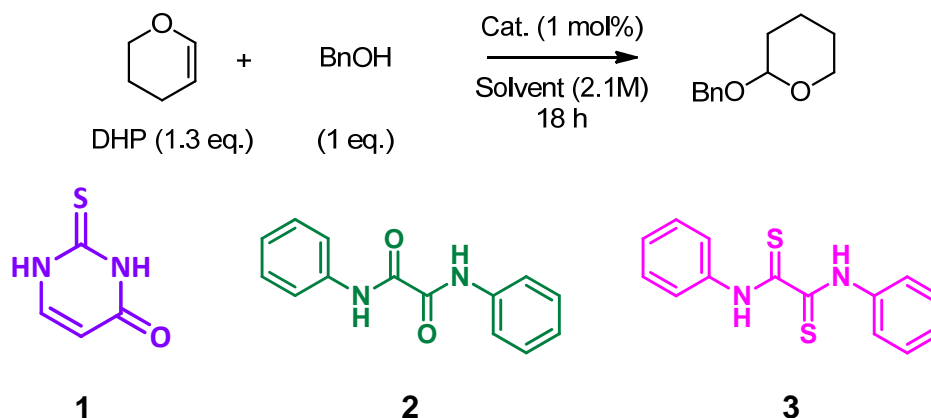


APPLICATIONS OF (THIO)OXALAMIDES IN ORGANOCATALYSIS: SYNTHESIS AND ACTIVITY OF OXALIC DERIVATIVES

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Hydrogen bond donating motifs, such as those found in *N,N*-dialkyl(aryl)thioureas, croconamides and 2-thiouracil **1**, have been extensively studied due to their ability to engage in strong hydrogen bonds.^{[1][2]} Our aim is to synthesise new amide structures and study their potential as organocatalysts. In this work a new family of organocatalysts - (thio)oxalamides **3** - characterised by electron-deficient (thio)amide moieties with the capacity to act as hydrogen bond donors/acceptors has been introduced.^[3] (Thio)amides, such as thiouracil and Schreiner's catalyst, are known to catalyse glycosylation and THP-protection reactions of alcohols. Here we demonstrate that incorporation of an extra carbonyl group into the structure, as in (thio)oxalamides, has significant benefits in terms of improved solubility. Rotational energy profiles of (thio)oxalamides **3** have been analysed to explore plausible interactions of different catalyst conformations with alcohol substrates. DFT calculations suggest that complex structures formed upon addition of an alcohol to the (thio)oxalamide catalyst **3** may be responsible for their catalytic activity.



[1] A. G. Doyle, E. N. Jacobsen. *Chem. Rev.* 2007, 107, 5713-5743.

[2] G. A. Bradshaw, A. C. Colgan, N. P. Allen, I. Pongener, M. B. Boland, Y. Ortin, E. M. McGarrigle, *Chem. Sci.* 2019, 10, 508-514.

[3] M. Kotke, P. Schreiner, *Synthesis.* 2007, 779-790.