently high interest in small-molecule fluorophores demand a highly flexible and direct synthesis with the use of stable reagents.

Motivated by our previous results in the synthesis of arenes, we set out to investigate a one-step synthesis of heterocycles from carboxylic acid esters in combination of 1,5-bifunctional organomagnesium reagents. With a heteroatom incorporated in the 3-position of the 1,5-bifunctional reagent ($Z = O$ or SiMe_2), we would obtain a heterocyclohexadienolate intermediate which forms a fluorescent salt upon acidic work-up, when substituted with an amino group.

This highly modular approach led to the formation of aryl, alkyl and alkenyl xanthylium dyes ($X = O$) and SiR-dyes ($X = \text{SiMe}_2$) dyes in up to 90% yield. This approach is expected to become the preferred method for the formation of fluorescent dyes with tailored physicochemical properties.



- [1] A. Link, C. Fischer, C. Sparr, *Angew. Chem.* **2015**, *127*, 12331–12334; *Angew. Chem. Int. Ed.* **2015**, *54*, 12163–12166.
- [2] C. Fischer, C. Sparr, *manuscript in preparation*.