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OR15 – Mechanistic Investigations of Catalytic C–H Functionalization:
A Combined Experimental and Computational Approach

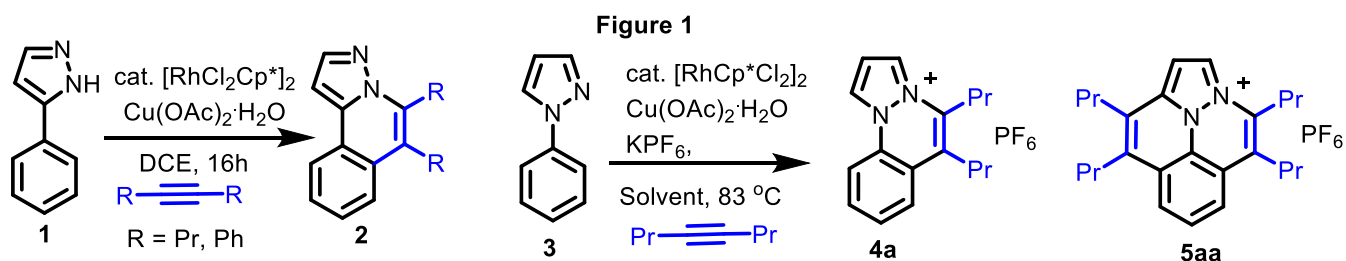
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Methods to form polycyclic heterocycles through the construction of C–Y bonds (Y = C, N and O) are of vital importance for the synthesis of molecules for applications in pharmaceuticals and materials science. Dramatic progress has been made with rhodium-catalysed oxidative functionalisation of C–H bonds with high selectivity and functional group tolerance without the need for pre-functionalisation.¹ Here we present some of our mechanistic investigations of Rh-catalysed carboxylate assisted C–H functionalization of pyrazoles (for example Fig 1).^{2,3} We will show that the nature of the C–H activation step is controlled by the solvent² and that C–H activation or reductive elimination can be rate determining. The importance of the computational methodology to accurately model the experimental results will also be discussed.



References

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3. Algarra, A. G., W. B. Cross, D. L. Davies, Q. Khamker, S. A. Macgregor, C. L. McMullin and K. Singh, *J. Org. Chem.* **2014**, *79*, 1954.